EUROPEAN COMMISSION
Directorate-General for Communications Networks, Content and Technology

Digital Excellence and Science Infrastructure
Flagships

GRANT AGREEMENT

NUMBER 957189 — BIG-MAP

This **Agreement** ('the Agreement') is **between** the following parties:

on the one part,

*the **European Union** ('the EU'), represented by the European Commission ('the Commission'), represented for the purposes of signature of this Agreement by Head of Unit, Authorised Representative of the Director General, Directorate-General for Communications Networks, Content and Technology, Artificial Intelligence and Digital Industry, Administration and Finance, Jose Manuel BASTOS,*

and

on the other part,

1. 'the coordinator':

DANMARKS TEKNISKE UNIVERSITET (DTU), established in ANKER ENGELUNDSVEJ 1 BYGNING 101 A, KGS LYNGBY 2800, Denmark, VAT number: DK30060946, represented for the purposes of signing the Agreement by Head of Department, Søren LINDEROTH

and the following other beneficiaries, if they sign their 'Accession Form' (see Annex 3 and Article 56):

2. **UPPSALA UNIVERSITET (UU)**, established in VON KRAEMERS ALLE 4, UPPSALA 751 05, Sweden, VAT number: SE202100293201,

3. **KARLSRUHER INSTITUT FUER TECHNOLOGIE (KIT)**, established in KAISERSTRASSE 12, KARLSRUHE 76131, Germany, VAT number: DE266749428,

4. **CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS)**, established in RUE MICHEL ANGE 3, PARIS 75794, France, VAT number: FR40180089013,

5. **WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER (WWU)**, established in SCHLOSSPLATZ 2, MUENSTER 48149, Germany, VAT number: DE126118759,

6. **COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES (CEA)**, established in RUE LEBLANC 25, PARIS 15 75015, France, VAT number: FR43775685019,

7. **KEMIJSKI INSTITUT (NIC)**, established in HAJDRIHOVA 19, LJUBLJANA 1000, Slovenia, VAT number: SI33840890,

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8. **SINTEF AS (SINTEF)**, established in STRINDVEGEN 4, TRONDHEIM 7034, Norway, VAT number: NO919303808MVA,

9. **POLITECNICO DI TORINO (PDT)**, established in CORSO DUCA DEGLI ABRUZZI 24, TORINO 10129, Italy, VAT number: IT00518460019,

10. **FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V. (Fraunhofer)**, established in HANSASTRASSE 27C, MUNCHEN 80686, Germany, VAT number: DE129515865,

11. **CHALMERS TEKNISKA HOEGSKOLA AB (CTH)**, established in -, GOETEBORG 41296, Sweden, VAT number: SE556479559801,

12. **POLITECHNIKA WARSZAWSKA (WUT)**, established in PLAC POLITECHNIKI 1, WARSZAWA 00 661, Poland, VAT number: PL5250005834,

13. **AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS (CSIC)**, established in CALLE SERRANO 117, MADRID 28006, Spain, VAT number: ESQ2818002D,

14. **TECHNISCHE UNIVERSITEIT DELFT (TUD)**, established in STEVINWEG 1, DELFT 2628 CN, Netherlands, VAT number: NL001569569B01,

15. **CONSIGLIO NAZIONALE DELLE RICERCHE (CNR)**, established in PIAZZALE ALDO MORO 7, ROMA 00185, Italy, VAT number: IT02118311006,

16. **ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)**, established in BATIMENT CE 3316 STATION 1, LAUSANNE 1015, Switzerland, VAT number: CHE116075613TVA,

17. **THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE (UCAM)**, established in TRINITY LANE THE OLD SCHOOLS, CAMBRIDGE CB2 1TN, United Kingdom, VAT number: GB823847609,

18. **THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD (UOXF)**, established in WELLINGTON SQUARE UNIVERSITY OFFICES, OXFORD OX1 2JD, United Kingdom, VAT number: GB125506730,

19. **TARTU ULIKOOL (UT)**, established in ULIKOOLI 18, TARTU 50090, Estonia, VAT number: EE100030417,

20. **THE UNIVERSITY OF LIVERPOOL (ULIV)**, established in BROWNLOW HILL 765 FOUNDATION BUILDING, LIVERPOOL L69 7ZX, United Kingdom, VAT number: GB673598875,

21. **EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF)**, established in 71 AVENUE DES MARTYRS, GRENOBLE 38000, France, VAT number: FR60338723919,

22. **INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL)**, established in 71 AVENUE DES MARTYRS, GRENOBLE 38000, France, VAT number: FR01779555887,

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23. **SYNCHROTRON SOLEIL SOCIETE CIVILE (SOLEIL)**, established in L ORME DES MERISIERS, SAINT AUBIN 91190, France, VAT number: FR27439684903,

24. **FUNDACION CIDETEC (CID)**, established in PASEO MIRAMON 196 PARQUE TECNOLOGICO DE MIRAMON, SAN SEBASTIAN 20014, Spain, VAT number: ESG20588588,

25. **ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL (EMIRI)**, established in RUE DU MARAIS 31, BRUXELLES 1000, Belgium, VAT number: BE0500888006,

26. **UMICORE (UMI)**, established in RUE DU MARAIS 31, BRUXELLES 1000, Belgium, VAT number: BE0401574852,

27. **SOLVAY SA (SOLB)**, established in RUE DE RANSBEEK 310, BRUXELLES 1120, Belgium,

28. **BASF SE (BASF)**, established in CARL BOSCH STRASSE 38, LUDWIGSHAFEN AM RHEIN 67056, Germany, VAT number: DE149145247,

29. **NORTHVOLT AB (NVOLT)**, established in GAMLA BROGATAN 26, STOCKHOLM 111 20, Sweden, VAT number: SE559015889401,

30. **UNIVERSITAT BASEL (UNIBAS)**, established in PETERSPLATZ 1, BASEL 4051, Switzerland, VAT number: CHE115244907MWST,

31. **IT-UNIVERSITETET I KOBENHAVN (ITU)**, established in RUED LANGGAARDSVEJ 7, KOBENHAVN 2300, Denmark, VAT number: DK29057753,

32. **DASSAULT SYSTEMES DEUTSCHLAND GMBH (3DS)**, established in MEITNERSTRASSE 8, STUTTGART 70563, Germany, VAT number: DE147319694,

33. **FORSCHUNGSZENTRUM JULICH GMBH (FZJ)**, established in WILHELM JOHNEN STRASSE, JULICH 52428, Germany, VAT number: DE122624631,

34. **SAFT (SAFT)**, established in 26 QUAI CHARLES PASQUA, LEVALLOIS PERRET 92300, France, VAT number: FR21383703873,

Unless otherwise specified, references to ‘beneficiary’ or ‘beneficiaries’ include the coordinator.

The parties referred to above have agreed to enter into the Agreement under the terms and conditions below.

By signing the Agreement or the Accession Form, the beneficiaries accept the grant and agree to implement it under their own responsibility and in accordance with the Agreement, with all the obligations and conditions it sets out.

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The Agreement is composed of:

Terms and Conditions

Annex 1 Description of the action

Annex 2 Estimated budget for the action

2a Additional information on the estimated budget

Annex 3 Accession Forms

Annex 4 Model for the financial statements

Annex 5 Model for the certificate on the financial statements

Annex 6 Model for the certificate on the methodology

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TERMS AND CONDITIONS

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CHAPTER 1 GENERAL

ARTICLE 1 — SUBJECT OF THE AGREEMENT

This Agreement sets out the rights and obligations and the terms and conditions applicable to the grant awarded to the beneficiaries for implementing the action set out in Chapter 2.

CHAPTER 2 ACTION

ARTICLE 2 — ACTION TO BE IMPLEMENTED — *COMPLEMENTARY GRANT*

The grant is awarded for the action entitled '***Battery Interface Genome - Materials Acceleration Platform***' — '***BIG-MAP***' **('action')**, as described in Annex 1.

*The grant is a '**complementary grant**' to the grant agreement(s) under the call(s) for proposals LC-BAT-2020-3.*

ARTICLE 3 — DURATION AND STARTING DATE OF THE ACTION

The duration of the action will be ***36*** **months** as of *1 September 2020* ('**starting date of the action**').

ARTICLE 4 — ESTIMATED BUDGET AND BUDGET TRANSFERS

4.1 Estimated budget

The '**estimated budget**' for the action is set out in Annex 2.

It contains the estimated eligible costs and the forms of costs, broken down by beneficiary *(and linked third party)* and budget category (see Articles 5, 6*, and 14*).

4.2 Budget transfers

The estimated budget breakdown indicated in Annex 2 may be adjusted — without an amendment (see Article 55) — by transfers of amounts between beneficiaries, budget categories and/or forms of costs set out in Annex 2, if the action is implemented as described in Annex 1.

However, the beneficiaries may not add costs relating to subcontracts not provided for in Annex 1, unless such additional subcontracts are approved by an amendment or in accordance with Article 13.

CHAPTER 3 GRANT

ARTICLE 5 — GRANT AMOUNT, FORM OF GRANT, REIMBURSEMENT RATES AND FORMS OF COSTS

5.1 Maximum grant amount

The '**maximum grant amount**' is **EUR 19 997 812.50** (nineteen million nine hundred and ninety seven thousand eight hundred and twelve EURO and fifty eurocents).

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5.2 Form of grant, reimbursement rates and forms of costs

The grant reimburses ***100% of the action's eligible costs*** (see Article 6) ('**reimbursement of eligible costs grant**') (see Annex 2).

The estimated eligible costs of the action are EUR **19 997 812.50** (nineteen million nine hundred and ninety seven thousand eight hundred and twelve EURO and fifty eurocents).

Eligible costs (see Article 6) must be declared under the following forms ('**forms of costs**'):

(a) for **direct personnel costs**:

- as actually incurred costs ('**actual costs**') or
- on the basis of an amount per unit calculated by the beneficiary in accordance with its usual cost accounting practices ('**unit costs**').

Personnel **costs for SME owners** or **beneficiaries that are natural persons** not receiving a salary (see Article 6.2, Points A.4 and A.5) must be declared on the basis of the amount per unit set out in Annex 2a (**unit costs**);

(b) for **direct costs for subcontracting**: as actually incurred costs (**actual costs**);

(c) for **direct costs of providing financial support to third parties**: *not applicable;*

(d) for **other direct costs**:

- for costs of internally invoiced goods and services: on the basis of an amount per unit calculated by the beneficiary in accordance with its usual cost accounting practices ('**unit costs**');
- for all other costs: as actually incurred costs (**actual costs**);

(e) for **indirect costs**: on the basis of a flat-rate applied as set out in Article 6.2, Point E ('**flat-rate costs**');

(f) ***specific cost category(ies):*** *not applicable.*

5.3 Final grant amount — Calculation

The '**final grant amount**' depends on the actual extent to which the action is implemented in accordance with the Agreement's terms and conditions.

This amount is calculated by the *Commission* — when the payment of the balance is made (see Article 21.4) — in the following steps:

Step 1 — Application of the reimbursement rates to the eligible costs

Step 2 — Limit to the maximum grant amount

Step 3 — Reduction due to the no-profit rule

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Step 4 — Reduction due to substantial errors, irregularities or fraud or serious breach of obligations

5.3.1 Step 1 — Application of the reimbursement rates to the eligible costs

The reimbursement rate(s) (see Article 5.2) are applied to the eligible costs (actual costs, unit costs and flat-rate costs; see Article 6) declared by the beneficiaries *and linked third parties* (see Article 20) and approved by the *Commission* (see Article 21).

5.3.2 Step 2 — Limit to the maximum grant amount

If the amount obtained following Step 1 is higher than the maximum grant amount set out in Article 5.1, it will be limited to the latter.

5.3.3 Step 3 — Reduction due to the no-profit rule

The grant must not produce a profit.

'**Profit**' means the surplus of the amount obtained following Steps 1 and 2 plus the action's total receipts, over the action's total eligible costs.

The '**action's total eligible costs**' are the consolidated total eligible costs approved by the *Commission*.

The '**action's total receipts**' are the consolidated total receipts generated during its duration (see Article 3).

The following are considered **receipts**:

(a) income generated by the action; if the income is generated from selling equipment or other assets purchased under the Agreement, the receipt is up to the amount declared as eligible under the Agreement;

(b) financial contributions given by third parties to the beneficiary *or to a linked third party* specifically to be used for the action, and

(c) in-kind contributions provided by third parties free of charge and specifically to be used for the action, if they have been declared as eligible costs.

The following are however not considered receipts:

(a) income generated by exploiting the action's results (see Article 28);

(b) financial contributions by third parties, if they may be used to cover costs other than the eligible costs (see Article 6);

(c) financial contributions by third parties with no obligation to repay any amount unused at the end of the period set out in Article 3.

If there is a profit, it will be deducted from the amount obtained following Steps 1 and 2.

5.3.4 Step 4 — Reduction due to substantial errors, irregularities or fraud or serious breach of obligations — Reduced grant amount — Calculation

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If the grant is reduced (see Article 43), the *Commission* will calculate the reduced grant amount by deducting the amount of the reduction (calculated in proportion to the seriousness of the errors, irregularities or fraud or breach of obligations, in accordance with Article 43.2) from the maximum grant amount set out in Article 5.1.

The final grant amount will be the lower of the following two:

- the amount obtained following Steps 1 to 3 or
- the reduced grant amount following Step 4.

5.4 Revised final grant amount — Calculation

If — after the payment of the balance (in particular, after checks, reviews, audits or investigations; see Article 22) — the *Commission* rejects costs (see Article 42) or reduces the grant (see Article 43), it will calculate the '**revised final grant amount**' for the beneficiary concerned by the findings.

This amount is calculated by the *Commission* on the basis of the findings, as follows:

- in case of **rejection of costs**: by applying the reimbursement rate to the revised eligible costs approved by the *Commission* for the beneficiary concerned;
- in case of **reduction of the grant**: by calculating the concerned beneficiary's share in the grant amount reduced in proportion to the seriousness of the errors, irregularities or fraud or breach of obligations (see Article 43.2).

In case of **rejection of costs and reduction of the grant**, the revised final grant amount for the beneficiary concerned will be the lower of the two amounts above.

ARTICLE 6 — ELIGIBLE AND INELIGIBLE COSTS

6.1 General conditions for costs to be eligible

'**Eligible costs**' are costs that meet the following criteria:

(a) for **actual costs**:

(i) they must be actually incurred by the beneficiary;

(ii) they must be incurred in the period set out in Article 3, with the exception of costs relating to the submission of the periodic report for the last reporting period and the final report (see Article 20);

(iii) they must be indicated in the estimated budget set out in Annex 2;

(iv) they must be incurred in connection with the action as described in Annex 1 and necessary for its implementation;

(v) they must be identifiable and verifiable, in particular recorded in the beneficiary's accounts in accordance with the accounting standards applicable in the country where the beneficiary is established and with the beneficiary's usual cost accounting practices;

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(vi) they must comply with the applicable national law on taxes, labour and social security, and

(vii) they must be reasonable, justified and must comply with the principle of sound financial management, in particular regarding economy and efficiency;

(b) for **unit costs**:

(i) they must be calculated as follows:

{amounts per unit set out in Annex 2a or calculated by the beneficiary in accordance with its usual cost accounting practices (see Article 6.2, Point A and Article 6.2.D.5)

multiplied by

the number of actual units};

(ii) the number of actual units must comply with the following conditions:

- the units must be actually used or produced in the period set out in Article 3;
- the units must be necessary for implementing the action or produced by it, and
- the number of units must be identifiable and verifiable, in particular supported by records and documentation (see Article 18);

(c) for **flat-rate costs**:

(i) they must be calculated by applying the flat-rate set out in Annex 2, and

(ii) the costs (actual costs or unit costs) to which the flat-rate is applied must comply with the conditions for eligibility set out in this Article.

6.2 Specific conditions for costs to be eligible

Costs are eligible if they comply with the general conditions (see above) and the specific conditions set out below for each of the following budget categories:

A. direct personnel costs;
B. direct costs of subcontracting;
C. *not applicable;*
D. other direct costs;
E. indirect costs;
F. *not applicable.*

'Direct costs' are costs that are directly linked to the action implementation and can therefore be attributed to it directly. They must not include any indirect costs (see Point E below).

'Indirect costs' are costs that are not directly linked to the action implementation and therefore cannot be attributed directly to it.

A. Direct personnel costs

<u>Types of eligible personnel costs</u>

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A.1 Personnel costs are eligible, if they are related to personnel working for the beneficiary under an employment contract (or equivalent appointing act) and assigned to the action ('**costs for employees (or equivalent)**'). They must be limited to salaries (including during parental leave), social security contributions, taxes and other costs included in the **remuneration**, if they arise from national law or the employment contract (or equivalent appointing act).

Beneficiaries that are non-profit legal entities[1] may also declare as personnel costs **additional remuneration** for personnel assigned to the action (including payments on the basis of supplementary contracts regardless of their nature), if:

(a) it is part of the beneficiary's usual remuneration practices and is paid in a consistent manner whenever the same kind of work or expertise is required;

(b) the criteria used to calculate the supplementary payments are objective and generally applied by the beneficiary, regardless of the source of funding used.

'Additional remuneration' means any part of the remuneration which exceeds what the person would be paid for time worked in projects funded by national schemes.

Additional remuneration for personnel assigned to the action is eligible up to the following amount:

(a) if the person works full time and exclusively on the action during the full year: up to EUR 8 000;

(b) if the person works exclusively on the action but not full-time or not for the full year: up to the corresponding pro-rata amount of EUR 8 000, or

(c) if the person does not work exclusively on the action: up to a pro-rata amount calculated as follows:

{{EUR 8 000

divided by

the number of annual productive hours (see below)},

multiplied by

the number of hours that the person has worked on the action during the year}.

A.2 The **costs for natural persons working under a direct contract** with the beneficiary other than an employment contract are eligible personnel costs, if:

(a) the person works under conditions similar to those of an employee (in particular regarding the way the work is organised, the tasks that are performed and the premises where they are performed);

(b) the result of the work carried out belongs to the beneficiary (unless exceptionally agreed otherwise), and

[1] For the definition, see Article 2.1(14) of the Rules for Participation Regulation No 1290/2013: '**non-profit legal entity**' means a legal entity which by its legal form is non-profit-making or which has a legal or statutory obligation not to distribute profits to its shareholders or individual members.

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(c) the costs are not significantly different from those for personnel performing similar tasks under an employment contract with the beneficiary.

A.3 The **costs of personnel seconded by a third party against payment** are eligible personnel costs, if the conditions in Article 11.1 are met.

A.4 **Costs of owners** of beneficiaries that are small and medium-sized enterprises ('**SME owners**') who are working on the action and who do not receive a salary are eligible personnel costs, if they correspond to the amount per unit set out in Annex 2a multiplied by the number of actual hours worked on the action.

A.5 **Costs of 'beneficiaries that are natural persons'** not receiving a salary are eligible personnel costs, if they correspond to the amount per unit set out in Annex 2a multiplied by the number of actual hours worked on the action.

Calculation

Personnel costs must be calculated by the beneficiaries as follows:

{{hourly rate

multiplied by

the number of actual hours worked on the action},

plus

for non-profit legal entities: additional remuneration to personnel assigned to the action under the conditions set out above (Point A.1)}.

The number of actual hours declared for a person must be identifiable and verifiable (see Article 18).

The total number of hours declared in *EU or Euratom* grants, for a person for a year, cannot be higher than the annual productive hours used for the calculations of the hourly rate. Therefore, the maximum number of hours that can be declared for the grant are:

{number of annual productive hours for the year (see below)

minus

total number of hours declared by the beneficiary, for that person in that year, for other *EU or Euratom* grants}.

The '**hourly rate**' is one of the following:

(a) for personnel costs declared as **actual costs** (i.e. budget categories A.1, A.2, A.3): the hourly rate is calculated *per full financial year*, as follows:

{actual annual personnel costs (excluding additional remuneration) for the person

divided by

number of annual productive hours}.

using the personnel costs and the number of productive hours for each full financial year covered by the reporting period concerned. If a financial year is not closed at the end of the

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reporting period, the beneficiaries must use the hourly rate of the last closed financial year available.

For the 'number of annual productive hours', the beneficiaries may choose one of the following:

(i) 'fixed number of hours': 1 720 hours for persons working full time (or corresponding pro-rata for persons not working full time);

(ii) 'individual annual productive hours': the total number of hours worked by the person in the year for the beneficiary, calculated as follows:

{annual workable hours of the person (according to the employment contract, applicable collective labour agreement or national law)

plus

overtime worked

minus

absences (such as sick leave and special leave)}.

'Annual workable hours' means the period during which the personnel must be working, at the employer's disposal and carrying out his/her activity or duties under the employment contract, applicable collective labour agreement or national working time legislation.

If the contract (or applicable collective labour agreement or national working time legislation) does not allow to determine the annual workable hours, this option cannot be used;

(iii) 'standard annual productive hours': the 'standard number of annual hours' generally applied by the beneficiary for its personnel in accordance with its usual cost accounting practices. This number must be at least 90% of the 'standard annual workable hours'.

If there is no applicable reference for the standard annual workable hours, this option cannot be used.

For all options, the actual time spent on **parental leave** by a person assigned to the action may be deducted from the number of annual productive hours.

As an alternative, beneficiaries may calculate the hourly rate *per month*, as follows:

{actual monthly personnel cost (excluding additional remuneration) for the person

divided by

{number of annual productive hours / 12}}

using the personnel costs for each month and (one twelfth of) the annual productive hours calculated according to either option (i) or (iii) above, i.e.:

- fixed number of hours or
- standard annual productive hours.

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Time spent on **parental leave** may not be deducted when calculating the hourly rate per month. However, beneficiaries may declare personnel costs incurred in periods of parental leave in proportion to the time the person worked on the action in that financial year.

If parts of a basic remuneration are generated over a period longer than a month, the beneficiaries may include only the share which is generated in the month (irrespective of the amount actually paid for that month).

Each beneficiary must use only one option (per full financial year or per month) for each full financial year;

(b) for personnel costs declared on the basis of **unit costs** (i.e. budget categories A.1, A.2, A.4, A.5): the hourly rate is one of the following:

(i) for SME owners or beneficiaries that are natural persons: the hourly rate set out in Annex 2a (see Points A.4 and A.5 above), or

(ii) for personnel costs declared on the basis of the beneficiary's usual cost accounting practices: the hourly rate calculated by the beneficiary in accordance with its usual cost accounting practices, if:

- the cost accounting practices used are applied in a consistent manner, based on objective criteria, regardless of the source of funding;

- the hourly rate is calculated using the actual personnel costs recorded in the beneficiary's accounts, excluding any ineligible cost or costs included in other budget categories.

  The actual personnel costs may be adjusted by the beneficiary on the basis of budgeted or estimated elements. Those elements must be relevant for calculating the personnel costs, reasonable and correspond to objective and verifiable information;

and

- the hourly rate is calculated using the number of annual productive hours (see above).

B. Direct costs of subcontracting (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible if the conditions in Article 13.1.1 are met.

C. Direct costs of providing financial support to third parties

Not applicable

D. Other direct costs

D.1 **Travel costs and related subsistence allowances** (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible if they are in line with the beneficiary's usual practices on travel.

D.2 The **depreciation costs of equipment, infrastructure or other assets** (new or second-hand) as recorded in the beneficiary's accounts are eligible, if they were purchased in accordance with

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Article 10.1.1 and written off in accordance with international accounting standards and the beneficiary's usual accounting practices.

The **costs of renting or leasing** equipment, infrastructure or other assets (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are also eligible, if they do not exceed the depreciation costs of similar equipment, infrastructure or assets and do not include any financing fees.

The costs of equipment, infrastructure or other assets **contributed in-kind against payment** are eligible, if they do not exceed the depreciation costs of similar equipment, infrastructure or assets, do not include any financing fees and if the conditions in Article 11.1 are met.

The only portion of the costs that will be taken into account is that which corresponds to the duration of the action and rate of actual use for the purposes of the action.

D.3 **Costs of other goods and services** (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible, if they are:

(a) purchased specifically for the action and in accordance with Article 10.1.1 or

(b) contributed in kind against payment and in accordance with Article 11.1.

Such goods and services include, for instance, consumables and supplies, dissemination (including open access), protection of results, certificates on the financial statements (if they are required by the Agreement), certificates on the methodology, translations and publications.

D.4 **Capitalised and operating costs of 'large research infrastructure'**[2] directly used for the action are eligible, if:

(a) the value of the large research infrastructure represents at least 75% of the total fixed assets (at historical value in its last closed balance sheet before the date of the signature of the Agreement or as determined on the basis of the rental and leasing costs of the research infrastructure[3]);

(b) the beneficiary's methodology for declaring the costs for large research infrastructure has been positively assessed by the Commission ('**ex-ante assessment**');

(c) the beneficiary declares as direct eligible costs only the portion which corresponds to the duration of the action and the rate of actual use for the purposes of the action, and

(d) they comply with the conditions as further detailed in the annotations to the H2020 grant agreements.

[2] '**Large research infrastructure**' means research infrastructure of a total value of at least EUR 20 million, for a beneficiary, calculated as the sum of historical asset values of each individual research infrastructure of that beneficiary, as they appear in its last closed balance sheet before the date of the signature of the Agreement or as determined on the basis of the rental and leasing costs of the research infrastructure.

[3] For the definition, see Article 2(6) of the H2020 Framework Programme Regulation No 1291/2013: '**Research infrastructure**' are facilities, resources and services that are used by the research communities to conduct research and foster innovation in their fields. Where relevant, they may be used beyond research, e.g. for education or public services. They include: major scientific equipment (or sets of instruments); knowledge-based resources such as collections, archives or scientific data; e-infrastructures such as data and computing systems and communication networks; and any other infrastructure of a unique nature essential to achieve excellence in research and innovation. Such infrastructures may be 'single-sited', 'virtual' or 'distributed'.

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D.5 **Costs of internally invoiced goods and services** directly used for the action are eligible, if:

(a) they are declared on the basis of a unit cost calculated in accordance with the beneficiary's usual cost accounting practices;

(b) the cost accounting practices used are applied in a consistent manner, based on objective criteria, regardless of the source of funding;

(c) the unit cost is calculated using the actual costs for the good or service recorded in the beneficiary's accounts, excluding any ineligible cost or costs included in other budget categories.

The actual costs may be adjusted by the beneficiary on the basis of budgeted or estimated elements. Those elements must be relevant for calculating the costs, reasonable and correspond to objective and verifiable information;

(d) the unit cost excludes any costs of items which are not directly linked to the production of the invoiced goods or service.

'Internally invoiced goods and services' means goods or services which are provided by the beneficiary directly for the action and which the beneficiary values on the basis of its usual cost accounting practices.

E. Indirect costs

Indirect costs are eligible if they are declared on the basis of the flat-rate of 25% of the eligible direct costs (see Article 5.2 and Points A to D above), from which are excluded:

(a) costs of subcontracting and

(b) costs of in-kind contributions provided by third parties which are not used on the beneficiary's premises*;*

(c) *not applicable;*

(d) *not applicable.*

Beneficiaries receiving an operating grant[4] financed by the EU or Euratom budget cannot declare indirect costs for the period covered by the operating grant, unless they can demonstrate that the operating grant does not cover any costs of the action.

F. *Specific cost category(ies)*

Not applicable

6.3 Conditions for costs of linked third parties to be eligible

[4] For the definition, see Article 121(1)(b) of Regulation (EU, Euratom) No 966/2012 of the European Parliament and of the Council of 25 October 2012 on the financial rules applicable to the general budget of the Union and repealing Council Regulation (EC, Euratom) No 1605/2002 ('**Financial Regulation No 966/2012**')(OJ L 218, 26.10.2012, p.1): '**operating grant**' means direct financial contribution, by way of donation, from the budget in order to finance the functioning of a body which pursues an aim of general EU interest or has an objective forming part of and supporting an EU policy.

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Costs incurred by linked third parties *are eligible if they fulfil — mutatis mutandis — the general and specific conditions for eligibility set out in this Article (Article 6.1 and 6.2) and Article 14.1.1.*

6.4 Conditions for in-kind contributions provided by third parties free of charge to be eligible

In-kind contributions provided free of charge are eligible direct costs (for the beneficiary *or linked third party*), if the costs incurred by the third party fulfil — *mutatis mutandis* — the general and specific conditions for eligibility set out in this Article (Article 6.1 and 6.2) and Article 12.1.

6.5 Ineligible costs

'**Ineligible costs**' are:

(a) costs that do not comply with the conditions set out above (Article 6.1 to 6.4), in particular:

(i) costs related to return on capital;

(ii) debt and debt service charges;

(iii) provisions for future losses or debts;

(iv) interest owed;

(v) doubtful debts;

(vi) currency exchange losses;

(vii) bank costs charged by the beneficiary's bank for transfers from the *Commission*;

(viii) excessive or reckless expenditure;

(ix) deductible VAT;

(x) costs incurred during suspension of the implementation of the action (see Article 49);

(b) costs declared under another EU or Euratom grant (including grants awarded by a Member State and financed by the EU or Euratom budget and grants awarded by bodies other than the *Commission* for the purpose of implementing the EU or Euratom budget); in particular, indirect costs if the beneficiary is already receiving an operating grant financed by the EU or Euratom budget in the same period, unless it can demonstrate that the operating grant does not cover any costs of the action.

6.6 Consequences of declaration of ineligible costs

Declared costs that are ineligible will be rejected (see Article 42).

This may also lead to any of the other measures described in Chapter 6.

CHAPTER 4 RIGHTS AND OBLIGATIONS OF THE PARTIES

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SECTION 1 RIGHTS AND OBLIGATIONS RELATED TO IMPLEMENTING THE ACTION

ARTICLE 7 — GENERAL OBLIGATION TO PROPERLY IMPLEMENT THE ACTION

7.1 General obligation to properly implement the action

The beneficiaries must implement the action as described in Annex 1 and in compliance with the provisions of the Agreement and all legal obligations under applicable EU, international and national law.

7.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 8 — RESOURCES TO IMPLEMENT THE ACTION — THIRD PARTIES INVOLVED IN THE ACTION

The beneficiaries must have the appropriate resources to implement the action.

If it is necessary to implement the action, the beneficiaries may:

- purchase goods, works and services (see Article 10);
- use in-kind contributions provided by third parties against payment (see Article 11);
- use in-kind contributions provided by third parties free of charge (see Article 12);
- call upon subcontractors to implement action tasks described in Annex 1 (see Article 13);
- call upon linked third parties to implement action tasks described in Annex 1 (see Article 14);
- call upon international partners to implement action tasks described in Annex 1 (see Article 14a).

In these cases, the beneficiaries retain sole responsibility towards the *Commission* and the other beneficiaries for implementing the action.

ARTICLE 9 — IMPLEMENTATION OF ACTION TASKS BY BENEFICIARIES NOT RECEIVING EU FUNDING

Not applicable

ARTICLE 10 — PURCHASE OF GOODS, WORKS OR SERVICES

10.1 Rules for purchasing goods, works or services

10.1.1 If necessary to implement the action, the beneficiaries may purchase goods, works or services.

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The beneficiaries must make such purchases ensuring the best value for money or, if appropriate, the lowest price. In doing so, they must avoid any conflict of interests (see Article 35).

The beneficiaries must ensure that the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards their contractors.

10.1.2 Beneficiaries that are 'contracting authorities' within the meaning of Directive 2004/18/EC[5] (or 2014/24/EU[6]) or 'contracting entities' within the meaning of Directive 2004/17/EC[7] (or 2014/25/EU[8]) must comply with the applicable national law on public procurement.

10.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under Article 10.1.1, the costs related to the contract concerned will be ineligible (see Article 6) and will be rejected (see Article 42).

If a beneficiary breaches any of its obligations under Article 10.1.2, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 11 — USE OF IN-KIND CONTRIBUTIONS PROVIDED BY THIRD PARTIES AGAINST PAYMENT

11.1 Rules for the use of in-kind contributions against payment

If necessary to implement the action, the beneficiaries may use in-kind contributions provided by third parties against payment.

The beneficiaries may declare costs related to the payment of in-kind contributions as eligible (see Article 6.1 and 6.2), up to the third parties' costs for the seconded persons, contributed equipment, infrastructure or other assets or other contributed goods and services.

The third parties and their contributions must be set out in Annex 1. The *Commission* may however approve in-kind contributions not set out in Annex 1 without amendment (see Article 55), if:

- they are specifically justified in the periodic technical report and
- their use does not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

The beneficiaries must ensure that the Commission, the European Court of Auditors (ECA) and the

[5] Directive 2004/18/EC of the European Parliament and of the Council of 31 March 2004 on the coordination of procedures for the award of public work contracts, public supply contracts and public service contracts (OJ L 134, 30.04.2004, p. 114).

[6] Directive 2014/24/EU of the European Parliament and of the Council of 26 February 2014 on public procurement and repealing Directive 2004/18/EC. (OJ L 94, 28.03.2014, p. 65).

[7] Directive 2004/17/EC of the European Parliament and of the Council of 31 March 2004 coordinating the procurement procedures of entities operating in the water, energy, transport and postal services sectors (OJ L 134, 30.04.2004, p. 1)

[8] Directive 2014/25/EU of the European Parliament and of the Council of 26 February 2014 on procurement by entities operating in the water, energy, transport and postal services sectors and repealing Directive 2004/17/EC (OJ L 94, 28.03.2014, p. 243).

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European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards the third parties.

11.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the costs related to the payment of the in-kind contribution will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 12 — USE OF IN-KIND CONTRIBUTIONS PROVIDED BY THIRD PARTIES FREE OF CHARGE

12.1 Rules for the use of in-kind contributions free of charge

If necessary to implement the action, the beneficiaries may use in-kind contributions provided by third parties free of charge.

The beneficiaries may declare costs incurred by the third parties for the seconded persons, contributed equipment, infrastructure or other assets or other contributed goods and services as eligible in accordance with Article 6.4.

The third parties and their contributions must be set out in Annex 1. The *Commission* may however approve in-kind contributions not set out in Annex 1 without amendment (see Article 55), if:

- they are specifically justified in the periodic technical report and
- their use does not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

The beneficiaries must ensure that the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards the third parties.

12.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the costs incurred by the third parties related to the in-kind contribution will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 13 — IMPLEMENTATION OF ACTION TASKS BY SUBCONTRACTORS

13.1 Rules for subcontracting action tasks

13.1.1 If necessary to implement the action, the beneficiaries may award subcontracts covering the implementation of certain action tasks described in Annex 1.

Subcontracting may cover only a limited part of the action.

The beneficiaries must award the subcontracts ensuring the best value for money or, if appropriate, the lowest price. In doing so, they must avoid any conflict of interests (see Article 35).

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The tasks to be implemented and the estimated cost for each subcontract must be set out in Annex 1 and the total estimated costs of subcontracting per beneficiary must be set out in Annex 2. The *Commission* may however approve subcontracts not set out in Annex 1 and 2 without amendment (see Article 55), if:

- they are specifically justified in the periodic technical report and
- they do not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

The beneficiaries must ensure that the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards their subcontractors.

13.1.2 The beneficiaries must ensure that their obligations under Articles 35, 36, 38 and 46 also apply to the subcontractors.

Beneficiaries that are 'contracting authorities' within the meaning of Directive 2004/18/EC (or 2014/24/EU) or 'contracting entities' within the meaning of Directive 2004/17/EC (or 2014/25/EU) must comply with the applicable national law on public procurement.

13.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under Article 13.1.1, the costs related to the subcontract concerned will be ineligible (see Article 6) and will be rejected (see Article 42).

If a beneficiary breaches any of its obligations under Article 13.1.2, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 14 — IMPLEMENTATION OF ACTION TASKS BY LINKED THIRD PARTIES

14.1 Rules for calling upon linked third parties to implement part of the action

*14.1.1 The following **affiliated entities**[10] and **third parties with a legal link to a beneficiary**[11] ('**linked third parties**') may implement the action tasks attributed to them in Annex 1:*

[10] For the definition see Article 2.1(2) Rules for Participation Regulation No 1290/2013: '**affiliated entity**' means any legal entity that is:
- under the direct or indirect control of a participant, or
- under the same direct or indirect control as the participant, or
- directly or indirectly controlling a participant.

'Control' may take any of the following forms:
(a) the direct or indirect holding of more than 50% of the nominal value of the issued share capital in the legal entity concerned, or of a majority of the voting rights of the shareholders or associates of that entity;
(b) the direct or indirect holding, in fact or in law, of decision-making powers in the legal entity concerned.

However the following relationships between legal entities shall not in themselves be deemed to constitute controlling relationships:
(a) the same public investment corporation, institutional investor or venture-capital company has a direct or indirect holding of more than 50% of the nominal value of the issued share capital or a majority of voting rights of the shareholders or associates;
(b) the legal entities concerned are owned or supervised by the same public body.

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The linked third parties may declare as eligible the costs they incur for implementing the action tasks in accordance with Article 6.3.

The beneficiaries must ensure that the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards their linked third parties.

14.1.2 The beneficiaries must ensure that their obligations under Articles 18, 20, 35, 36 and 38 also apply to their linked third parties.

14.2 Consequences of non-compliance

If any obligation under Article 14.1.1 is breached, the costs of the linked third party will be ineligible (see Article 6) and will be rejected (see Article 42).

If any obligation under Article 14.1.2 is breached, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 14a — IMPLEMENTATION OF ACTION TASKS BY INTERNATIONAL PARTNERS

Not applicable

ARTICLE 15 — FINANCIAL SUPPORT TO THIRD PARTIES

15.1 Rules for providing financial support to third parties

Not applicable

15.2 Financial support in the form of prizes

Not applicable

15.3 Consequences of non-compliance

Not applicable

ARTICLE 16 — PROVISION OF TRANS-NATIONAL OR VIRTUAL ACCESS TO RESEARCH INFRASTRUCTURE

16.1 Rules for providing trans-national access to research infrastructure

Not applicable

16.2 Rules for providing virtual access to research infrastructure

[11] '**Third party with a legal link to a beneficiary**' is any legal entity which has a legal link to the beneficiary implying collaboration that is not limited to the action.

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Not applicable

16.3 Consequences of non-compliance

Not applicable

SECTION 2 RIGHTS AND OBLIGATIONS RELATED TO THE GRANT ADMINISTRATION

ARTICLE 17 — GENERAL OBLIGATION TO INFORM

17.1 General obligation to provide information upon request

The beneficiaries must provide — during implementation of the action or afterwards and in accordance with Article 41.2 — any information requested in order to verify eligibility of the costs, proper implementation of the action and compliance with any other obligation under the Agreement.

17.2 Obligation to keep information up to date and to inform about events and circumstances likely to affect the Agreement

Each beneficiary must keep information stored in the Participant Portal Beneficiary Register (via the electronic exchange system; see Article 52) up to date, in particular, its name, address, legal representatives, legal form and organisation type.

Each beneficiary must immediately inform the coordinator — which must immediately inform the *Commission* and the other beneficiaries — of any of the following:

(a) **events** which are likely to affect significantly or delay the implementation of the action or the EU's financial interests, in particular:

(i) changes in its legal, financial, technical, organisational or ownership situation *or those of its linked third parties and*

(ii) changes in the name, address, legal form, organisation type of its linked third parties;

(b) **circumstances** affecting:

(i) the decision to award the grant or

(ii) compliance with requirements under the Agreement.

17.3 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 18 — KEEPING RECORDS — SUPPORTING DOCUMENTATION

18.1 Obligation to keep records and other supporting documentation

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The beneficiaries must — for a period of *five* years after the payment of the balance — keep records and other supporting documentation in order to prove the proper implementation of the action and the costs they declare as eligible.

They must make them available upon request (see Article 17) or in the context of checks, reviews, audits or investigations (see Article 22).

If there are on-going checks, reviews, audits, investigations, litigation or other pursuits of claims under the Agreement (including the extension of findings; see Article 22), the beneficiaries must keep the records and other supporting documentation until the end of these procedures.

The beneficiaries must keep the original documents. Digital and digitalised documents are considered originals if they are authorised by the applicable national law. The *Commission* may accept non-original documents if it considers that they offer a comparable level of assurance.

18.1.1 Records and other supporting documentation on the scientific and technical implementation

The beneficiaries must keep records and other supporting documentation on scientific and technical implementation of the action in line with the accepted standards in the respective field.

18.1.2 Records and other documentation to support the costs declared

The beneficiaries must keep the records and documentation supporting the costs declared, in particular the following:

(a) for **actual costs**: adequate records and other supporting documentation to prove the costs declared, such as contracts, subcontracts, invoices and accounting records. In addition, the beneficiaries' usual cost accounting practices and internal control procedures must enable direct reconciliation between the amounts declared, the amounts recorded in their accounts and the amounts stated in the supporting documentation;

(b) for **unit costs**: adequate records and other supporting documentation to prove the number of units declared. Beneficiaries do not need to identify the actual eligible costs covered or to keep or provide supporting documentation (such as accounting statements) to prove the amount per unit.

In addition, **for unit costs calculated in accordance with the beneficiary's usual cost accounting practices**, the beneficiaries must keep adequate records and documentation to prove that the cost accounting practices used comply with the conditions set out in Article 6.2.

The beneficiaries *and linked third parties* may submit to the Commission, for approval, a certificate (drawn up in accordance with Annex 6) stating that their usual cost accounting practices comply with these conditions ('**certificate on the methodology**'). If the certificate is approved, costs declared in line with this methodology will not be challenged subsequently, unless the beneficiaries have concealed information for the purpose of the approval.

(c) for **flat-rate costs**: adequate records and other supporting documentation to prove the eligibility of the costs to which the flat-rate is applied. The beneficiaries do not need to identify the costs covered or provide supporting documentation (such as accounting statements) to prove the amount declared at a flat-rate.

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In addition, for **personnel costs** (declared as actual costs or on the basis of unit costs), the beneficiaries must keep **time records** for the number of hours declared. The time records must be in writing and approved by the persons working on the action and their supervisors, at least monthly. In the absence of reliable time records of the hours worked on the action, the *Commission* may accept alternative evidence supporting the number of hours declared, if it considers that it offers an adequate level of assurance.

As an exception, for **persons working exclusively on the action**, there is no need to keep time records, if the beneficiary signs a **declaration** confirming that the persons concerned have worked exclusively on the action.

For costs declared by linked third parties (see Article 14), it is the beneficiary that must keep the originals of the financial statements and the certificates on the financial statements of the linked third parties.

18.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, costs insufficiently substantiated will be ineligible (see Article 6) and will be rejected (see Article 42), and the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 19 — SUBMISSION OF DELIVERABLES

19.1 Obligation to submit deliverables

The coordinator must submit the '**deliverables**' identified in Annex 1, in accordance with the timing and conditions set out in it.

19.2 Consequences of non-compliance

If the coordinator breaches any of its obligations under this Article, the *Commission* may apply any of the measures described in Chapter 6.

ARTICLE 20 — REPORTING — PAYMENT REQUESTS

20.1 Obligation to submit reports

The coordinator must submit to the *Commission* (see Article 52) the technical and financial reports set out in this Article. These reports include requests for payment and must be drawn up using the forms and templates provided in the electronic exchange system (see Article 52).

20.2 Reporting periods

The action is divided into the following '**reporting periods**':

- RP1: from month 1 to month 18
- *RP2: from month 19 to month 36*

20.3 Periodic reports — Requests for interim payments

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The coordinator must submit a periodic report within 60 days following the end of each reporting period.

The **periodic report** must include the following:

(a) a '**periodic technical report**' containing:

(i) an **explanation of the work carried out** by the beneficiaries;

(ii) an **overview of the progress** towards the objectives of the action, including milestones and deliverables identified in Annex 1.

This report must include explanations justifying the differences between work expected to be carried out in accordance with Annex 1 and that actually carried out.

The report must detail the exploitation and dissemination of the results and — if required in Annex 1 — an updated '**plan for the exploitation and dissemination of the results**'.

The report must indicate the communication activities*;*

(iii) a **summary** for publication by the *Commission*;

(iv) the answers to the '**questionnaire**', covering issues related to the action implementation and the economic and societal impact, notably in the context of the Horizon 2020 key performance indicators and the Horizon 2020 monitoring requirements;

(b) a '**periodic financial report**' containing:

(i) an '**individual financial statement**' (see Annex 4) from each beneficiary *and from each linked third party*, for the reporting period concerned.

The individual financial statement must detail the eligible costs (actual costs, unit costs and flat-rate costs; see Article 6) for each budget category (see Annex 2).

The beneficiaries *and linked third parties* must declare all eligible costs, even if — for actual costs, unit costs and flat-rate costs — they exceed the amounts indicated in the estimated budget (see Annex 2). Amounts which are not declared in the individual financial statement will not be taken into account by the *Commission*.

If an individual financial statement is not submitted for a reporting period, it may be included in the periodic financial report for the next reporting period.

The individual financial statements of the last reporting period must also detail the **receipts of the action** (see Article 5.3.3).

Each beneficiary *and each linked third party* must **certify** that:

- the information provided is full, reliable and true;
- the costs declared are eligible (see Article 6);
- the costs can be substantiated by adequate records and supporting documentation

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(see Article 18) that will be produced upon request (see Article 17) or in the context of checks, reviews, audits and investigations (see Article 22), and

- for the last reporting period: that all the receipts have been declared (see Article 5.3.3);

(ii) an **explanation of the use of resources** and the information on subcontracting (see Article 13) and in-kind contributions provided by third parties (see Articles 11 and 12) from each beneficiary *and from each linked third party*, for the reporting period concerned;

(iii) *not applicable;*

(iv) a '**periodic summary financial statement**', created automatically by the electronic exchange system, consolidating the individual financial statements for the reporting period concerned and including — except for the last reporting period — the **request for interim payment**.

20.4 Final report — Request for payment of the balance

In addition to the periodic report for the last reporting period, the coordinator must submit the final report within 60 days following the end of the last reporting period.

The **final report** must include the following:

(a) a '**final technical report**' with a **summary** for publication containing:

(i) an overview of the results and their exploitation and dissemination;

(ii) the conclusions on the action, and

(iii) the socio-economic impact of the action;

(b) a '**final financial report**' containing:

(i) a '**final summary financial statement**', created automatically by the electronic exchange system, consolidating the individual financial statements for all reporting periods and including the **request for payment of the balance** and

(ii) a '**certificate on the financial statements**' (drawn up in accordance with Annex 5) for each beneficiary *and for each linked third party*, if it requests a total contribution of EUR 325 000 or more, as reimbursement of actual costs and unit costs calculated on the basis of its usual cost accounting practices (see Article 5.2 and Article 6.2).

20.5 Information on cumulative expenditure incurred

Not applicable

20.6 Currency for financial statements and conversion into euro

Financial statements must be drafted in euro.

Beneficiaries *and linked third parties* with accounting established in a currency other than the euro

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must convert the costs recorded in their accounts into euro, at the average of the daily exchange rates published in the C series of the *Official Journal of the European Union*, calculated over the corresponding reporting period.

If no daily euro exchange rate is published in the *Official Journal of the European Union* for the currency in question, they must be converted at the average of the monthly accounting rates published on the Commission's website, calculated over the corresponding reporting period.

Beneficiaries *and linked third parties* with accounting established in euro must convert costs incurred in another currency into euro according to their usual accounting practices.

20.7 Language of reports

All reports (technical and financial reports, including financial statements) must be submitted in the language of the Agreement.

20.8 Consequences of non-compliance

If the reports submitted do not comply with this Article, the *Commission* may suspend the payment deadline (see Article 47) and apply any of the other measures described in Chapter 6.

If the coordinator breaches its obligation to submit the reports and if it fails to comply with this obligation within 30 days following a written reminder, the *Commission* may terminate the Agreement (see Article 50) or apply any of the other measures described in Chapter 6.

ARTICLE 21 — PAYMENTS AND PAYMENT ARRANGEMENTS

21.1 Payments to be made

The following payments will be made to the coordinator:

- one **pre-financing payment**;
- one or more **interim payments**, on the basis of the request(s) for interim payment (see Article 20), and
- one **payment of the balance**, on the basis of the request for payment of the balance (see Article 20).

21.2 Pre-financing payment — Amount — Amount retained for the Guarantee Fund

The aim of the pre-financing is to provide the beneficiaries with a float.

It remains the property of the EU until the payment of the balance.

The amount of the pre-financing payment will be EUR **15 998 250.00** (fifteen million nine hundred and ninety eight thousand two hundred and fifty EURO).

The *Commission* will — except if Article 48 applies — make the pre-financing payment to the coordinator within 30 days, either from the entry into force of the Agreement (see Article 58) or from 10 days before the starting date of the action (see Article 3), whichever is the latest.

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An amount of EUR **999 890.63** (nine hundred and ninety nine thousand eight hundred and ninety EURO and sixty three eurocents), corresponding to 5% of the maximum grant amount (see Article 5.1), is retained by the *Commission* from the pre-financing payment and transferred into the '**Guarantee Fund**'.

21.3 Interim payments — Amount — Calculation

Interim payments reimburse the eligible costs incurred for the implementation of the action during the corresponding reporting periods.

The *Commission* will pay to the coordinator the amount due as interim payment within 90 days from receiving the periodic report (see Article 20.3), except if Articles 47 or 48 apply.

Payment is subject to the approval of the periodic report. Its approval does not imply recognition of the compliance, authenticity, completeness or correctness of its content.

The **amount due as interim payment** is calculated by the *Commission* in the following steps:

Step 1 — Application of the reimbursement rates

Step 2 — Limit to 90% of the maximum grant amount

21.3.1 Step 1 — Application of the reimbursement rates

The reimbursement rate(s) (see Article 5.2) are applied to the eligible costs (actual costs, unit costs and flat-rate costs; see Article 6) declared by the beneficiaries *and the linked third parties* (see Article 20) and approved by the *Commission* (see above) for the concerned reporting period.

21.3.2 Step 2 — Limit to 90% of the maximum grant amount

The total amount of pre-financing and interim payments must not exceed 90% of the maximum grant amount set out in Article 5.1. The maximum amount for the interim payment will be calculated as follows:

{90% of the maximum grant amount (see Article 5.1)

minus

{pre-financing and previous interim payments}}.

21.4 Payment of the balance — Amount — Calculation — Release of the amount retained for the Guarantee Fund

The payment of the balance reimburses the remaining part of the eligible costs incurred by the beneficiaries for the implementation of the action.

If the total amount of earlier payments is greater than the final grant amount (see Article 5.3), the payment of the balance takes the form of a recovery (see Article 44).

If the total amount of earlier payments is lower than the final grant amount, the *Commission* will pay the balance within 90 days from receiving the final report (see Article 20.4), except if Articles 47 or 48 apply.

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Payment is subject to the approval of the final report. Its approval does not imply recognition of the compliance, authenticity, completeness or correctness of its content.

The **amount due as the balance** is calculated by the *Commission* by deducting the total amount of pre-financing and interim payments (if any) already made, from the final grant amount determined in accordance with Article 5.3:

{final grant amount (see Article 5.3)

minus

{pre-financing and interim payments (if any) made}}.

At the payment of the balance, the amount retained for the Guarantee Fund (see above) will be released and:

- if the balance is positive: the amount released will be paid in full to the coordinator together with the amount due as the balance;
- if the balance is negative (payment of the balance taking the form of recovery): it will be deducted from the amount released (see Article 44.1.2). If the resulting amount:
    - is positive, it will be paid to the coordinator
    - is negative, it will be recovered.

The amount to be paid may however be offset — without the beneficiaries' consent — against any other amount owed by a beneficiary to the Commission or an executive agency (under the EU or Euratom budget), up to the maximum EU contribution indicated, for that beneficiary, in the estimated budget (see Annex 2).

21.5 Notification of amounts due

When making payments, the *Commission* will formally notify to the coordinator the amount due, specifying whether it concerns an interim payment or the payment of the balance.

For the payment of the balance, the notification will also specify the final grant amount.

In the case of reduction of the grant or recovery of undue amounts, the notification will be preceded by the contradictory procedure set out in Articles 43 and 44.

21.6 Currency for payments

The *Commission* will make all payments in euro.

21.7 Payments to the coordinator — Distribution to the beneficiaries

Payments will be made to the coordinator.

Payments to the coordinator will discharge the *Commission* from its payment obligation.

The coordinator must distribute the payments between the beneficiaries without unjustified delay.

Pre-financing may however be distributed only:

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(a) if the minimum number of beneficiaries set out in the call for proposals has acceded to the Agreement (see Article 56) and

(b) to beneficiaries that have acceded to the Agreement (see Article 56).

21.8 Bank account for payments

All payments will be made to the following bank account:

Name of bank: DANSKE BANK A/S
Full name of the account holder: DANMARKS TEKNISKE UNIVERSITETTECHNICAL UNIVERSITY OF DENMARK
IBAN code: DK9730004180011773

21.9 Costs of payment transfers

The cost of the payment transfers is borne as follows:

- the *Commission* bears the cost of transfers charged by its bank;
- the beneficiary bears the cost of transfers charged by its bank;
- the party causing a repetition of a transfer bears all costs of the repeated transfer.

21.10 Date of payment

Payments by the *Commission* are considered to have been carried out on the date when they are debited to its account.

21.11 Consequences of non-compliance

21.11.1 If the *Commission* does not pay within the payment deadlines (see above), the beneficiaries are entitled to **late-payment interest** at the rate applied by the European Central Bank (ECB) for its main refinancing operations in euros ('reference rate'), plus three and a half points. The reference rate is the rate in force on the first day of the month in which the payment deadline expires, as published in the C series of the *Official Journal of the European Union*.

If the late-payment interest is lower than or equal to EUR 200, it will be paid to the coordinator only upon request submitted within two months of receiving the late payment.

Late-payment interest is not due if all beneficiaries are EU Member States (including regional and local government authorities or other public bodies acting on behalf of a Member State for the purpose of this Agreement).

Suspension of the payment deadline or payments (see Articles 47 and 48) will not be considered as late payment.

Late-payment interest covers the period running from the day following the due date for payment (see above), up to and including the date of payment.

Late-payment interest is not considered for the purposes of calculating the final grant amount.

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21.11.2 If the coordinator breaches any of its obligations under this Article, the grant may be reduced (see Article 43) and the Agreement or the participation of the coordinator may be terminated (see Article 50).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 22 — CHECKS, REVIEWS, AUDITS AND INVESTIGATIONS — EXTENSION OF FINDINGS

22.1 Checks, reviews and audits by the Commission

22.1.1 Right to carry out checks

The Commission will — during the implementation of the action or afterwards — check the proper implementation of the action and compliance with the obligations under the Agreement, including assessing deliverables and reports.

For this purpose the Commission may be assisted by external persons or bodies.

The Commission may also request additional information in accordance with Article 17. The Commission may request beneficiaries to provide such information to it directly.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

22.1.2 Right to carry out reviews

The Commission may — during the implementation of the action or afterwards — carry out reviews on the proper implementation of the action (including assessment of deliverables and reports), compliance with the obligations under the Agreement and continued scientific or technological relevance of the action.

Reviews may be started up to two years after the payment of the balance. They will be formally notified to the coordinator or beneficiary concerned and will be considered to have started on the date of the formal notification.

If the review is carried out on a third party (see Articles 10 to 16), the beneficiary concerned must inform the third party.

The Commission may carry out reviews directly (using its own staff) or indirectly (using external persons or bodies appointed to do so). It will inform the coordinator or beneficiary concerned of the identity of the external persons or bodies. They have the right to object to the appointment on grounds of commercial confidentiality.

The coordinator or beneficiary concerned must provide — within the deadline requested — any information and data in addition to deliverables and reports already submitted (including information on the use of resources). The Commission may request beneficiaries to provide such information to it directly.

The coordinator or beneficiary concerned may be requested to participate in meetings, including with external experts.

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For **on-the-spot** reviews, the beneficiaries must allow access to their sites and premises, including to external persons or bodies, and must ensure that information requested is readily available.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

On the basis of the review findings, a '**review report**' will be drawn up.

The Commission will formally notify the review report to the coordinator or beneficiary concerned, which has 30 days to formally notify observations ('**contradictory review procedure**').

Reviews (including review reports) are in the language of the Agreement.

22.1.3 Right to carry out audits

The Commission may — during the implementation of the action or afterwards — carry out audits on the proper implementation of the action and compliance with the obligations under the Agreement.

Audits may be started up to two years after the payment of the balance. They will be formally notified to the coordinator or beneficiary concerned and will be considered to have started on the date of the formal notification.

If the audit is carried out on a third party (see Articles 10 to 16), the beneficiary concerned must inform the third party.

The Commission may carry out audits directly (using its own staff) or indirectly (using external persons or bodies appointed to do so). It will inform the coordinator or beneficiary concerned of the identity of the external persons or bodies. They have the right to object to the appointment on grounds of commercial confidentiality.

The coordinator or beneficiary concerned must provide — within the deadline requested — any information (including complete accounts, individual salary statements or other personal data) to verify compliance with the Agreement. The Commission may request beneficiaries to provide such information to it directly.

For **on-the-spot** audits, the beneficiaries must allow access to their sites and premises, including to external persons or bodies, and must ensure that information requested is readily available.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

On the basis of the audit findings, a '**draft audit report**' will be drawn up.

The Commission will formally notify the draft audit report to the coordinator or beneficiary concerned, which has 30 days to formally notify observations ('**contradictory audit procedure**'). This period may be extended by the Commission in justified cases.

The '**final audit report**' will take into account observations by the coordinator or beneficiary concerned. The report will be formally notified to it.

Audits (including audit reports) are in the language of the Agreement.

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The Commission may also access the beneficiaries' statutory records for the periodical assessment of unit costs or flat-rate amounts.

22.2 Investigations by the European Anti-Fraud Office (OLAF)

Under Regulations No 883/2013[16] and No 2185/96[17] (and in accordance with their provisions and procedures), the European Anti-Fraud Office (OLAF) may — at any moment during implementation of the action or afterwards — carry out investigations, including on-the-spot checks and inspections, to establish whether there has been fraud, corruption or any other illegal activity affecting the financial interests of the EU.

22.3 Checks and audits by the European Court of Auditors (ECA)

Under Article 287 of the Treaty on the Functioning of the European Union (TFEU) and Article 161 of the Financial Regulation No 966/2012[18], the European Court of Auditors (ECA) may — at any moment during implementation of the action or afterwards — carry out audits.

The ECA has the right of access for the purpose of checks and audits.

22.4 Checks, reviews, audits and investigations for international organisations

Not applicable

22.5 Consequences of findings in checks, reviews, audits and investigations — Extension of findings

22.5.1 Findings in this grant

Findings in checks, reviews, audits or investigations carried out in the context of this grant may lead to the rejection of ineligible costs (see Article 42), reduction of the grant (see Article 43), recovery of undue amounts (see Article 44) or to any of the other measures described in Chapter 6.

Rejection of costs or reduction of the grant after the payment of the balance will lead to a revised final grant amount (see Article 5.4).

Findings in checks, reviews, audits or investigations may lead to a request for amendment for the modification of Annex 1 (see Article 55).

Checks, reviews, audits or investigations that find systemic or recurrent errors, irregularities, fraud or breach of obligations may also lead to consequences in other EU or Euratom grants awarded under similar conditions ('**extension of findings from this grant to other grants**').

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[16] Regulation (EU, Euratom) No 883/2013 of the European Parliament and of the Council of 11 September 2013 concerning investigations conducted by the European Anti-Fraud Office (OLAF) and repealing Regulation (EC) No 1073/1999 of the European Parliament and of the Council and Council Regulation (Euratom) No 1074/1999 (OJ L 248, 18.09.2013, p. 1).

[17] Council Regulation (Euratom, EC) No 2185/1996 of 11 November 1996 concerning on-the-spot checks and inspections carried out by the Commission in order to protect the European Communities' financial interests against fraud and other irregularities (OJ L 292, 15.11.1996, p. 2).

[18] Regulation (EU, Euratom) No 966/2012 of the European Parliament and of the Council of 25 October 2012 on the financial rules applicable to the general budget of the Union and repealing Council Regulation (EC, Euratom) No 1605/2002 (OJ L 298, 26.10.2012, p. 1).

Moreover, findings arising from an OLAF investigation may lead to criminal prosecution under national law.

22.5.2 Findings in other grants

The Commission may extend findings from other grants to this grant ('**extension of findings from other grants to this grant**'), if:

(a) the beneficiary concerned is found, in other EU or Euratom grants awarded under similar conditions, to have committed systemic or recurrent errors, irregularities, fraud or breach of obligations that have a material impact on this grant and

(b) those findings are formally notified to the beneficiary concerned — together with the list of grants affected by the findings — no later than two years after the payment of the balance of this grant.

The extension of findings may lead to the rejection of costs (see Article 42), reduction of the grant (see Article 43), recovery of undue amounts (see Article 44), suspension of payments (see Article 48), suspension of the action implementation (see Article 49) or termination (see Article 50).

22.5.3 Procedure

The Commission will formally notify the beneficiary concerned the systemic or recurrent errors and its intention to extend these audit findings, together with the list of grants affected.

22.5.3.1 If the findings concern **eligibility of costs**: the formal notification will include:

(a) an invitation to submit observations on the list of grants affected by the findings;

(b) the request to submit **revised financial statements** for all grants affected;

(c) the **correction rate for extrapolation** established by the Commission on the basis of the systemic or recurrent errors, to calculate the amounts to be rejected if the beneficiary concerned:

(i) considers that the submission of revised financial statements is not possible or practicable or

(ii) does not submit revised financial statements.

The beneficiary concerned has 90 days from receiving notification to submit observations, revised financial statements or to propose a duly substantiated **alternative correction method**. This period may be extended by the Commission in justified cases.

The Commission may then start a rejection procedure in accordance with Article 42, on the basis of:

- the revised financial statements, if approved;

- the proposed alternative correction method, if accepted

or

- the initially notified correction rate for extrapolation, if it does not receive any observations

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or revised financial statements, does not accept the observations or the proposed alternative correction method or does not approve the revised financial statements.

22.5.3.2 If the findings concern **substantial errors**, **irregularities or fraud** or **serious breach of obligations**: the formal notification will include:

(a) an invitation to submit observations on the list of grants affected by the findings and

(b) the flat-rate the Commission intends to apply according to the principle of proportionality.

The beneficiary concerned has 90 days from receiving notification to submit observations or to propose a duly substantiated alternative flat-rate.

The Commission may then start a reduction procedure in accordance with Article 43, on the basis of:

- the proposed alternative flat-rate, if accepted

or

- the initially notified flat-rate, if it does not receive any observations or does not accept the observations or the proposed alternative flat-rate.

22.6 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, any insufficiently substantiated costs will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 23 — EVALUATION OF THE IMPACT OF THE ACTION

23.1 Right to evaluate the impact of the action

The Commission may carry out interim and final evaluations of the impact of the action measured against the objective of the *EU* programme.

Evaluations may be started during implementation of the action and up to *five* years after the payment of the balance. The evaluation is considered to start on the date of the formal notification to the coordinator or beneficiaries.

The Commission may make these evaluations directly (using its own staff) or indirectly (using external bodies or persons it has authorised to do so).

The coordinator or beneficiaries must provide any information relevant to evaluate the impact of the action, including information in electronic format.

23.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the *Commission* may apply the measures described in Chapter 6.

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SECTION 3 RIGHTS AND OBLIGATIONS RELATED TO BACKGROUND AND RESULTS

SUBSECTION 1 GENERAL

ARTICLE 23a — MANAGEMENT OF INTELLECTUAL PROPERTY

23a.1 Obligation to take measures to implement the Commission Recommendation on the management of intellectual property in knowledge transfer activities

Beneficiaries that are universities or other public research organisations must take measures to implement the principles set out in Points 1 and 2 of the Code of Practice annexed to the Commission Recommendation on the management of intellectual property in knowledge transfer activities[19].

This does not change the obligations set out in Subsections 2 and 3 of this Section.

The beneficiaries must ensure that researchers and third parties involved in the action are aware of them.

23a.2 Consequences of non-compliance

If a beneficiary breaches its obligations under this Article, the *Commission* may apply any of the measures described in Chapter 6.

SUBSECTION 2 RIGHTS AND OBLIGATIONS RELATED TO BACKGROUND

ARTICLE 24 — AGREEMENT ON BACKGROUND

24.1 Agreement on background

The beneficiaries must identify and agree (in writing) on the background for the action ('**agreement on background**').

'**Background**' means any data, know-how or information — whatever its form or nature (tangible or intangible), including any rights such as intellectual property rights — that:

(a) is held by the beneficiaries before they acceded to the Agreement, and

(b) is needed to implement the action or exploit the results.

24.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

[19] Commission Recommendation C(2008) 1329 of 10.4.2008 on the management of intellectual property in knowledge transfer activities and the Code of Practice for universities and other public research institutions attached to this recommendation.

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ARTICLE 25 — ACCESS RIGHTS TO BACKGROUND

25.1 Exercise of access rights — Waiving of access rights — No sub-licensing

To exercise access rights, this must first be requested in writing ('**request for access**').

'**Access rights**' means rights to use results or background under the terms and conditions laid down in this Agreement.

Waivers of access rights are not valid unless in writing.

Unless agreed otherwise, access rights do not include the right to sub-license.

25.2 Access rights for other beneficiaries, for implementing their own tasks under the action

The beneficiaries must give each other access — on a royalty-free basis — to background needed to implement their own tasks under the action, unless the beneficiary that holds the background has — before acceding to the Agreement —:

(a) informed the other beneficiaries that access to its background is subject to legal restrictions or limits, including those imposed by the rights of third parties (including personnel), or

(b) agreed with the other beneficiaries that access would not be on a royalty-free basis.

25.3 Access rights for other beneficiaries, for exploiting their own results

The beneficiaries must give each other access — under fair and reasonable conditions — to background needed for exploiting their own results, unless the beneficiary that holds the background has — before acceding to the Agreement — informed the other beneficiaries that access to its background is subject to legal restrictions or limits, including those imposed by the rights of third parties (including personnel).

'**Fair and reasonable conditions**' means appropriate conditions, including possible financial terms or royalty-free conditions, taking into account the specific circumstances of the request for access, for example the actual or potential value of the results or background to which access is requested and/or the scope, duration or other characteristics of the exploitation envisaged.

Requests for access may be made — unless agreed otherwise — up to one year after the period set out in Article 3.

25.4 Access rights for affiliated entities

Unless otherwise agreed in the consortium agreement, access to background must also be given — under fair and reasonable conditions (see above; Article 25.3) and unless it is subject to legal restrictions or limits, including those imposed by the rights of third parties (including personnel) — to affiliated entities[20] established in an EU Member State or '**associated country**'[21], if this is needed to exploit the results generated by the beneficiaries to which they are affiliated.

[20] For the definition, see 'affiliated entity' footnote (Article 14.1).

[21] For the definition, see Article 2.1(3) of the Rules for Participation Regulation No 1290/2013: '**associated country**' means a third country which is party to an international agreement with the Union, as identified in *Article 7 of*

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Unless agreed otherwise (see above; Article 25.1), the affiliated entity concerned must make the request directly to the beneficiary that holds the background.

Requests for access may be made — unless agreed otherwise — up to one year after the period set out in Article 3.

25.5 Access rights for third parties

Not applicable

25.6 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

SUBSECTION 3 RIGHTS AND OBLIGATIONS RELATED TO RESULTS

ARTICLE 26 — OWNERSHIP OF RESULTS

26.1 Ownership by the beneficiary that generates the results

Results are owned by the beneficiary that generates them.

'**Results**' means any (tangible or intangible) output of the action such as data, knowledge or information — whatever its form or nature, whether it can be protected or not — that is generated in the action, as well as any rights attached to it, including intellectual property rights.

26.2 Joint ownership by several beneficiaries

Two or more beneficiaries own results jointly if:

(a) they have jointly generated them and

(b) it is not possible to:

(i) establish the respective contribution of each beneficiary, or

(ii) separate them for the purpose of applying for, obtaining or maintaining their protection (see Article 27).

The joint owners must agree (in writing) on the allocation and terms of exercise of their joint ownership ('**joint ownership agreement**'), to ensure compliance with their obligations under this Agreement.

Unless otherwise agreed in the joint ownership agreement, each joint owner may grant non-exclusive licences to third parties to exploit jointly-owned results (without any right to sub-license), if the other joint owners are given:

Horizon 2020 Framework Programme Regulation No 1291/2013. Article 7 sets out the conditions for association of non-EU countries to Horizon 2020.

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(a) at least 45 days advance notice and

(b) fair and reasonable compensation.

Once the results have been generated, joint owners may agree (in writing) to apply another regime than joint ownership (such as, for instance, transfer to a single owner (see Article 30) with access rights for the others).

26.3 Rights of third parties (including personnel)

If third parties (including personnel) may claim rights to the results, the beneficiary concerned must ensure that it complies with its obligations under the Agreement.

If a third party generates results, the beneficiary concerned must obtain all necessary rights (transfer, licences or other) from the third party, in order to be able to respect its obligations as if those results were generated by the beneficiary itself.

If obtaining the rights is impossible, the beneficiary must refrain from using the third party to generate the results.

26.4 *EU* ownership, to protect results

26.4.1 *The EU* may — with the consent of the beneficiary concerned — assume ownership of results to protect them, if a beneficiary intends — up to four years after the period set out in Article 3 — to disseminate its results without protecting them, except in any of the following cases:

(a) the lack of protection is because protecting the results is not possible, reasonable or justified (given the circumstances);

(b) the lack of protection is because there is a lack of potential for commercial or industrial exploitation, or

(c) the beneficiary intends to transfer the results to another beneficiary or third party established in an EU Member State or associated country, which will protect them.

Before the results are disseminated and unless any of the cases above under Points (a), (b) or (c) applies, the beneficiary must formally notify the *Commission* and at the same time inform it of any reasons for refusing consent. The beneficiary may refuse consent only if it can show that its legitimate interests would suffer significant harm.

If the *Commission* decides to assume ownership, it will formally notify the beneficiary concerned within 45 days of receiving notification.

No dissemination relating to these results may take place before the end of this period or, if the *Commission* takes a positive decision, until it has taken the necessary steps to protect the results.

26.4.2 *The EU* may — with the consent of the beneficiary concerned — assume ownership of results to protect them, if a beneficiary intends — up to four years after the period set out in Article 3 — to stop protecting them or not to seek an extension of protection, except in any of the following cases:

(a) the protection is stopped because of a lack of potential for commercial or industrial exploitation;

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(b) an extension would not be justified given the circumstances.

A beneficiary that intends to stop protecting results or not seek an extension must — unless any of the cases above under Points (a) or (b) applies — formally notify the *Commission* at least 60 days before the protection lapses or its extension is no longer possible and at the same time inform it of any reasons for refusing consent. The beneficiary may refuse consent only if it can show that its legitimate interests would suffer significant harm.

If the *Commission* decides to assume ownership, it will formally notify the beneficiary concerned within 45 days of receiving notification.

26.5 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to the any of the other measures described in Chapter 6.

ARTICLE 27 — PROTECTION OF RESULTS — VISIBILITY OF EU FUNDING

27.1 Obligation to protect the results

Each beneficiary must examine the possibility of protecting its results and must adequately protect them — for an appropriate period and with appropriate territorial coverage — if:

(a) the results can reasonably be expected to be commercially or industrially exploited and

(b) protecting them is possible, reasonable and justified (given the circumstances).

When deciding on protection, the beneficiary must consider its own legitimate interests and the legitimate interests (especially commercial) of the other beneficiaries.

27.2 *EU* ownership, to protect the results

If a beneficiary intends not to protect its results, to stop protecting them or not seek an extension of protection, *the EU* may — under certain conditions (see Article 26.4) — assume ownership to ensure their (continued) protection.

27.3 Information on EU funding

Applications for protection of results (including patent applications) filed by or on behalf of a beneficiary must — unless the *Commission* requests or agrees otherwise or unless it is impossible — include the following:

> "The project leading to this application has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 957189".

27.4 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

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Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 28 — EXPLOITATION OF RESULTS

28.1 Obligation to exploit the results

Each beneficiary must — up to four years after the period set out in Article 3 — take measures aiming to ensure '**exploitation**' of its results (either directly or indirectly, in particular through transfer or licensing; see Article 30) by:

(a) using them in further research activities (outside the action);

(b) developing, creating or marketing a product or process;

(c) creating and providing a service, or

(d) using them in standardisation activities.

This does not change the security obligations in Article 37, which still apply.

28.2 Results that could contribute to European or international standards — Information on EU funding

If results are incorporated in a standard, the beneficiary concerned must — unless the *Commission* requests or agrees otherwise or unless it is impossible — ask the standardisation body to include the following statement in (information related to) the standard:

> "Results incorporated in this standard received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 957189".

28.3 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced in accordance with Article 43.

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 29 — DISSEMINATION OF RESULTS — OPEN ACCESS — VISIBILITY OF EU FUNDING

29.1 Obligation to disseminate results

Unless it goes against their legitimate interests, each beneficiary must — as soon as possible — '**disseminate**' its results by disclosing them to the public by appropriate means (other than those resulting from protecting or exploiting the results), including in scientific publications (in any medium).

This does not change the obligation to protect results in Article 27, the confidentiality obligations in Article 36, the security obligations in Article 37 or the obligations to protect personal data in Article 39, all of which still apply.

A beneficiary that intends to disseminate its results must give advance notice to the other beneficiaries

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of — unless agreed otherwise — at least 45 days, together with sufficient information on the results it will disseminate.

Any other beneficiary may object within — unless agreed otherwise — 30 days of receiving notification, if it can show that its legitimate interests in relation to the results or background would be significantly harmed. In such cases, the dissemination may not take place unless appropriate steps are taken to safeguard these legitimate interests.

If a beneficiary intends not to protect its results, it may — under certain conditions (see Article 26.4.1) — need to formally notify the *Commission* before dissemination takes place.

29.2 Open access to scientific publications

Each beneficiary must ensure open access (free of charge online access for any user) to all peer-reviewed scientific publications relating to its results.

In particular, it must:

(a) as soon as possible and at the latest on publication, deposit a machine-readable electronic copy of the published version or final peer-reviewed manuscript accepted for publication in a repository for scientific publications;

Moreover, the beneficiary must aim to deposit at the same time the research data needed to validate the results presented in the deposited scientific publications.

(b) ensure open access to the deposited publication — via the repository — at the latest:

(i) on publication, if an electronic version is available for free via the publisher, or

(ii) within six months of publication (twelve months for publications in the social sciences and humanities) in any other case.

(c) ensure open access — via the repository — to the bibliographic metadata that identify the deposited publication.

The bibliographic metadata must be in a standard format and must include all of the following:

- the terms *"European Union (EU)" and "Horizon 2020"*;
- the name of the action, acronym and grant number;
- the publication date, and length of embargo period if applicable, and
- a persistent identifier.

29.3 Open access to research data

*Regarding the digital research data generated in the action ('**data**'), the beneficiaries must:*

(a) deposit in a research data repository and take measures to make it possible for third parties to access, mine, exploit, reproduce and disseminate — free of charge for any user — the following:

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(i) the data, including associated metadata, needed to validate the results presented in scientific publications, as soon as possible;

(ii) not applicable;

(iii) other data, including associated metadata, as specified and within the deadlines laid down in the 'data management plan' (see Annex 1);

(b) provide information — via the repository — about tools and instruments at the disposal of the beneficiaries and necessary for validating the results (and — where possible — provide the tools and instruments themselves).

This does not change the obligation to protect results in Article 27, the confidentiality obligations in Article 36, the security obligations in Article 37 or the obligations to protect personal data in Article 39, all of which still apply.

As an exception, the beneficiaries do not have to ensure open access to specific parts of their research data under Point (a)(i) and (iii), if the achievement of the action's main objective (as described in Annex 1) would be jeopardised by making those specific parts of the research data openly accessible. In this case, the data management plan must contain the reasons for not giving access.

29.4 Information on EU funding — Obligation and right to use the EU emblem

Unless the *Commission* requests or agrees otherwise or unless it is impossible, any dissemination of results (in any form, including electronic) must:

(a) display the EU emblem and

(b) include the following text:

"This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 957189".

When displayed together with another logo, the EU emblem must have appropriate prominence.

For the purposes of their obligations under this Article, the beneficiaries may use the EU emblem without first obtaining approval from the *Commission*.

This does not however give them the right to exclusive use.

Moreover, they may not appropriate the EU emblem or any similar trademark or logo, either by registration or by any other means.

29.5 Disclaimer excluding *Commission* responsibility

Any dissemination of results must indicate that it reflects only the author's view and that the *Commission* is not responsible for any use that may be made of the information it contains.

29.6 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

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Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 30 — TRANSFER AND LICENSING OF RESULTS

30.1 Transfer of ownership

Each beneficiary may transfer ownership of its results.

It must however ensure that its obligations under Articles 26.2, 26.4, 27, 28, 29, 30 and 31 also apply to the new owner and that this owner has the obligation to pass them on in any subsequent transfer.

This does not change the security obligations in Article 37, which still apply.

Unless agreed otherwise (in writing) for specifically-identified third parties or unless impossible under applicable EU and national laws on mergers and acquisitions, a beneficiary that intends to transfer ownership of results must give at least 45 days advance notice (or less if agreed in writing) to the other beneficiaries that still have (or still may request) access rights to the results. This notification must include sufficient information on the new owner to enable any beneficiary concerned to assess the effects on its access rights.

Unless agreed otherwise (in writing) for specifically-identified third parties, any other beneficiary may object within 30 days of receiving notification (or less if agreed in writing), if it can show that the transfer would adversely affect its access rights. In this case, the transfer may not take place until agreement has been reached between the beneficiaries concerned.

30.2 Granting licenses

Each beneficiary may grant licences to its results (or otherwise give the right to exploit them), if:

(a) this does not impede the access rights under Article 31 and

(b) *not applicable.*

In addition to Points (a) and (b), exclusive licences for results may be granted only if all the other beneficiaries concerned have waived their access rights (see Article 31.1).

This does not change the dissemination obligations in Article 29 or security obligations in Article 37, which still apply.

30.3 *Commission* right to object to transfers or licensing

The Commission may — up to four years after the period set out in Article 3 — object to a transfer of ownership or the exclusive licensing of results, if:

(a) it is to a third party established in a non-EU country not associated with Horizon 2020 and

(b) the Commission considers that the transfer or licence is not in line with EU interests regarding competitiveness or is inconsistent with ethical principles or security considerations.

A beneficiary that intends to transfer ownership or grant an exclusive licence must formally notify the Commission before the intended transfer or licensing takes place and:

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- *identify the specific results concerned;*
- *describe in detail the new owner or licensee and the planned or potential exploitation of the results, and*
- *include a reasoned assessment of the likely impact of the transfer or licence on EU competitiveness and its consistency with ethical principles and security considerations.*

The Commission may request additional information.

If the Commission decides to object to a transfer or exclusive licence, it must formally notify the beneficiary concerned within 60 days of receiving notification (or any additional information it has requested).

No transfer or licensing may take place in the following cases:

- *pending the Commission decision, within the period set out above;*
- *if the Commission objects;*
- *until the conditions are complied with, if the Commission objection comes with conditions.*

30.4 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 31 — ACCESS RIGHTS TO RESULTS

31.1 Exercise of access rights — Waiving of access rights — No sub-licensing

The conditions set out in Article 25.1 apply.

The obligations set out in this Article do not change the security obligations in Article 37, which still apply.

31.2 Access rights for other beneficiaries, for implementing their own tasks under the action

The beneficiaries must give each other access — on a royalty-free basis — to results needed for implementing their own tasks under the action.

31.3 Access rights for other beneficiaries, for exploiting their own results

The beneficiaries must give each other — under fair and reasonable conditions (see Article 25.3) — access to results needed for exploiting their own results.

Requests for access may be made — unless agreed otherwise — up to one year after the period set out in Article 3.

31.4 Access rights of affiliated entities

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Unless agreed otherwise in the consortium agreement, access to results must also be given — under fair and reasonable conditions (Article 25.3) — to affiliated entities established in an EU Member State or associated country, if this is needed for those entities to exploit the results generated by the beneficiaries to which they are affiliated.

Unless agreed otherwise (see above; Article 31.1), the affiliated entity concerned must make any such request directly to the beneficiary that owns the results.

Requests for access may be made — unless agreed otherwise — up to one year after the period set out in Article 3.

31.5 Access rights for the EU institutions, bodies, offices or agencies and EU Member States

The beneficiaries must give access to their results — on a royalty-free basis — to EU institutions, bodies, offices or agencies, for developing, implementing or monitoring EU policies or programmes.

Such access rights are limited to non-commercial and non-competitive use.

This does not change the right to use any material, document or information received from the beneficiaries for communication and publicising activities (see Article 38.2).

31.6 Access rights for third parties

The beneficiaries must give — under the conditions set out in Article 31.2 and 31.3 — access to their results to complementary beneficiaries[22], for the purposes of the complementary grant agreement(s) (see Article 2).

31.7 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

SECTION 4 OTHER RIGHTS AND OBLIGATIONS

ARTICLE 32 — RECRUITMENT AND WORKING CONDITIONS FOR RESEARCHERS

32.1 Obligation to take measures to implement the European Charter for Researchers and Code of Conduct for the Recruitment of Researchers

The beneficiaries must take all measures to implement the principles set out in the Commission Recommendation on the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers[23], in particular regarding:

- working conditions;

[22] '**Complementary beneficiary**' means a beneficiary of a complementary grant agreement.

[23] Commission Recommendation 2005/251/EC of 11 March 2005 on the European Charter for Researchers and on a Code of Conduct for the Recruitment of Researchers (OJ L 75, 22.3.2005, p. 67).

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- transparent recruitment processes based on merit, and
- career development.

The beneficiaries must ensure that researchers and third parties involved in the action are aware of them.

32.2 Consequences of non-compliance

If a beneficiary breaches its obligations under this Article, the *Commission* may apply any of the measures described in Chapter 6.

ARTICLE 33 — GENDER EQUALITY

33.1 Obligation to aim for gender equality

The beneficiaries must take all measures to promote equal opportunities between men and women in the implementation of the action. They must aim, to the extent possible, for a gender balance at all levels of personnel assigned to the action, including at supervisory and managerial level.

33.2 Consequences of non-compliance

If a beneficiary breaches its obligations under this Article, the *Commission* may apply any of the measures described in Chapter 6.

ARTICLE 34 — ETHICS AND RESEARCH INTEGRITY

34.1 Obligation to comply with ethical and research integrity principles

The beneficiaries must carry out the action in compliance with:

(a) ethical principles (including the highest standards of research integrity)

and

(b) applicable international, EU and national law.

Funding will not be granted for activities carried out outside the EU if they are prohibited in all Member States or for activities which destroy human embryos (for example, for obtaining stem cells).

The beneficiaries must ensure that the activities under the action have an exclusive focus on civil applications.

The beneficiaries must ensure that the activities under the action do not:

(a) aim at human cloning for reproductive purposes;

(b) intend to modify the genetic heritage of human beings which could make such changes heritable (with the exception of research relating to cancer treatment of the gonads, which may be financed), or

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(c) intend to create human embryos solely for the purpose of research or for the purpose of stem cell procurement, including by means of somatic cell nuclear transfer.

In addition, the beneficiaries must respect the fundamental principle of research integrity — as set out, for instance, in the European Code of Conduct for Research Integrity[24].

This implies compliance with the following fundamental principles:

- **reliability** in ensuring the quality of research reflected in the design, the methodology, the analysis and the use of resources;
- **honesty** in developing, undertaking, reviewing, reporting and communicating research in a transparent, fair and unbiased way;
- **respect** for colleagues, research participants, society, ecosystems, cultural heritage and the environment;
- **accountability** for the research from idea to publication, for its management and organisation, for training, supervision and mentoring, and for its wider impacts

and means that beneficiaries must ensure that persons carrying out research tasks follow the good research practices and refrain from the research integrity violations described in this Code.

This does not change the other obligations under this Agreement or obligations under applicable international, EU or national law, all of which still apply.

34.2 Activities raising ethical issues

Activities raising ethical issues must comply with the '**ethics requirements**' set out as deliverables in Annex 1.

Before the beginning of an activity raising an ethical issue, each beneficiary must have obtained:

(a) any ethics committee opinion required under national law and

(b) any notification or authorisation for activities raising ethical issues required under national and/or European law

needed for implementing the action tasks in question.

The documents must be kept on file and be submitted upon request by the coordinator to the *Commission* (see Article 52). If they are not in English, they must be submitted together with an English summary, which shows that the action tasks in question are covered and includes the conclusions of the committee or authority concerned (if available).

34.3 Activities involving human embryos or human embryonic stem cells

Activities involving research on human embryos or human embryonic stem cells may be carried out, in addition to Article 34.1, only if:

[24] European Code of Conduct for Research Integrity of ALLEA (All European Academies) http://ec.europa.eu/research/participants/data/ref/h2020/other/hi/h2020-ethics_code-of-conduct_en.pdf

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- they are set out in Annex 1 or
- the coordinator has obtained explicit approval (in writing) from the *Commission* (see Article 52).

34.4 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43) and the Agreement or participation of the beneficiary may be terminated (see Article 50).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 35 — CONFLICT OF INTERESTS

35.1 Obligation to avoid a conflict of interests

The beneficiaries must take all measures to prevent any situation where the impartial and objective implementation of the action is compromised for reasons involving economic interest, political or national affinity, family or emotional ties or any other shared interest ('**conflict of interests**').

They must formally notify to the *Commission* without delay any situation constituting or likely to lead to a conflict of interests and immediately take all the necessary steps to rectify this situation.

The *Commission* may verify that the measures taken are appropriate and may require additional measures to be taken by a specified deadline.

35.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43) and the Agreement or participation of the beneficiary may be terminated (see Article 50).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 36 — CONFIDENTIALITY

36.1 General obligation to maintain confidentiality

During implementation of the action and for four years after the period set out in Article 3, the parties must keep confidential any data, documents or other material (in any form) that is identified as confidential at the time it is disclosed ('**confidential information**').

If a beneficiary requests, the *Commission* may agree to keep such information confidential for an additional period beyond the initial four years.

If information has been identified as confidential only orally, it will be considered to be confidential only if this is confirmed in writing within 15 days of the oral disclosure.

Unless otherwise agreed between the parties, they may use confidential information only to implement the Agreement.

The beneficiaries may disclose confidential information to their personnel or third parties involved in the action only if they:

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(a) need to know to implement the Agreement and

(b) are bound by an obligation of confidentiality.

This does not change the security obligations in Article 37, which still apply.

The *Commission* may disclose confidential information to its staff, other EU institutions and bodies. It may disclose confidential information to third parties, if:

(a) this is necessary to implement the Agreement or safeguard the EU's financial interests and

(b) the recipients of the information are bound by an obligation of confidentiality.

Under the conditions set out in Article 4 of the Rules for Participation Regulation No 1290/2013[25], the Commission must moreover make available information on the results to other EU institutions, bodies, offices or agencies as well as Member States or associated countries.

The confidentiality obligations no longer apply if:

(a) the disclosing party agrees to release the other party;

(b) the information was already known by the recipient or is given to him without obligation of confidentiality by a third party that was not bound by any obligation of confidentiality;

(c) the recipient proves that the information was developed without the use of confidential information;

(d) the information becomes generally and publicly available, without breaching any confidentiality obligation, or

(e) the disclosure of the information is required by EU or national law.

36.2 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 37 — SECURITY-RELATED OBLIGATIONS

37.1 Results with a security recommendation

Not applicable

37.2 Classified information

Not applicable

[25] Regulation (EU) No 1290/2013 of the European Parliament and of the Council of 11 December 2013 laying down the rules for participation and dissemination in "Horizon 2020 - the Framework Programme for Research and Innovation (2014-2020)" (OJ L 347, 20.12.2013 p.81).

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37.3 Activities involving dual-use goods or dangerous materials and substances

Not applicable

37.4 Consequences of non-compliance

Not applicable

ARTICLE 38 — PROMOTING THE ACTION — VISIBILITY OF EU FUNDING

38.1 Communication activities by beneficiaries

38.1.1 Obligation to promote the action and its results

The beneficiaries must promote the action and its results, by providing targeted information to multiple audiences (including the media and the public) in a strategic and effective manner.

This does not change the dissemination obligations in Article 29, the confidentiality obligations in Article 36 or the security obligations in Article 37, all of which still apply.

Before engaging in a communication activity expected to have a major media impact, the beneficiaries must inform the *Commission* (see Article 52).

38.1.2 Information on EU funding — Obligation and right to use the EU emblem

Unless the *Commission* requests or agrees otherwise or unless it is impossible, any communication activity related to the action (including in electronic form, via social media, etc.) and any infrastructure, equipment and major results funded by the grant must:

(a) display the EU emblem and

(b) include the following text:

For communication activities:

"This project has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 957189".

For infrastructure, equipment and major results:

"This *[infrastructure][equipment][insert type of result]* is part of a project that has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 957189".

When displayed together with another logo, the EU emblem must have appropriate prominence.

For the purposes of their obligations under this Article, the beneficiaries may use the EU emblem without first obtaining approval from the *Commission*.

This does not, however, give them the right to exclusive use.

Moreover, they may not appropriate the EU emblem or any similar trademark or logo, either by registration or by any other means.

38.1.3 Disclaimer excluding Commission responsibility

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Any communication activity related to the action must indicate that it reflects only the author's view and that the Commission *is* not responsible for any use that may be made of the information it contains.

38.2 Communication activities by the Commission

38.2.1 Right to use beneficiaries' materials, documents or information

The Commission may use, for its communication and publicising activities, information relating to the action, documents notably summaries for publication and public deliverables as well as any other material, such as pictures or audio-visual material received from any beneficiary (including in electronic form).

This does not change the confidentiality obligations in Article 36 and the security obligations in Article 37, all of which still apply.

If the Commission's use of these materials, documents or information would risk compromising legitimate interests, the beneficiary concerned may request the Commission not to use it (see Article 52).

The right to use a beneficiary's materials, documents and information includes:

(a) **use for its own purposes** (in particular, making them available to persons working for the Commission or any other EU institution, body, office or agency or body or institutions in EU Member States; and copying or reproducing them in whole or in part, in unlimited numbers);

(b) **distribution to the public** (in particular, publication as hard copies and in electronic or digital format, publication on the internet, as a downloadable or non-downloadable file, broadcasting by any channel, public display or presentation, communicating through press information services, or inclusion in widely accessible databases or indexes);

(c) **editing or redrafting** for communication and publicising activities (including shortening, summarising, inserting other elements (such as meta-data, legends, other graphic, visual, audio or text elements), extracting parts (e.g. audio or video files), dividing into parts, use in a compilation);

(d) translation;

(e) giving **access in response to individual requests** under Regulation No 1049/2001[27], without the right to reproduce or exploit;

(f) **storage** in paper, electronic or other form;

(g) **archiving**, in line with applicable document-management rules, and

(h) the right to authorise **third parties** to act on its behalf or sub-license the modes of use set out in Points (b), (c), (d) and (f) to third parties if needed for the communication and publicising activities of the Commission.

If the right of use is subject to rights of a third party (including personnel of the beneficiary), the

[27] Regulation (EC) No 1049/2001 of the European Parliament and of the Council of 30 May 2001 regarding public access to European Parliament, Council and Commission documents, OJ L 145, 31.5.2001, p. 43.

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beneficiary must ensure that it complies with its obligations under this Agreement (in particular, by obtaining the necessary approval from the third parties concerned).

Where applicable (and if provided by the beneficiaries), the Commission will insert the following information:

> "© – [year] – [name of the copyright owner]. All rights reserved. Licensed to the *European Union (EU)* under conditions."

38.3 Consequences of non-compliance

If a beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 39 — PROCESSING OF PERSONAL DATA

39.1 Processing of personal data by the Commission

Any personal data under the Agreement will be processed by the Commission under Regulation No 45/2001[28] and according to the 'notifications of the processing operations' to the Data Protection Officer (DPO) of the Commission (publicly accessible in the DPO register).

Such data will be processed by the '**data controller**' of the Commission for the purposes of implementing, managing and monitoring the Agreement or protecting the financial interests of the EU or Euratom (including checks, reviews, audits and investigations; see Article 22).

The persons whose personal data are processed have the right to access and correct their own personal data. For this purpose, they must send any queries about the processing of their personal data to the data controller, via the contact point indicated in the privacy statement(s) that are published on the Commission websites.

They also have the right to have recourse at any time to the European Data Protection Supervisor (EDPS).

39.2 Processing of personal data by the beneficiaries

The beneficiaries must process personal data under the Agreement in compliance with applicable EU and national law on data protection (including authorisations or notification requirements).

The beneficiaries may grant their personnel access only to data that is strictly necessary for implementing, managing and monitoring the Agreement.

The beneficiaries must inform the personnel whose personal data are collected and processed by the Commission. For this purpose, they must provide them with the privacy statement(s) (see above), before transmitting their data to the Commission.

[28] Regulation (EC) No 45/2001 of the European Parliament and of the Council of 18 December 2000 on the protection of individuals with regard to the processing of personal data by the Community institutions and bodies and on the free movement of such data (OJ L 8, 12.01.2001, p. 1).

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39.3 Consequences of non-compliance

If a beneficiary breaches any of its obligations under Article 39.2, the *Commission* may apply any of the measures described in Chapter 6.

ARTICLE 40 — ASSIGNMENTS OF CLAIMS FOR PAYMENT AGAINST THE *COMMISSION*

The beneficiaries may not assign any of their claims for payment against the *Commission* to any third party, except if approved by the *Commission* on the basis of a reasoned, written request by the coordinator (on behalf of the beneficiary concerned).

If the *Commission* has not accepted the assignment or the terms of it are not observed, the assignment will have no effect on it.

In no circumstances will an assignment release the beneficiaries from their obligations towards the *Commission*.

CHAPTER 5 DIVISION OF BENEFICIARIES' ROLES AND RESPONSIBILITIES — RELATIONSHIP WITH COMPLEMENTARY BENEFICIARIES — RELATIONSHIP WITH PARTNERS OF A JOINT ACTION

ARTICLE 41 — DIVISION OF BENEFICIARIES' ROLES AND RESPONSIBILITIES — RELATIONSHIP WITH COMPLEMENTARY BENEFICIARIES — RELATIONSHIP WITH PARTNERS OF A JOINT ACTION

41.1 Roles and responsibility towards the *Commission*

The beneficiaries have full responsibility for implementing the action and complying with the Agreement.

The beneficiaries are jointly and severally liable for the **technical implementation** of the action as described in Annex 1. If a beneficiary fails to implement its part of the action, the other beneficiaries become responsible for implementing this part (without being entitled to any additional EU funding for doing so), unless the *Commission* expressly relieves them of this obligation.

The **financial responsibility** of each beneficiary is governed by Article 44.

41.2 Internal division of roles and responsibilities

The internal roles and responsibilities of the beneficiaries are divided as follows:

(a) Each **beneficiary** must:

(i) keep information stored in the Participant Portal Beneficiary Register (via the electronic exchange system) up to date (see Article 17);

(ii) inform the coordinator immediately of any events or circumstances likely to affect significantly or delay the implementation of the action (see Article 17);

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(iii) submit to the coordinator in good time:

- individual financial statements for itself *and its linked third parties* and, if required, certificates on the financial statements (see Article 20);
- the data needed to draw up the technical reports (see Article 20);
- ethics committee opinions and notifications or authorisations for activities raising ethical issues (see Article 34);
- any other documents or information required by the Commission under the Agreement, unless the Agreement requires the beneficiary to submit this information directly to the Commission.

(b) The **coordinator** must:

(i) monitor that the action is implemented properly (see Article 7);

(ii) act as the intermediary for all communications between the beneficiaries and the *Commission* (in particular, providing the *Commission* with the information described in Article 17), unless the Agreement specifies otherwise;

(iii) request and review any documents or information required by the *Commission* and verify their completeness and correctness before passing them on to the *Commission*;

(iv) submit the deliverables and reports to the *Commission* (see Articles 19 and 20);

(v) ensure that all payments are made to the other beneficiaries without unjustified delay (see Article 21);

(vi) inform the *Commission* of the amounts paid to each beneficiary, when required under the Agreement (see Articles 44 and 50) or requested by the *Commission*.

The coordinator may not delegate or subcontract the above-mentioned tasks to any other beneficiary or third party (including linked third parties).

41.3 Internal arrangements between beneficiaries — Consortium agreement

*The beneficiaries must have internal arrangements regarding their operation and co-ordination to ensure that the action is implemented properly. These internal arrangements must be set out in a written '**consortium agreement**' between the beneficiaries, which may cover:*

- *internal organisation of the consortium;*
- *management of access to the electronic exchange system;*
- *distribution of EU funding;*
- *additional rules on rights and obligations related to background and results (including whether access rights remain or not, if a beneficiary is in breach of its obligations) (see Section 3 of Chapter 4);*

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- *settlement of internal disputes;*
- *liability, indemnification and confidentiality arrangements between the beneficiaries.*

The consortium agreement must not contain any provision contrary to the Agreement.

41.4 Relationship with complementary beneficiaries — Collaboration agreement

The beneficiaries must conclude a written 'collaboration agreement' with the complementary beneficiaries to coordinate the work under the Agreement and the complementary grant agreement(s) (see Article 2), covering for instance:

- *efficient decision making processes and*
- *settlement of disputes.*

The collaboration agreement must not contain any provision contrary to the Agreement.

The beneficiaries and complementary beneficiaries must create and participate in common boards and advisory structures to decide on collaboration and synchronisation of activities, including on management of outcomes, common approaches towards standardisation, SME involvement, links with regulatory and policy activities, and commonly shared dissemination and awareness raising activities.

The beneficiaries must give access to their results to the complementary beneficiaries, for the purposes of the complementary grant agreement(s) (see Article 31.6).

The beneficiaries must share the technical reports (see Article 20.3 and 20.4). The confidentiality obligations in Article 36 apply.

41.5 Relationship with partners of a joint action — Coordination agreement

Not applicable

CHAPTER 6 REJECTION OF COSTS — REDUCTION OF THE GRANT — RECOVERY — SANCTIONS — DAMAGES — SUSPENSION — TERMINATION — FORCE MAJEURE

SECTION 1 REJECTION OF COSTS — REDUCTION OF THE GRANT — RECOVERY — SANCTIONS

ARTICLE 42 — REJECTION OF INELIGIBLE COSTS

42.1 Conditions

The *Commission* will — after **termination of the participation of a beneficiary**, at the time of an **interim payment**, **at the payment of the balance** or **afterwards** — reject any costs which are ineligible (see Article 6), in particular following checks, reviews, audits or investigations (see Article 22).

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The rejection may also be based on the **extension of findings from other grants to this grant** (see Article 22.5.2).

42.2 Ineligible costs to be rejected — Calculation — Procedure

Ineligible costs will be rejected in full.

If the rejection of costs does not lead to a recovery (see Article 44), the *Commission* will formally notify the coordinator or beneficiary concerned of the rejection of costs, the amounts and the reasons why (if applicable, together with the notification of amounts due; see Article 21.5). The coordinator or beneficiary concerned may — within 30 days of receiving notification — formally notify the *Commission* of its disagreement and the reasons why.

If the rejection of costs leads to a recovery, the *Commission* will follow the contradictory procedure with pre-information letter set out in Article 44.

42.3 Effects

If the *Commission* rejects costs at the time of an **interim payment** or **the payment of the balance**, it will deduct them from the total eligible costs declared, for the action, in the periodic or final summary financial statement (see Articles 20.3 and 20.4). It will then calculate the interim payment or payment of the balance as set out in Articles 21.3 or 21.4.

If the *Commission* rejects costs **after termination of the participation of a beneficiary**, it will deduct them from the costs declared by the beneficiary in the termination report and include the rejection in the calculation after termination (see Article 50.2 and 50.3).

If the *Commission* — **after an interim payment but before the payment of the balance** — rejects costs declared in a periodic summary financial statement, it will deduct them from the total eligible costs declared, for the action, in the next periodic summary financial statement or in the final summary financial statement. It will then calculate the interim payment or payment of the balance as set out in Articles 21.3 or 21.4.

If the *Commission* rejects costs **after the payment of the balance**, it will deduct the amount rejected from the total eligible costs declared, by the beneficiary, in the final summary financial statement. It will then calculate the revised final grant amount as set out in Article 5.4.

ARTICLE 43 — REDUCTION OF THE GRANT

43.1 Conditions

The *Commission* may — **after termination of the participation of a beneficiary**, **at the payment of the balance** or **afterwards** — reduce the grant amount (see Article 5.1), if :

(a) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed:

(i) substantial errors, irregularities or fraud or

(ii) serious breach of obligations under the Agreement or during the award procedure

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(including improper implementation of the action, submission of false information, failure to provide required information, breach of ethical principles) or

(b) a beneficiary (or a natural person who has the power to represent or take decision on its behalf) has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2).

43.2 Amount to be reduced — Calculation — Procedure

The amount of the reduction will be proportionate to the seriousness of the errors, irregularities or fraud or breach of obligations.

Before reduction of the grant, the *Commission* will formally notify a '**pre-information letter**' to the coordinator or beneficiary concerned:

- informing it of its intention to reduce the grant, the amount it intends to reduce and the reasons why and

- inviting it to submit observations within 30 days of receiving notification.

If the *Commission* does not receive any observations or decides to pursue reduction despite the observations it has received, it will formally notify **confirmation** of the reduction (if applicable, together with the notification of amounts due; see Article 21).

43.3 Effects

If the *Commission* reduces the grant **after termination of the participation of a beneficiary**, it will calculate the reduced grant amount for that beneficiary and then determine the amount due to that beneficiary (see Article 50.2 and 50.3).

If the *Commission* reduces the grant **at the payment of the balance**, it will calculate the reduced grant amount for the action and then determine the amount due as payment of the balance (see Articles 5.3.4 and 21.4).

If the *Commission* reduces the grant **after the payment of the balance**, it will calculate the revised final grant amount for the beneficiary concerned (see Article 5.4). If the revised final grant amount for the beneficiary concerned is lower than its share of the final grant amount, the *Commission* will recover the difference (see Article 44).

ARTICLE 44 — RECOVERY OF UNDUE AMOUNTS

44.1 Amount to be recovered — Calculation — Procedure

The *Commission* will — after **termination of the participation of a beneficiary, at the payment of the balance** or **afterwards** — claim back any amount that was paid, but is not due under the Agreement.

Each beneficiary's financial responsibility in case of recovery is limited to its own debt *(including*

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undue amounts paid by the Commission for costs declared by its linked third parties), except for the amount retained for the Guarantee Fund (see Article 21.4).

44.1.1 Recovery after termination of a beneficiary's participation

If recovery takes place after termination of a beneficiary's participation (including the coordinator), the *Commission* will claim back the undue amount from the beneficiary concerned, by formally notifying it a debit note (see Article 50.2 and 50.3). This note will specify the amount to be recovered, the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Commission will **recover** the amount:

(a) by '**offsetting**' it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Commission or an executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Commission may offset before the payment date specified in the debit note;

(b) *not applicable;*

(c) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date specified in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the payment date in the debit note, up to and including the date the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC[29] applies.

44.1.2 Recovery at payment of the balance

If the payment of the balance takes the form of a recovery (see Article 21.4), the *Commission* will formally notify a '**pre-information letter**' to the coordinator:

- informing it of its intention to recover, the amount due as the balance and the reasons why;
- specifying that it intends to deduct the amount to be recovered from the amount retained for the Guarantee Fund;
- requesting the coordinator to submit a report on the distribution of payments to the beneficiaries within 30 days of receiving notification, and

[29] Directive 2007/64/EC of the European Parliament and of the Council of 13 November 2007 on payment services in the internal market amending Directives 97/7/EC, 2002/65/EC, 2005/60/EC and 2006/48/EC and repealing Directive 97/5/EC (OJ L 319, 05.12.2007, p. 1).

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- inviting the coordinator to submit observations within 30 days of receiving notification.

If no observations are submitted or the *Commission* decides to pursue recovery despite the observations it has received, it will **confirm recovery** (together with the notification of amounts due; see Article 21.5) and:

- pay the difference between the amount to be recovered and the amount retained for the Guarantee Fund, **if the difference is positive** or

- formally notify to the coordinator a **debit note** for the difference between the amount to be recovered and the amount retained for the Guarantee Fund, **if the difference is negative**. This note will also specify the terms and the date for payment.

If the coordinator does not repay the *Commission* by the date in the debit note and has not submitted the report on the distribution of payments: the Commission will **recover** the amount set out in the debit note from the coordinator (see below).

If the coordinator does not repay the *Commission* by the date in the debit note, but has submitted the report on the distribution of payments: the *Commission* will:

(a) identify the beneficiaries for which the amount calculated as follows is negative:

{{{{beneficiary's costs declared in the final summary financial statement and approved by the *Commission* multiplied by the reimbursement rate set out in Article 5.2 for the beneficiary concerned

plus

its linked third parties' costs declared in the final summary financial statement and approved by the Commission multiplied by the reimbursement rate set out in Article 5.2 for each linked third party concerned}

divided by

the EU contribution for the action calculated according to Article 5.3.1}

multiplied by

the final grant amount (see Article 5.3)},

minus

{pre-financing and interim payments received by the beneficiary}}.

(b) formally notify to each beneficiary identified according to point (a) a **debit note** specifying the terms and date for payment. The amount of the debit note is calculated as follows:

{{amount calculated according to point (a) for the beneficiary concerned

divided by

the sum of the amounts calculated according to point (a) for all the beneficiaries identified according to point (a)}

multiplied by

the amount set out in the debit note formally notified to the coordinator}.

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If payment is not made by the date specified in the debit note, the Commission will **recover** the amount:

(a) by **offsetting** it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Commission or an executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Commission may offset before the payment date specified in the debit note;

(b) by **drawing on the Guarantee Fund**. The Commission will formally notify the beneficiary concerned the debit note on behalf of the Guarantee Fund and recover the amount:

(i) *not applicable;*

(ii) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the payment date in the debit note, up to and including the date the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

44.1.3 Recovery of amounts after payment of the balance

If, for a beneficiary, the revised final grant amount (see Article 5.4) is lower than its share of the final grant amount, it must repay the difference to the *Commission*.

The beneficiary's share of the final grant amount is calculated as follows:

{{{beneficiary's costs declared in the final summary financial statement and approved by the *Commission* multiplied by the reimbursement rate set out in Article 5.2 for the beneficiary concerned

plus

its linked third parties' costs declared in the final summary financial statement and approved by the Commission multiplied by the reimbursement rate set out in Article 5.2 for each linked third party concerned}

divided by

the EU contribution for the action calculated according to Article 5.3.1}

multiplied by

the final grant amount (see Article 5.3)}.

If the coordinator has not distributed amounts received (see Article 21.7), the *Commission* will also recover these amounts.

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The *Commission* will formally notify a **pre-information letter** to the beneficiary concerned:

- informing it of its intention to recover, the due amount and the reasons why and
- inviting it to submit observations within 30 days of receiving notification.

If no observations are submitted or the *Commission* decides to pursue recovery despite the observations it has received, it will **confirm** the amount to be recovered and formally notify to the beneficiary concerned a **debit note**. This note will also specify the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Commission will **recover** the amount:

(a) by **offsetting** it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Commission or an executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Commission may offset before the payment date specified in the debit note;

(b) by **drawing on the Guarantee Fund**. The Commission will formally notify the beneficiary concerned the debit note on behalf of the Guarantee Fund and recover the amount:

(i) *not applicable;*

(ii) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the date for payment in the debit note, up to and including the date the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

ARTICLE 45 — ADMINISTRATIVE SANCTIONS

In addition to contractual measures, the Commission may also adopt administrative sanctions under *Articles 106 and 131(4) of the Financial Regulation No 966/2012* (i.e. exclusion from future procurement contracts, grants, prizes and expert contracts and/or financial penalties).

SECTION 2 LIABILITY FOR DAMAGES

ARTICLE 46 — LIABILITY FOR DAMAGES

46.1 Liability of the *Commission*

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The *Commission* cannot be held liable for any damage caused to the beneficiaries or to third parties as a consequence of implementing the Agreement, including for gross negligence.

The *Commission* cannot be held liable for any damage caused by any of the beneficiaries or third parties involved in the action, as a consequence of implementing the Agreement.

46.2 Liability of the beneficiaries

Except in case of force majeure (see Article 51), the beneficiaries must compensate the *Commission* for any damage it sustains as a result of the implementation of the action or because the action was not implemented in full compliance with the Agreement.

SECTION 3 SUSPENSION AND TERMINATION

ARTICLE 47 — SUSPENSION OF PAYMENT DEADLINE

47.1 Conditions

The *Commission* may — at any moment — suspend the payment deadline (see Article 21.2 to 21.4) if a request for payment (see Article 20) cannot be approved because:

(a) it does not comply with the provisions of the Agreement (see Article 20);

(b) the technical or financial reports have not been submitted or are not complete or additional information is needed, or

(c) there is doubt about the eligibility of the costs declared in the financial statements and additional checks, reviews, audits or investigations are necessary.

47.2 Procedure

The *Commission* will formally notify the coordinator of the suspension and the reasons why.

The suspension will **take effect** the day notification is sent by the *Commission* (see Article 52).

If the conditions for suspending the payment deadline are no longer met, the suspension will be **lifted** — and the remaining period will resume.

If the suspension exceeds two months, the coordinator may request the *Commission* if the suspension will continue.

If the payment deadline has been suspended due to the non-compliance of the technical or financial reports (see Article 20) and the revised report or statement is not submitted or was submitted but is also rejected, the *Commission* may also terminate the Agreement or the participation of the beneficiary (see Article 50.3.1(l)).

ARTICLE 48 — SUSPENSION OF PAYMENTS

48.1 Conditions

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The *Commission* may — at any moment — suspend payments, in whole or in part and interim payments or the payment of the balance for one or more beneficiaries, if:

(a) a beneficiary (or a natural person who has the power to represent or take decision on its behalf) has committed or is suspected of having committed:

(i) substantial errors, irregularities or fraud or

(ii) serious breach of obligations under the Agreement or during the award procedure (including improper implementation of the action, submission of false information, failure to provide required information, breach of ethical principles) or

(b) a beneficiary (or a natural person who has the power to represent or take decision on its behalf) has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2).

If payments are suspended for one or more beneficiaries, the *Commission* will make partial payment(s) for the part(s) not suspended. If suspension concerns the payment of the balance, — once suspension is lifted — the payment or the recovery of the amount(s) concerned will be considered the payment of the balance that closes the action.

48.2 Procedure

Before suspending payments, the *Commission* will formally notify the coordinator or beneficiary concerned:

- informing it of its intention to suspend payments and the reasons why and
- inviting it to submit observations within 30 days of receiving notification.

If the *Commission* does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify **confirmation** of the suspension. Otherwise, it will formally notify that the suspension procedure is not continued.

The suspension will **take effect** the day the confirmation notification is sent by the *Commission*.

If the conditions for resuming payments are met, the suspension will be **lifted**. The *Commission* will formally notify the coordinator or beneficiary concerned.

During the suspension, the periodic report(s) for all reporting periods except the last one (see Article 20.3), must not contain any individual financial statements from the beneficiary concerned *and its linked third parties*. The coordinator must include them in the next periodic report after the suspension is lifted or — if suspension is not lifted before the end of the action — in the last periodic report.

The beneficiaries may suspend implementation of the action (see Article 49.1) or terminate the Agreement or the participation of the beneficiary concerned (see Article 50.1 and 50.2).

ARTICLE 49 — SUSPENSION OF THE ACTION IMPLEMENTATION

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49.1 Suspension of the action implementation, by the beneficiaries

49.1.1 Conditions

The beneficiaries may suspend implementation of the action or any part of it, if exceptional circumstances — in particular *force majeure* (see Article 51) — make implementation impossible or excessively difficult.

49.1.2 Procedure

The coordinator must immediately formally notify to the *Commission* the suspension (see Article 52), stating:

- the reasons why and
- the expected date of resumption.

The suspension will **take effect** the day this notification is received by the *Commission*.

Once circumstances allow for implementation to resume, the coordinator must immediately formally notify the *Commission* and request an **amendment** of the Agreement to set the date on which the action will be resumed, extend the duration of the action and make other changes necessary to adapt the action to the new situation (see Article 55) — unless the Agreement or the participation of a beneficiary has been terminated (see Article 50).

The suspension will be **lifted** with effect from the resumption date set out in the amendment. This date may be before the date on which the amendment enters into force.

Costs incurred during suspension of the action implementation are not eligible (see Article 6).

49.2 Suspension of the action implementation, by the *Commission*

49.2.1 Conditions

The *Commission* may suspend implementation of the action or any part of it, if:

(a) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed or is suspected of having committed:

  (i) substantial errors, irregularities or fraud or

  (ii) serious breach of obligations under the Agreement or during the award procedure (including improper implementation of the action, submission of false information, failure to provide required information, breach of ethical principles);

(b) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2), or

(c) the action is suspected of having lost its scientific or technological relevance.

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49.2.2 Procedure

Before suspending implementation of the action, the *Commission* will formally notify the coordinator or beneficiary concerned:

- informing it of its intention to suspend the implementation and the reasons why and
- inviting it to submit observations within 30 days of receiving notification.

If the *Commission* does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify **confirmation** of the suspension. Otherwise, it will formally notify that the procedure is not continued.

The suspension will **take effect** five days after confirmation notification is received (or on a later date specified in the notification).

It will be **lifted** if the conditions for resuming implementation of the action are met.

The coordinator or beneficiary concerned will be formally notified of the lifting and the Agreement will be **amended** to set the date on which the action will be resumed, extend the duration of the action and make other changes necessary to adapt the action to the new situation (see Article 55) — unless the Agreement has already been terminated (see Article 50).

The suspension will be lifted with effect from the resumption date set out in the amendment. This date may be before the date on which the amendment enters into force.

Costs incurred during suspension are not eligible (see Article 6).

The beneficiaries may not claim damages due to suspension by the *Commission* (see Article 46).

Suspension of the action implementation does not affect the *Commission's* right to terminate the Agreement or participation of a beneficiary (see Article 50), reduce the grant or recover amounts unduly paid (see Articles 43 and 44).

ARTICLE 50 — TERMINATION OF THE AGREEMENT OR OF THE PARTICIPATION OF ONE OR MORE BENEFICIARIES

50.1 Termination of the Agreement, by the beneficiaries

50.1.1 Conditions and procedure

The beneficiaries may terminate the Agreement.

The coordinator must formally notify termination to the *Commission* (see Article 52), stating:

- the reasons why and
- the date the termination will take effect. This date must be after the notification.

If no reasons are given or if the *Commission* considers the reasons do not justify termination, the Agreement will be considered to have been '**terminated improperly**'.

The termination will **take effect** on the day specified in the notification.

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50.1.2 Effects

The coordinator must — within 60 days from when termination takes effect — submit:

(i) a periodic report (for the open reporting period until termination; see Article 20.3) and

(ii) the final report (see Article 20.4).

If the *Commission* does not receive the reports within the deadline (see above), only costs which are included in an approved periodic report will be taken into account.

The *Commission* will **calculate** the final grant amount (see Article 5.3) and the balance (see Article 21.4) on the basis of the reports submitted. Only costs incurred until termination are eligible (see Article 6). Costs relating to contracts due for execution only after termination are not eligible.

Improper termination may lead to a reduction of the grant (see Article 43).

After termination, the beneficiaries' obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38, 40, 42, 43 and 44) continue to apply.

50.2 Termination of the participation of one or more beneficiaries, by the beneficiaries

50.2.1 Conditions and procedure

The participation of one or more beneficiaries may be terminated by the coordinator, on request of the beneficiary concerned or on behalf of the other beneficiaries.

The coordinator must formally notify termination to the *Commission* (see Article 52) and inform the beneficiary concerned.

If the coordinator's participation is terminated without its agreement, the formal notification must be done by another beneficiary (acting on behalf of the other beneficiaries).

The notification must include:

- the reasons why;
- the opinion of the beneficiary concerned (or proof that this opinion has been requested in writing);
- the date the termination takes effect. This date must be after the notification, and
- a request for amendment (see Article 55), with a proposal for reallocation of the tasks and the estimated budget of the beneficiary concerned (see Annexes 1 and 2) and, if necessary, the addition of one or more new beneficiaries (see Article 56). If termination takes effect after the period set out in Article 3, no request for amendment must be included unless the beneficiary concerned is the coordinator. In this case, the request for amendment must propose a new coordinator.

If this information is not given or if the *Commission* considers that the reasons do not justify termination, the participation will be considered to have been **terminated improperly**.

The termination will **take effect** on the day specified in the notification.

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50.2.2 Effects

The coordinator must — within 30 days from when termination takes effect — submit:

(i) a report on the distribution of payments to the beneficiary concerned and

(ii) if termination takes effect during the period set out in Article 3, a '**termination report**' from the beneficiary concerned, for the open reporting period until termination, containing an overview of the progress of the work, an overview of the use of resources, the individual financial statement and, if applicable, the certificate on the financial statement (see Articles 20.3 and 20.4).

The information in the termination report must also be included in the periodic report for the next reporting period (see Article 20.3).

If the request for amendment is rejected by the *Commission* (because it calls into question the decision awarding the grant or breaches the principle of equal treatment of applicants), the Agreement may be terminated according to Article 50.3.1(c).

If the request for amendment is accepted by the *Commission*, the Agreement is **amended** to introduce the necessary changes (see Article 55).

The *Commission* will — on the basis of the periodic reports, the termination report and the report on the distribution of payments — **calculate** the amount which is due to the beneficiary and if the (pre-financing and interim) payments received by the beneficiary exceed this amount.

The **amount which is due** is calculated in the following steps:

Step 1 — Application of the reimbursement rate to the eligible costs

The grant amount for the beneficiary is calculated by applying the reimbursement rate(s) to the total eligible costs declared by the beneficiary *and its linked third parties* in the termination report and approved by the *Commission*.

Only costs incurred by the beneficiary concerned until termination takes effect are eligible (see Article 6). Costs relating to contracts due for execution only after termination are not eligible.

Step 2 — Reduction due to substantial errors, irregularities or fraud or serious breach of obligations

In case of a reduction (see Article 43), the *Commission* will calculate the reduced grant amount for the beneficiary by deducting the amount of the reduction (calculated in proportion to the seriousness of the errors, irregularities or fraud or breach of obligations, in accordance with Article 43.2) from the grant amount for the beneficiary.

If the payments received **exceed the amounts due**:

- if termination takes effect during the period set out in Article 3 and the request for amendment is accepted, the beneficiary concerned must repay to the coordinator the amount unduly received. The *Commission* will formally notify the amount unduly received and

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request the beneficiary concerned to repay it to the coordinator within 30 days of receiving notification. If it does not repay the coordinator, the *Commission* will draw upon the Guarantee Fund to pay the coordinator and then notify a **debit note** on behalf of the Guarantee Fund to the beneficiary concerned (see Article 44);

- in all other cases, in particular if termination takes effect after the period set out in Article 3, the *Commission* will formally notify a **debit note** to the beneficiary concerned. If payment is not made by the date in the debit note, the Guarantee Fund will pay to the *Commission* the amount due and the *Commission* will notify a debit note on behalf of the Guarantee Fund to the beneficiary concerned (see Article 44);

- if the beneficiary concerned is the former coordinator, it must repay the new coordinator according to the procedure above, unless:

  - termination takes effect after an interim payment and

  - the former coordinator has not distributed amounts received as pre-financing or interim payments (see Article 21.7).

  In this case, the *Commission* will formally notify a **debit note** to the former coordinator. If payment is not made by the date in the debit note, the Guarantee Fund will pay to the *Commission* the amount due. The *Commission* will then pay the new coordinator and notify a debit note on behalf of the Guarantee Fund to the former coordinator (see Article 44).

If the payments received **do not exceed the amounts due**: amounts owed to the beneficiary concerned will be included in the next interim or final payment.

If the *Commission* does not receive the termination report within the deadline (see above), only costs included in an approved periodic report will be taken into account.

If the *Commission* does not receive the report on the distribution of payments within the deadline (see above), it will consider that:

- the coordinator did not distribute any payment to the beneficiary concerned and that

- the beneficiary concerned must not repay any amount to the coordinator.

Improper termination may lead to a reduction of the grant (see Article 43) or termination of the Agreement (see Article 50).

After termination, the concerned beneficiary's obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38, 40, 42, 43 and 44) continue to apply.

50.3 Termination of the Agreement or the participation of one or more beneficiaries, by the *Commission*

50.3.1 Conditions

The *Commission* may terminate the Agreement or the participation of one or more beneficiaries, if:

(a) one or more beneficiaries do not accede to the Agreement (see Article 56);

(b) a change to their legal, financial, technical, organisational or ownership situation *(or those*

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of its linked third parties) is likely to substantially affect or delay the implementation of the action or calls into question the decision to award the grant;

(c) following termination of participation for one or more beneficiaries (see above), the necessary changes to the Agreement would call into question the decision awarding the grant or breach the principle of equal treatment of applicants (see Article 55);

(d) implementation of the action is prevented by force majeure (see Article 51) or suspended by the coordinator (see Article 49.1) and either:

(i) resumption is impossible, or

(ii) the necessary changes to the Agreement would call into question the decision awarding the grant or breach the principle of equal treatment of applicants;

(e) a beneficiary is declared bankrupt, being wound up, having its affairs administered by the courts, has entered into an arrangement with creditors, has suspended business activities, or is subject to any other similar proceedings or procedures under national law;

(f) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has been found guilty of professional misconduct, proven by any means;

(g) a beneficiary does not comply with the applicable national law on taxes and social security;

(h) the action has lost scientific or technological relevance;

(i) *not applicable;*

(j) *not applicable;*

(k) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed fraud, corruption, or is involved in a criminal organisation, money laundering or any other illegal activity;

(l) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed:

(i) substantial errors, irregularities or fraud or

(ii) serious breach of obligations under the Agreement or during the award procedure (including improper implementation of the action, submission of false information, failure to provide required information, breach of ethical principles);

(m) a beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2);

(n) *despite a specific request by the Commission, a beneficiary does not request — through the coordinator — an amendment to the Agreement to end the participation of one of its linked third parties or international partners that is in one of the situations under points (e), (f), (g), (k), (l) or (m) and to reallocate its tasks.*

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50.3.2 Procedure

Before terminating the Agreement or participation of one or more beneficiaries, the *Commission* will formally notify the coordinator or beneficiary concerned:

- informing it of its intention to terminate and the reasons why and
- inviting it, within 30 days of receiving notification, to submit observations and — in case of Point (l.ii) above — to inform the *Commission* of the measures to ensure compliance with the obligations under the Agreement.

If the *Commission* does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify to the coordinator or beneficiary concerned **confirmation** of the termination and the date it will take effect. Otherwise, it will formally notify that the procedure is not continued.

The termination will **take effect**:

- for terminations under Points (b), (c), (e), (g), (h), (j), (l.ii) and (n) above: on the day specified in the notification of the confirmation (see above);
- for terminations under Points (a), (d), (f), (i), (k), (l.i) and (m) above: on the day after the notification of the confirmation is received.

50.3.3 Effects

(a) for **termination of the Agreement**:

The coordinator must — within 60 days from when termination takes effect — submit:

(i) a periodic report (for the last open reporting period until termination; see Article 20.3) and

(ii) a final report (see Article 20.4).

If the Agreement is terminated for breach of the obligation to submit reports (see Articles 20.8 and 50.3.1(l)), the coordinator may not submit any reports after termination.

If the *Commission* does not receive the reports within the deadline (see above), only costs which are included in an approved periodic report will be taken into account.

The *Commission* will **calculate** the final grant amount (see Article 5.3) and the balance (see Article 21.4) on the basis of the reports submitted. Only costs incurred until termination takes effect are eligible (see Article 6). Costs relating to contracts due for execution only after termination are not eligible.

This does not affect the *Commission's* right to reduce the grant (see Article 43) or to impose administrative sanctions (Article 45).

The beneficiaries may not claim damages due to termination by the *Commission* (see Article 46).

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After termination, the beneficiaries' obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38, 40, 42, 43 and 44) continue to apply.

(b) for **termination of the participation of one or more beneficiaries**:

The coordinator must — within 60 days from when termination takes effect — submit:

(i) a report on the distribution of payments to the beneficiary concerned;

(ii) a request for amendment (see Article 55), with a proposal for reallocation of the tasks and estimated budget of the beneficiary concerned (see Annexes 1 and 2) and, if necessary, the addition of one or more new beneficiaries (see Article 56). If termination is notified after the period set out in Article 3, no request for amendment must be submitted unless the beneficiary concerned is the coordinator. In this case the request for amendment must propose a new coordinator, and

(iii) if termination takes effect during the period set out in Article 3, a **termination report** from the beneficiary concerned, for the open reporting period until termination, containing an overview of the progress of the work, an overview of the use of resources, the individual financial statement and, if applicable, the certificate on the financial statement (see Article 20).

The information in the termination report must also be included in the periodic report for the next reporting period (see Article 20.3).

If the request for amendment is rejected by the *Commission* (because it calls into question the decision awarding the grant or breaches the principle of equal treatment of applicants), the Agreement may be terminated according to Article 50.3.1(c).

If the request for amendment is accepted by the *Commission*, the Agreement is **amended** to introduce the necessary changes (see Article 55).

The *Commission* will — on the basis of the periodic reports, the termination report and the report on the distribution of payments — **calculate** the amount which is due to the beneficiary and if the (pre-financing and interim) payments received by the beneficiary exceed this amount.

The **amount which is due** is calculated in the following steps:

Step 1 — Application of the reimbursement rate to the eligible costs

The grant amount for the beneficiary is calculated by applying the reimbursement rate(s) to the total eligible costs declared by the beneficiary *and its linked third parties* in the termination report and approved by the *Commission*.

Only costs incurred by the beneficiary concerned until termination takes effect are eligible (see Article 6). Costs relating to contracts due for execution only after termination are not eligible.

Step 2 — Reduction due to substantial errors, irregularities or fraud or serious breach of obligations

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In case of a reduction (see Article 43), the *Commission* will calculate the reduced grant amount for the beneficiary by deducting the amount of the reduction (calculated in proportion to the seriousness of the errors, irregularities or fraud or breach of obligations, in accordance with Article 43.2) from the grant amount for the beneficiary.

If the payments received **exceed the amounts due**:

- if termination takes effect during the period set out in Article 3 and the request for amendment is accepted, the beneficiary concerned must repay to the coordinator the amount unduly received. The *Commission* will formally notify the amount unduly received and request the beneficiary concerned to repay it to the coordinator within 30 days of receiving notification. If it does not repay the coordinator, the *Commission* will draw upon the Guarantee Fund to pay the coordinator and then notify a **debit note** on behalf of the Guarantee Fund to the beneficiary concerned (see Article 44);

- in all other cases, in particular if termination takes effect after the period set out in Article 3, the *Commission* will formally notify a **debit note** to the beneficiary concerned. If payment is not made by the date in the debit note, the Guarantee Fund will pay to the *Commission* the amount due and the *Commission* will notify a debit note on behalf of the Guarantee Fund to the beneficiary concerned (see Article 44);

- if the beneficiary concerned is the former coordinator, it must repay the new coordinator according to the procedure above, unless:

  - termination takes effect after an interim payment and

  - the former coordinator has not distributed amounts received as pre-financing or interim payments (see Article 21.7).

  In this case, the *Commission* will formally notify a **debit note** to the former coordinator. If payment is not made by the date in the debit note, the Guarantee Fund will pay to the *Commission* the amount due. The *Commission* will then pay the new coordinator and notify a debit note on behalf of the Guarantee Fund to the former coordinator (see Article 44).

If the payments received **do not exceed the amounts due**: amounts owed to the beneficiary concerned will be included in the next interim or final payment.

If the *Commission* does not receive the termination report within the deadline (see above), only costs included in an approved periodic report will be taken into account.

If the *Commission* does not receive the report on the distribution of payments within the deadline (see above), it will consider that:

- the coordinator did not distribute any payment to the beneficiary concerned and that

- the beneficiary concerned must not repay any amount to the coordinator.

After termination, the concerned beneficiary's obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38, 40, 42, 43 and 44) continue to apply.

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SECTION 4 FORCE MAJEURE

ARTICLE 51 — FORCE MAJEURE

'Force majeure' means any situation or event that:

- prevents either party from fulfilling their obligations under the Agreement,
- was unforeseeable, exceptional situation and beyond the parties' control,
- was not due to error or negligence on their part (or on the part of third parties involved in the action), and
- proves to be inevitable in spite of exercising all due diligence.

The following cannot be invoked as force majeure:

- any default of a service, defect in equipment or material or delays in making them available, unless they stem directly from a relevant case of force majeure,
- labour disputes or strikes, or
- financial difficulties.

Any situation constituting force majeure must be formally notified to the other party without delay, stating the nature, likely duration and foreseeable effects.

The parties must immediately take all the necessary steps to limit any damage due to force majeure and do their best to resume implementation of the action as soon as possible.

The party prevented by force majeure from fulfilling its obligations under the Agreement cannot be considered in breach of them.

CHAPTER 7 FINAL PROVISIONS

ARTICLE 52 — COMMUNICATION BETWEEN THE PARTIES

52.1 Form and means of communication

Communication under the Agreement (information, requests, submissions, 'formal notifications', etc.) must:

- be made in writing and
- bear the number of the Agreement.

All communication must be made through the Participant Portal **electronic** exchange system and using the forms and templates provided there.

If — after the payment of the balance — the *Commission* finds that a formal notification was not

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accessed, a second formal notification will be made by registered post with proof of delivery ('formal notification on **paper**'). Deadlines will be calculated from the moment of the second notification.

Communications in the electronic exchange system must be made by persons authorised according to the Participant Portal Terms & Conditions. For naming the authorised persons, each beneficiary must have designated — before the signature of this Agreement — a 'legal entity appointed representative (LEAR)'. The role and tasks of the LEAR are stipulated in his/her appointment letter (see Participant Portal Terms & Conditions).

If the electronic exchange system is temporarily unavailable, instructions will be given on the Commission website.

52.2 Date of communication

Communications are considered to have been made when they are sent by the sending party (i.e. on the date and time they are sent through the electronic exchange system).

Formal notifications through the **electronic** exchange system are considered to have been made when they are received by the receiving party (i.e. on the date and time of acceptance by the receiving party, as indicated by the time stamp). A formal notification that has not been accepted within 10 days after sending is considered to have been accepted.

Formal notifications **on paper** sent by **registered post** with proof of delivery (only after the payment of the balance) are considered to have been made on either:

- the delivery date registered by the postal service or
- the deadline for collection at the post office.

If the electronic exchange system is temporarily unavailable, the sending party cannot be considered in breach of its obligation to send a communication within a specified deadline.

52.3 Addresses for communication

The **electronic** exchange system must be accessed via the following URL:

https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/myarea/projects

The *Commission* will formally notify the coordinator and beneficiaries in advance any changes to this URL.

Formal notifications on paper (only after the payment of the balance) addressed **to the *Commission*** must be sent to the official mailing address indicated on the *Commission's* website.

Formal notifications on paper (only after the payment of the balance) addressed **to the beneficiaries** must be sent to their legal address as specified in the Participant Portal Beneficiary Register.

ARTICLE 53 — INTERPRETATION OF THE AGREEMENT

53.1 Precedence of the Terms and Conditions over the Annexes

The provisions in the Terms and Conditions of the Agreement take precedence over its Annexes.

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Annex 2 takes precedence over Annex 1.

53.2 Privileges and immunities

Not applicable

ARTICLE 54 — CALCULATION OF PERIODS, DATES AND DEADLINES

In accordance with Regulation No 1182/71[30], periods expressed in days, months or years are calculated from the moment the triggering event occurs.

The day during which that event occurs is not considered as falling within the period.

ARTICLE 55 — AMENDMENTS TO THE AGREEMENT

55.1 Conditions

The Agreement may be amended, unless the amendment entails changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

Amendments may be requested by any of the parties.

55.2 Procedure

The party requesting an amendment must submit a request for amendment signed in the electronic exchange system (see Article 52).

The coordinator submits and receives requests for amendment on behalf of the beneficiaries (see Annex 3).

If a change of coordinator is requested without its agreement, the submission must be done by another beneficiary (acting on behalf of the other beneficiaries).

The request for amendment must include:

- the reasons why;
- the appropriate supporting documents, and
- for a change of coordinator without its agreement: the opinion of the coordinator (or proof that this opinion has been requested in writing).

The *Commission* may request additional information.

If the party receiving the request agrees, it must sign the amendment in the electronic exchange system within 45 days of receiving notification (or any additional information the *Commission* has requested). If it does not agree, it must formally notify its disagreement within the same deadline. The deadline

[30] Regulation (EEC, Euratom) No 1182/71 of the Council of 3 June 1971 determining the rules applicable to periods, dates and time-limits (OJ L 124, 8.6.1971, p. 1).

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may be extended, if necessary for the assessment of the request. If no notification is received within the deadline, the request is considered to have been rejected.

An amendment **enters into force** on the day of the signature of the receiving party.

An amendment **takes effect** on the date agreed by the parties or, in the absence of such an agreement, on the date on which the amendment enters into force.

ARTICLE 56 — ACCESSION TO THE AGREEMENT

56.1 Accession of the beneficiaries mentioned in the Preamble

The other beneficiaries must accede to the Agreement by signing the Accession Form (see Annex 3) in the electronic exchange system (see Article 52) within 30 days after its entry into force (see Article 58).

They will assume the rights and obligations under the Agreement with effect from the date of its entry into force (see Article 58).

If a beneficiary does not accede to the Agreement within the above deadline, the coordinator must — within 30 days — request an amendment to make any changes necessary to ensure proper implementation of the action. This does not affect the *Commission's* right to terminate the Agreement (see Article 50).

56.2 Addition of new beneficiaries

In justified cases, the beneficiaries may request the addition of a new beneficiary.

For this purpose, the coordinator must submit a request for amendment in accordance with Article 55. It must include an Accession Form (see Annex 3) signed by the new beneficiary in the electronic exchange system (see Article 52).

New beneficiaries must assume the rights and obligations under the Agreement with effect from the date of their accession specified in the Accession Form (see Annex 3).

ARTICLE 57 — APPLICABLE LAW AND SETTLEMENT OF DISPUTES

57.1 Applicable law

The Agreement is governed by the applicable EU law, supplemented if necessary by the law of Belgium.

57.2 Dispute settlement

If a dispute concerning the interpretation, application or validity of the Agreement cannot be settled amicably, the General Court — or, on appeal, the Court of Justice of the European Union — has sole jurisdiction. Such actions must be brought under Article 272 of the Treaty on the Functioning of the EU (TFEU).

As an exception, if such a dispute is between the Commission and SINTEF AS, ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE, UNIVERSITAT BASEL, the competent Belgian courts have sole jurisdiction.

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If a dispute concerns administrative sanctions, offsetting or an enforceable decision under Article 299 TFEU (see Articles 44, 45 and 46), the beneficiaries must bring action before the General Court — or, on appeal, the Court of Justice of the European Union — under Article 263 TFEU.

ARTICLE 58 — ENTRY INTO FORCE OF THE AGREEMENT

The Agreement will enter into force on the day of signature by the *Commission* or the coordinator, depending on which is later.

SIGNATURES

For the coordinator

For the *Commission*

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EUROPEAN COMMISSION

Directorate-General for Communications Networks, Content and Technology

CNECT.C – Digital Excellence and Science Infrastructure

C.4 – Flagships

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ANNEX 1 (part A)

Research and Innovation action

NUMBER — 957189 — BIG-MAP

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1.1. The project summary

Project Number [1]	957189	Project Acronym [2]	BIG-MAP

One form per project

General information	
Project title [3]	Battery Interface Genome - Materials Acceleration Platform
Starting date [4]	01/09/2020
Duration in months [5]	36
Call (part) identifier [6]	H2020-LC-BAT-2020-3
Topic	LC-BAT-12-2020 Novel methodologies for autonomous discovery of advanced battery chemistries
Fixed EC Keywords	
Free keywords	Materials Acceleration Platform; battery value chain; artificial intelligence, machine learning

Abstract [7]

Today, energy production and transport are evolving fast to meet challenging environmental targets and growing demand. The Achilles' heel is energy storage, which is incapable of providing both low cost and high-performance solutions. The answer is not a simple evolution of existing batteries but disruptive technologies that must be discovered fast.

The BIG-MAP vision is to develop a modular, closed-loop infrastructure and methodology to bridge physical insights and data-driven approaches to accelerate the discovery of sustainable battery chemistries and technologies. BIG-MAP's strategy is to cohesively integrate machine learning, computer simulations and AI-orchestrated experiments and synthesis to accelerate battery materials discovery and optimization. The project will be a lever to create the infrastructural backbone of a versatile and chemistry-neutral European Materials Acceleration Platform, capable of reaching a 10-fold increase in the rate of discovery of novel battery materials and interfaces.

To succeed in this unprecedented international initiative, the BIG-MAP consortium covers the entire battery discovery value chain from atoms to battery cells, totaling 34 partners from 15 countries and spanning world-leading academic experts, research laboratories and industry leaders. The consortium is a joint European battery community effort, and the large-scale European Research Initiative BATTERY 2030+ stands united behind the BIG-MAP consortium. In addition to 13 core partners from BATTERY 2030+, the BIG-MAP consortium includes 21 leading European partners with complementary battery skills and essential competences from critical research areas such as quantum machine learning, deep learning and autonomous synthesis robotics. All partners will work to create an innovative methodology relying on unique competences and cross-cutting initiatives to deliver a shared infrastructure and 12 key demonstrators to showcase the value of AI-orchestrated materials discovery.

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1.2. List of Beneficiaries

Project Number [1]	957189	Project Acronym [2]	BIG-MAP

List of Beneficiaries

No	Name	Short name	Country	Project entry month[8]	Project exit month
1	DANMARKS TEKNISKE UNIVERSITET	DTU	Denmark	1	36
2	UPPSALA UNIVERSITET	UU	Sweden	1	36
3	KARLSRUHER INSTITUT FUER TECHNOLOGIE	KIT	Germany	1	36
4	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS	CNRS	France	1	36
5	WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER	WWU	Germany	1	36
6	COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES	CEA	France	1	36
7	KEMIJSKI INSTITUT	NIC	Slovenia	1	36
8	SINTEF AS	SINTEF	Norway	1	36
9	POLITECNICO DI TORINO	PDT	Italy	1	36
10	FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.	Fraunhofer	Germany	1	36
11	CHALMERS TEKNISKA HOEGSKOLA AB	CTH	Sweden	1	36
12	POLITECHNIKA WARSZAWSKA	WUT	Poland	1	36
13	AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS	CSIC	Spain	1	36
14	TECHNISCHE UNIVERSITEIT DELFT	TUD	Netherlands	1	36
15	CONSIGLIO NAZIONALE DELLE RICERCHE	CNR	Italy	1	36
16	ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE	EPFL	Switzerland	1	36
17	THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE	UCAM	United Kingdom	1	36
18	THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD	UOXF	United Kingdom	1	36
19	TARTU ULIKOOL	UT	Estonia	1	36
20	THE UNIVERSITY OF LIVERPOOL	ULIV	United Kingdom	1	36
21	EUROPEAN SYNCHROTRON RADIATION FACILITY	ESRF	France	1	36

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1.2. List of Beneficiaries

No	Name	Short name	Country	Project entry month[8]	Project exit month
22	INSTITUT MAX VON LAUE - PAUL LANGEVIN	ILL	France	1	36
23	SYNCHROTRON SOLEIL SOCIETE CIVILE	SOLEIL	France	1	36
24	FUNDACION CIDETEC	CID	Spain	1	36
25	ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL	EMIRI	Belgium	1	36
26	UMICORE	UMI	Belgium	1	36
27	SOLVAY SA	SOLB	Belgium	1	36
28	BASF SE	BASF	Germany	1	36
29	NORTHVOLT AB	NVOLT	Sweden	1	36
30	UNIVERSITAT BASEL	UNIBAS	Switzerland	1	36
31	IT-UNIVERSITETET I KOBENHAVN	ITU	Denmark	1	36
32	DASSAULT SYSTEMES DEUTSCHLAND GMBH	3DS	Germany	1	36
33	FORSCHUNGSZENTRUM JULICH GMBH	FZJ	Germany	1	36
34	SAFT	SAFT	France	1	36

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1.3. Workplan Tables - Detailed implementation

1.3.1. WT1 List of work packages

WP Number[9]	WP Title	Lead beneficiary[10]	Person-months[11]	Start month[12]	End month[13]
WP1	Project management, education, exploitation and outreach	1 - DTU	99.50	1	36
WP2	Accelerated atomic-scale simulations	2 - UU	227.40	1	36
WP3	Multiscale Modelling	3 - KIT	255.50	1	36
WP4	Modular Synthesis Robotics	10 - Fraunhofer	234.90	1	36
WP5	Characterization	6 - CEA	293.80	1	36
WP6	HTS and Testing	33 - FZJ	228.30	1	36
WP7	Battery Interface Ontology	8 - SINTEF	76.00	1	36
WP8	Standards and Protocols	4 - CNRS	168.50	1	36
WP9	Infrastructure and Interoperability	16 - EPFL	160.00	1	36
WP10	AI Accelerated Materials Discovery	3 - KIT	170.00	1	36
WP11	Battery Interface Genome	1 - DTU	192.00	1	36
		Total	2 105.90		

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1.3.2. WT2 list of deliverables

Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D1.1	BIG-MAP website	WP1	1 - DTU	Websites, patents filling, etc.	Public	5
D1.2	Data Management Plan	WP1	1 - DTU	ORDP: Open Research Data Pilot	Public	6
D1.3	Minutes of kick-off meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	2
D1.4	Minutes of 1. bi-annual project meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	7
D1.5	Minutes of 2. bi-annual project meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	13
D1.6	Minutes of 3. bi-annual project meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	19
D1.7	Minutes of 4. bi-annual project meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	25
D1.8	Minutes of 5. bi-annual project meeting	WP1	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	31
D1.9	Interim Dissemination and Communication plan	WP1	13 - CSIC	Report	Confidential, only for members of the consortium (including the	18

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
					Commission Services)	
D1.10	Proceedings from Early Stage Research Seminar	WP1	25 - EMIRI	Report	Public	18
D1.11	Proceeding from international workshop/ conference	WP1	25 - EMIRI	Report	Public	18
D1.12	Interim Exploitation plan	WP1	13 - CSIC	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D1.13	Final Dissemination report	WP1	13 - CSIC	Report	Public	36
D1.14	Final Exploitation plan	WP1	13 - CSIC	Report	Confidential, only for members of the consortium (including the Commission Services)	36
D1.15	Report and blueprint on the integration of input from LC-BAT-13/14 projects in BIG-MAP	WP1	6 - CEA	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D2.1	Initial QM data sets for ML-training and analysis	WP2	2 - UU	data sets, microdata, etc	Confidential, only for members of the consortium (including the Commission Services)	12
D2.2	1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system	WP2	17 - UCAM	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	18
D2.3	Full protocol to achieve the exploration of chemical space for selected battery systems and in a longer perspective for battery systems of an arbitrary chemistry	WP2	30 - UNIBAS	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	36

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D2.4	Protocol for SEI composition and degradation prediction	WP2	11 - CTH	Report	Public	33
D2.5	Initial protocols for experimental spectra prediction	WP2	15 - CNR	Report	Public	20
D3.1	Validated mesoscale models for SEI/CEI morphology	WP3	9 - PDT	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D3.2	Verification of scale bridging models against SEI/CEI experiment	WP3	6 - CEA	Report	Confidential, only for members of the consortium (including the Commission Services)	24
D3.3	Computational Framework for AI-enhanced models	WP3	3 - KIT	Other	Confidential, only for members of the consortium (including the Commission Services)	18
D3.4	Incorporation of Multiscale-Model into hybrid models based on HTS data	WP3	7 - NIC	Report	Confidential, only for members of the consortium (including the Commission Services)	32
D3.5	Workflow demonstrator	WP3	3 - KIT	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	32
D4.1	Specification (flow chart) of hardware and software architecture	WP4	31 - ITU	Report	Public	6
D4.2	Robotic system for organic synthesis installed including sensors	WP4	10 - Fraunhofer	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	30
D4.3	Robotic system for inorganic synthesis installed including sensors	WP4	20 - ULIV	Demonstrator	Confidential, only for members of the consortium (including the	30

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
					Commission Services)	
D4.4	Report on synthesis and upscale of molecules for SEI formation and electrolyte components	WP4	7 - NIC	Report	Confidential, only for members of the consortium (including the Commission Services)	30
D4.5	Report on inorganic coatings prepared by combinatorial syntheses	WP4	6 - CEA	Report	Public	30
D4.6	Demonstration of automated synthesis procedure	WP4	10 - Fraunhofer	Demonstrator	Public	36
D4.7	Design of robotic system for organic synthesis completed	WP4	10 - Fraunhofer	Report	Public	18
D4.8	Design of robotic system for inorganic synthesis completed	WP4	20 - ULIV	Report	Public	18
D5.1	State-of-the art experimental matrix, tier 1 experimental plan and workflow	WP5	14 - TUD	Report	Public	6
D5.2	Global BIG-MAP experimental matrix, proof-of-concept of BIG-MAP experimental workflow and definition of perspectives and future vision towards the European multimodal platform	WP5	6 - CEA	Report	Public	36
D5.3	Demonstration of the capability to run coordinated multi-techniques experiments to acquire multi-scale data, and practical application to a selected chemistry	WP5	21 - ESRF	Demonstrator	Public	32
D5.4	Report on lab-scale and large-scale facilities automated and standardized data analysis	WP5	22 - ILL	Report	Public	36
D5.5	Design of workflow for a European	WP5	6 - CEA	Report	Public	18

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
	experimental multimodal platform completed					
D6.1	Set up "feeding" units for the HTS assays at FZJ comprising advanced functional electrolyte components from Solvay and WUT (commercially available and newly synthesized) and compatible electrode materials	WP6	28 - BASF	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D6.2	Develop materials experiment embeddings for advanced functional liquid electrolytes in lithium-based battery cells containing compatible electrodes with proven capabilities	WP6	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D6.3	1st Deployment of HTS experimentally obtained raw results and subsequent analyses for data lineage tracking	WP6	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D6.4	Advanced direct SEI investigations for chemistry neutral lithium-based batteries by integrated high throughput electrochemistry with ex situ high throughput spectroscopy	WP6	3 - KIT	Report	Public	24
D6.5	Generate high quality, abundant pertinent interphase/interface/ device data across the entire lifetime of the battery cell	WP6	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	36
D7.1	Report on ontology standards and development strategy	WP7	12 - WUT	Report	Public	3
D7.2	Initial version of battery ontology	WP7	8 - SINTEF	Report	Public	6

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D7.3	First stable release of battery interface ontology	WP7	8 - SINTEF	Report	Public	18
D7.4	Report on battery interface ontology case study	WP7	16 - EPFL	Report	Public	24
D7.5	Battery Interface Ontology published according to standards in the European modelling community	WP7	8 - SINTEF	Report	Public	36
D8.1	Initial templates for standards and protocols completed	WP8	4 - CNRS	Report	Confidential, only for members of the consortium (including the Commission Services)	6
D8.2	DOI format for samples exchange made available online for the whole consortium	WP8	4 - CNRS	Other	Confidential, only for members of the consortium (including the Commission Services)	6
D8.3	Release of updated standards and protocols following the working group meeting at M6	WP8	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	6
D8.4	Update of standards and protocols following the working group meeting at M18	WP8	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D8.5	Update of standards and protocols following the working group meeting at M30	WP8	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	30
D8.6	Online data analysis tools made available to the consortium	WP8	4 - CNRS	Other	Confidential, only for members of the consortium (including the Commission Services)	12

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D8.7	Online data analysis tools made available to the whole community	WP8	4 - CNRS	Websites, patents filling, etc.	Public	36
D8.8	First European platform open to researchers/ industries outside of the consortium where batteries can be tested following the tests protocols defined in BIG-MAP	WP8	4 - CNRS	Websites, patents filling, etc.	Public	36
D9.1	Prototype of the BIG-MAP App-store	WP9	3 - KIT	Websites, patents filling, etc.	Public	6
D9.2	Automated workflows linking experiments and modelling for representative samples of battery materials	WP9	16 - EPFL	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D9.3	Integrated AiiDA, ASE, SimStack platform	WP9	16 - EPFL	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D9.4	Proprietary data management framework capable of ingesting data from materials experiments (e.g. data from high-throughput experimentation, or a materials library)	WP9	3 - KIT	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D9.5	Updated BIG-MAP App-store	WP9	16 - EPFL	ORDP: Open Research Data Pilot	Public	36
D9.6	Demonstrator of a simulation run by an experiment, and an experiment run by a simulation	WP9	11 - CTH	Demonstrator	Public	36
D10.1	Active learning package/module demonstrated to work on pre-generated	WP10	3 - KIT	Demonstrator	Public	18

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Deliverable Number[14]	Deliverable Title	WP number[9]	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
	simulation or experimental data sets					
D10.2	Modular package for analysis of pertinent spectroscopic data and electrochemistry	WP10	20 - ULIV	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D10.3	Demonstration of linking active learning accelerated HTS and simulations	WP10	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D10.4	Tiered theory and experiment screening pipeline as first test case for automatic reasoning calibration	WP10	3 - KIT	Report	Public	36
D11.1	Initial model for dynamic fidelity assignment	WP11	21 - ESRF	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D11.2	Identification of interphase descriptor dynamics for test system	WP11	1 - DTU	Report	Public	18
D11.3	Multi-scale representation of interface with scale bridging descriptors from simulation and experimental data	WP11	1 - DTU	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D11.4	1st generation uncertainty-guided hybrid physics- and data-driven model of battery interfaces	WP11	1 - DTU	Other	Confidential, only for members of the consortium (including the Commission Services)	32
D11.5	Demonstrate transfer of select model(s) to novel battery materials/ chemistry	WP11	24 - CID	Demonstrator	Public	36

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1.3.3. WT3 Work package descriptions

Work package number [9]	WP1	Lead beneficiary [10]	1 - DTU
Work package title	Project management, education, exploitation and outreach		
Start month	1	End month	36

Objectives

The main objectives of WP1 are:
• To ensure an effective implementation of the project in line with the GrA and the CA and guidelines from the EC, and to perform quality control and risk management.
• To ensure efficient and regular communication among the project partners and towards the European Commission (EC), including project reporting.
• Promotion of a web-platform (from WP9) to share project outcomes including computational tools and experimental in/output (including metadata), ensuring data reliability, traceability and interoperability.
• Create and promote a dissemination and training strategy for accelerated AI-based materials discovery to different groups of stakeholders throughout the whole battery chain value, and to ensure high visibility and awareness for the project outcome by selecting the right type of communication channels and timing.
• Create an exploitation strategy to envisage an optimal commercialization route for the innovative outcome of the project, and assure that the project IP is properly protected.
• Enable close contact with a broad network of stakeholders by taking part in networking events/conferences and by arranging project event like stakeholder meetings, seminars and workshop/conferences.
Tejs Vegge (DTU) will be the PC, the Scientific Coordinator and the leader of the EB. The PC will be the official point of contact between the project and the EC. The management structure is described in more details in section 3.2 of the proposal.

Description of work and role of partners

WP1 - Project management, education, exploitation and outreach [Months: 1-36]
DTU, UU, KIT, CNRS, WWU, CEA, NIC, SINTEF, PDT, Fraunhofer, CTH, WUT, CSIC, TUD, CNR, EPFL, UCAM, UOXF, UT, ULIV, ESRF, ILL, SOLEIL, CID, EMIRI, UMI, SOLB, BASF, NVOLT, UNIBAS, ITU, 3DS, FZJ, SAFT
Task 1.1: Administrative and financial management and reporting
Task leader: DTU; Partners involved: All; M1-M36
The PC will:
• Handle the strategic project management though periodic reviews with support of the EB, e.g. assessment of achievements towards the Scientific Objectives and plan described in the Grant Agreement (GrA).
• Consolidate the progress of the scientific and financial reports, and their delivery to the EC.
• Maintain the CA and resolve any technical, financial or contractual issues.
• Coordinate and implement requests and decisions for amendments to the GrA and/or CA.
• Resolve potential conflicts between the partners and propose solutions to critical situations that may arise and implement these in agreement with the partners.
Moreover, the PC and the PC Assistant will be the day-to-day contact persons of the project and will:
• Follow up on the day-to-day project progress, provide proactive support, consolidate project level data and ensure efficient communication channels.
• Organize, chairing and recording meetings.
• Collect financial status reports form all partners every six months.
• Organization and coordination of the activities between WPs to ensure complete coverage and technical consistency.
• Liaison with WP leaders to ensure the timely preparation and production of deliverables and an optimal flow of samples and results between the WPs.
The quality of the project results will be monitored closely by the PC through the day-to-day management and regular reporting from the WP leaders. If doubts arise regarding the quality of work performed, an external assessment of the work could be conducted. Together with the EB, the PC regularly assess the project risks. The initial risk table, which may be found in section 3.2.3, will be updated when needed and at least every 6 months. The General Assembly should decide if a contingency plan needs to be put in place.

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Task 1.2. Participation in the Future Battery Technologies initiative and collaboration with BATTERY 2030+ CSA and with other LC-BAT projects
Task leader: CEA; Partners involved: All; M1-M36
The objective of this task is to ensure synergies between the projects to reach the full impact of the common goals of the large-scale research initiatives of Future Battery Technologies. For this a strong collaboration with the other projects funded under the LC-BAT-12/13/14/15-2020 call topics is necessary. The BATTERY 2030+ CSA project funded under LC-BAT-15-2020 will be in charge of the overall coordination of the joint efforts. The partner CEA will lead the task of ensuring that the project partners actively contribute to the joint efforts coordinated by the BATTERY 2030+ CSA comprising the following tasks: communication & dissemination (Task 1.7), exploitation and IPR strategy (Tasks 1.4 and 1.5), Identify and contribute to guidelines and best practice for data sharing & FAIR Data (WP8), educational curricula, roadmap development, infrastructure and interoperability (WP9). With regards to costs and efforts, each of the LC-BAT-12,13,14,15-2020 project shall support the costs and efforts related to their participation to the collaboration on the different tasks mentioned above as well as to their participation to the bi-annual cross-project meetings and to specific meetings for addressing these tasks. This includes travelling and accommodation costs for participation in joint meetings and events.

Task 1.3: Research Data Management
Task leader: DTU; Partners involved: EPFL, All; M1-M36
A Data Management Coordinator (DMC) will be appointed, and in collaboration with all project partners, the DMC will prepare a Data Management Plan (DMP) by month 6 (D1.2). The DMP describes the management of the data collected, processed and generated in the project in order to ensure that the research data is findable, accessible, interoperable and re-usable (FAIR), as described in more detail in section 2.2. Other important aspects are ensuring data safety and the ability to operate with protected data, e.g. from industry (3 layers of access), as ensuring trackability in the data, DOI-protection for data sets, and alignment with other initiatives regarding data management. The DMC is responsible for setting up and updating the DMP when needed and at least once a year. The whole consortium is responsible to operate according to the DMP. The DMC will be responsible for matching the DMP to the Platform for Open Science developed in WP9 (Task 9.4) in partnership with the existing www.materialscloud.org for seamless sharing of resources in computational materials science, specifically devoted to batteries. The DMC will provide educational, research, and archiving tools; simulation software and services; and curated and raw data, ensuring data reliability, traceability and interoperability.

Task 1.4: Intellectual Property management and utilization
Task leader: CEA; Partners involved: All; M1-M36
An IP Manager (IPM) will be appointed to manage the IP generated during the project, according to the rules defined and agreed upon in the CA. Specific attention will be placed on defining a strategy for ensuring IP protection and sharing for co-developed methodologies, as well as for novel materials and interfaces identified and/or developed by BIG-MAP and/or individual modules.
Any partner wishing to protect, publish or disseminate project results must first inform the IPM in due time beforehand; the IPM will archive related documents on the dedicated collaborative tool and inform all partners so that each can ensure that their interests are protected.

Task 1.5: Development and implementation of an Exploitation Plan
Task leader: CSIC; Partners involved: All; M1-M36
Exploitation in general is making use of and deriving benefit from a resource. BIG-MAP outcomes will be used at different levels, by different actors during the initial 3-year ramp-up stage covered in this proposal, and after its end in a ~10 year horizon. CSIC will be responsible for the Exploitation plan, which should aim at synergizing efforts for partner-level exploitation, involving also stakeholders (Task 1.6), as well as a plan for exploitation beyond the BIG-MAP consortium, i.e. within the Future Battery Technologies initiative. Strategies will be defined to identify and successfully involve target groups, end-users, stakeholders and transferring the outcomes of the Project into their respective domains, aligned with their respective user requirements and technological objectives and goals. Exploitable results include data, knowledge, methods, processes, materials, agreements, will be are clearly identified and their direct and indirect value and impact for different stakeholders considered. The Plan will be compliant with the DMP (Task 1.3) and also include concrete measures to ensure that the results meet real needs, and will be taken up by potential and define the roles and responsibilities of partners in exploiting results or supporting results exploitation by others (intermediate or end) users.

Task 1.6: Stakeholder activities and management
Task leader: EMIRI; Partners involved: All; M1-M36
EMIRI will be responsible for coordinating the stakeholder management, e.g. organizing yearly stakeholder workshops and/or training events and webinars; all partners will contribute to these events. The task includes establishing an overview of the industrial sectors (apart from batteries) in which a 'Materials Acceleration Platform' or similar concepts

are developed or used, and identify best practices. The task will also include establishing the practical framework managing stakeholder requests for, e.g. priority status, access to models, (pre-release) apps in the BIG-MAP App-store, and/or resources to co-develop new apps, interfaces to community relevant soft/hardware modules. The Executive Board will be consulted in establishing and monitoring the guide lines for allocation of resources to stakeholders.

Task 1.7: Dissemination, outreach and communication
Task leader: CSIC; Partners involved: All; M1-M36
Development and implementation of a communication plan including also education and training targeting a wide spectrum of stakeholders involving different actions. The website www.BIG-MAP.eu will serve as a unification point for these activities. The specific plans are outlined in detail in Table 2.4 (Target groups for BIG-MAP) and Table 2.5 (Dissemination strategy of BIG-MAP partner). CSIC will be responsible for the coordination of the dissemination and outreach activities, but all partners are required to participate actively and to adhere to the guide lines in the Interim Dissemination and Communication plan (D1.9).

Participation per Partner

Partner number and short name	WP1 effort
1 - DTU	36.00
2 - UU	1.00
3 - KIT	1.00
4 - CNRS	1.00
5 - WWU	1.00
6 - CEA	3.00
7 - NIC	1.00
8 - SINTEF	1.00
9 - PDT	1.00
10 - Fraunhofer	1.00
11 - CTH	1.00
12 - WUT	1.00
13 - CSIC	12.00
14 - TUD	1.00
15 - CNR	1.00
16 - EPFL	6.00
17 - UCAM	1.00
18 - UOXF	1.00
19 - UT	1.00
20 - ULIV	1.00
21 - ESRF	1.00
22 - ILL	1.00
23 - SOLEIL	1.00
24 - CID	1.00
25 - EMIRI	12.00
26 - UMI	1.00

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Partner number and short name	WP1 effort
27 - SOLB	1.00
28 - BASF	2.50
29 - NVOLT	1.00
30 - UNIBAS	1.00
31 - ITU	1.00
32 - 3DS	1.00
33 - FZJ	1.00
34 - SAFT	1.00
Total	99.50

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D1.1	BIG-MAP website	1 - DTU	Websites, patents filling, etc.	Public	5
D1.2	Data Management Plan	1 - DTU	ORDP: Open Research Data Pilot	Public	6
D1.3	Minutes of kick-off meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	2
D1.4	Minutes of 1. bi-annual project meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	7
D1.5	Minutes of 2. bi-annual project meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	13
D1.6	Minutes of 3. bi-annual project meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	19
D1.7	Minutes of 4. bi-annual project meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	25

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List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D1.8	Minutes of 5. bi-annual project meeting	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	31
D1.9	Interim Dissemination and Communication plan	13 - CSIC	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D1.10	Proceedings from Early Stage Research Seminar	25 - EMIRI	Report	Public	18
D1.11	Proceeding from international workshop/ conference	25 - EMIRI	Report	Public	18
D1.12	Interim Exploitation plan	13 - CSIC	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D1.13	Final Dissemination report	13 - CSIC	Report	Public	36
D1.14	Final Exploitation plan	13 - CSIC	Report	Confidential, only for members of the consortium (including the Commission Services)	36
D1.15	Report and blueprint on the integration of input from LC-BAT-13/14 projects in BIG-MAP	6 - CEA	Report	Confidential, only for members of the consortium (including the Commission Services)	18

Description of deliverables

D1.1: BIG-MAP website (DTU, M3)
D1.2: Data Management Plan (DTU, M6)
D1.3: Minutes of kick-off meetings (DTU, M2)
D1.4: Minutes of 1. bi-annual project meeting (DTU, M7)
D1.5: Minutes of 2. bi-annual project meeting (DTU, M13)
D1.6: Minutes of 3. bi-annual project meeting (DTU, M19)
D1.7: Minutes of 4. bi-annual project meeting (DTU, M25)
D1.8: Minutes of 5. bi-annual project meeting (DTU, M31)
D1.9: Interim Dissemination and Communication plan (CSIC, M18)
D1.10: Proceedings from Early Stage Research Seminar (EMIRI, M18)
D1.11: Proceedings from international workshop/conference (EMIRI, M18)
D1.12: Interim Exploitation plan (CSIC, M12)
D1.13: Final dissemination report (CSIC, M36)
D1.14: Final Exploitation plan (CSIC, M36)

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D1.15: Report and blueprint on the integration of input from LC-BAT-13/14 projects in BIG-MAP (CEA, M18)

D1.1 : BIG-MAP website [5]

Launch of the http://www.BIG-MAP.eu web site with information about the project.

D1.2 : Data Management Plan [6]

A Data Management Plan will be prepared, which complies with the Open Research Data Pilot (ORDP) Requirements and the specific data requirements in the project.

D1.3 : Minutes of kick-off meeting [2]

Minutes of kick-off meeting.

D1.4 : Minutes of 1. bi-annual project meeting [7]

Minutes of 1. bi-annual project meeting.

D1.5 : Minutes of 2. bi-annual project meeting [13]

Minutes of 2. bi-annual project meeting.

D1.6 : Minutes of 3. bi-annual project meeting [19]

Minutes of 3. bi-annual project meeting.

D1.7 : Minutes of 4. bi-annual project meeting [25]

Minutes of 4. bi-annual project meeting.

D1.8 : Minutes of 5. bi-annual project meeting [31]

Minutes of 5. bi-annual project meeting.

D1.9 : Interim Dissemination and Communication plan [18]

Submission of the interim Dissemination and Communication plan.

D1.10 : Proceedings from Early Stage Research Seminar [18]

Submission of report with proceedings from the Early Stage Research Seminar.

D1.11 : Proceeding from international workshop/conference [18]

Submission of report with proceedings from the international workshop/conference.

D1.12 : Interim Exploitation plan [12]

Submission of an interim exploitation plan.

D1.13 : Final Dissemination report [36]

Submission of the Final Dissemination report.

D1.14 : Final Exploitation plan [36]

Submission of the Final Exploitation plan.

D1.15 : Report and blueprint on the integration of input from LC-BAT-13/14 projects in BIG-MAP [18]

Submission of report and blueprint on the integration of input from LC-BAT-13/14 projects in BIG-MAP. The report will be prepared in close collaboration with Battery2030Plus and the granted projects under LC-BAT-13/14.

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Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification

Work package number [9]	WP2	Lead beneficiary [10]	2 - UU
Work package title	Accelerated atomic-scale simulations		
Start month	1	End month	36

Objectives

Density Functional Theory (DFT) based molecular dynamics (MD) simulation is one of very few feasible approaches for modelling reactive solid-state chemistry, where these techniques provide unique information. However, for large scale simulations of complex systems –such as battery-relevant electrode-electrolyte interfaces– DFT can be prohibitively expensive, making property prediction and high-throughput screening not feasible. Machine learning (ML) based force fields (FFs) have been shown to speed up DFT-quality calculations by 10,000x for standard moderately sized systems (say, below 200 atoms), and much more for larger systems due to the poor scaling of QM methods. This has been demonstrated as a proof of concept for solids and molecular liquids separately, but not yet together for complex and challenging atomistic battery interface simulations, which are the target of this WP.
The focus of WP2 is in modelling batteries at the electronic and atomistic scales. This WP serves as a technology demonstrator, and necessarily will use example chemistries that are much simpler than those in commercial batteries, but nevertheless sufficiently complex to be relevant and push the boundaries of what is possible to simulate computationally. Strong interactions with primarily WP3 (Multiscale modelling) and WP11 (Battery Interface Genome) and WP5 (Characterization) are foreseen. The anode materials considered will be carbon and silicon based, including amorphous systems and graphite, and an example cathode will be nickel oxide based materials (in accordance with WP6). For electrolytes, we will have a hierarchy of systems typically based on simple cyclic carbonates (ethylene carbonate, propylene carbonate, vinylene carbonate) in combination with lithium hexafluorophosphate. We will develop an automated closed-loop workflow that demonstrates the (i) calculation of reliable QM data to complex battery materials, (ii) fitting of FFs and other property models to the QM data and (iii) predicts properties of electrolytes, electrodes and their combination. Together with experimental data, the workflow will be used to optimize relevant properties throughout compound space and identify sets of most promising new materials candidates. We will demonstrate the applicability of the AI/ML-generated interatomic potentials, and the insight from electronic structure calculations, in predicting enhanced properties of relevance to battery performance such as diffusivity of charge carriers in the electrolyte and the evolution of the structure of the electrode/electrolyte interface and generate automated workflows for simulations of spectra and images for prediction and analysis materials characterization technique.

Description of work and role of partners

WP2 - Accelerated atomic-scale simulations [Months: 1-36]
UU, DTU, WWU, CEA, SINTEF, CTH, CNR, EPFL, UCAM, UMI, UNIBAS, 3DS, SAFT
Task 2.1: Data from QM calculations
Task leader: UU; Partners involved: UCAM, SINTEF, UBAS, WWU, CTH; M1-M36
In Task 2.1 we will explore and assess the applicability of the various quantum mechanical (QM) approximations to battery interface systems. In this task, we will also create a large amount of consistent DFT data suitable for modelling the potential energy surface of the constituent molecules and solids. We will set up, design and perform QM calculations of varying cost efficiency and accuracy for equilibrium and redox properties of a broad selection of compounds from materials classes relevant for the BIG-MAP's targets. The resulting data will serve as input to Tasks 2.2 and 2.3 in order to work toward the aforementioned closed-loop scheme. This task involves extensive method testing to identify the most appropriate (sufficiently accurate and most cost-effective) level of QM treatment, including semi-empirical schemes such as tight-binding calculations for validation tests for FFs. The role of van der Waals interactions present in molecular clusters of the molecular electrolyte candidates, and systematic trends among the various levels of theory will be established by considering equilibrium and non-equilibrium clusters consisting of dimers, trimers, tetramers, pentamers, etc. and a sufficient number of solvation shells making the results reliable, yet affordable. Resulting data will continuously feed into Tasks 2.2 and 2.3, and feedback from both of these tasks will be used in order to define additional systems for subsequent QM treatment. We will treat Si-Graphite based anode material and Ni-oxide based cathode material accordingly. UU will be task leader and drive the DFT and tight-binding modelling, as well as hybrid QM/MM (quantum mechanics/molecular mechanics) calculations. UCAM and UBAS will together with UU design the overall workflow. WWU and CTH will assist in providing atomistic-based data for electrode and electrolyte systems. Wave-function based methods when needed such as MP2, CCSD, CCSD(T), and even MRCI for various basis-set sizes, and SINTEF will also provide benchmark properties of strongly correlated cathode materials with the FCIQMC method, efficiently making full CI quality results available for periodic systems and for calibrating DFT-based results.

Task 2.2: Train ML potentials
Task leader: UCAM; Partners involved: UU, DTU, UBAS, WWU; M1-M36
In this task, we will identify relevant representations for the ML-based protocols, and train potentials on QM output from Task 2.1. Currently the best representations are based on projections of the atomic neighbour density onto rotationally invariant bases - but there is considerable freedom in how this is done. We will take the best ideas in the field (such as the Smooth Overlap of Atomic Positions (SOAP), Atomic Cluster Expansion (ACE), Atomic Permutationally Invariant Polynomials (aPIPs), Moment Tensor Potentials (MTP), etc.) and apply them to battery chemistries. Validation of the machine learned potentials will be carried out in several stages using large scale DFT calculations both for static properties of complex systems and dynamical properties of simplified models (see Task 2.4). UCAM will be task leader and drive the construction of the ML-based potentials, and DTU will focus on the specific challenges for training ML potentials for interfaces. UBAS and UU will together with UCAM and DTU to design the overall workflow. WWU will provide ML-based potentials for electrolytes. The ML models will be tested in Task 2.4.
Task 2.3: ML in battery compound space
Task leader: UBAS; Partners involved: UCAM, UU, DTU; M1-M36
Based on the results obtained within Tasks 2.1 and 2.2, we will develop ML models which can serve the ranking and selection of new promising candidate systems. This will be done by studying and developing improved and purpose-tailored descriptors and representations, which capture the physics of those degrees of freedom which govern battery relevant properties. We will use these developments to train, test, and apply computationally efficient and transferable ML models which are applicable across many and various materials, the representative training instances being obtained from simulations with the new ML potentials (Task 2.2), as well as from the QM calculations (Task 2.4). In particular, we will consider, the chemical space of small organic electrolyte candidates (functionalizing derivatives of ethylene and propylene carbonates, the effect of doping on Li at Ni enriched cathode materials (such as Ni-oxides), as well as chemical modifications to Silicon-graphite based anode materials. After training, we will use the ML models to explore said materials compound spaces with well-established optimization algorithms (Monte Carlo, simplex, genetic algorithm, etc.) in order to converge towards ranked sets of promising new materials candidates with expected optimal property combinations. Our results will subsequently inform Tasks 2.1 and 2.2 about new promising input materials worthy of further study. UBAS will be task leader and drive the exploration of compound space. UU and UCAM will together with UBAS design the overall workflows, while DTU will work on the predictability of the chemical reactions.
Task 2.4: Battery simulations at the atomistic level
Task leader: CTH; Partners involved: WWU, DTU, 3DS, CEA, UMI, SAFT; M1-M36
In this applied task, a range of simulations will be performed for validation of potentials and to solve outstanding problems related to battery interface and interphase functionality. This task will thus involve structural and physical phenomena such as ionic conductivity, transference numbers, solubility, solvation and thermal transport and will be interlinked with experimental efforts. Initially, these modelling tasks will be carried out using ab initio MD (AIMD), and as the ML-based FFs become available from Task 2.2, they will be tested against AIMD and experimental predictions. In particular, CTH, will decipher the formation stages of the SEIs and how additives reduce at the anode surfaces, as well as design a simulation protocol for predicting the solubility of the SEI components in the electrolytes. WWU will perform QM calculations of electrochemical stabilities of novel electrolyte compounds such as bi- and multifunctional additives, thus complementing the experimental efforts of WP6 (fully automated HTS approach for liquid electrolytes). Moreover, the screening of putative decomposition reactions will be automated in line with workflows and protocols developed in WP9. 3DS will generate a technology demonstrator (KD1), which can be used for testing and validation of the ML derived potentials for MD, which will be developed in Task 2.2. There is already a collaboration work between 3DS and UCAM to build on. DTU will carry our long-term/large-scale test simulations on selected interface systems. UMI will test the ability of the ML models to predict e.g. (bulk) elastic properties, surface energies and electrolyte wetting on selected interface systems.
Task 2.5: Modelling operando spectroscopies and atomistic-level characterization
Task leader: CNR; Partners involved: EPFL, UU, CTH; M6-M36
Starting from atomic geometries obtained from Tasks 2.1-2.3, we will define and apply protocols for calculating electronic properties and predicting experimental spectra at different levels of accuracy (e.g. DFT simulation of scanning probe microscopies and spectroscopies, absorption spectra, Raman etc.) to match the experiments performed in e.g. WP5. CNR will generate automated workflows for simulations of spectra and images for prediction, analysis, and materials characterization, together with EPFL, UU and CTH. We will first focus on vibrational characterization at different levels of accuracy; more complex spectroscopies, e.g. XAS or ARPES, will be subsequently tackled, including some focused development.

Partner number and short name	WP2 effort
1 - DTU	24.00
2 - UU	35.00
5 - WWU	12.00
6 - CEA	1.00
8 - SINTEF	11.00
11 - CTH	23.00
15 - CNR	12.00
16 - EPFL	6.00
17 - UCAM	49.90
26 - UMI	5.00
30 - UNIBAS	36.00
32 - 3DS	12.00
34 - SAFT	0.50
Total	227.40

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D2.1	Initial QM data sets for ML-training and analysis	2 - UU	data sets, microdata, etc	Confidential, only for members of the consortium (including the Commission Services)	12
D2.2	1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system	17 - UCAM	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	18
D2.3	Full protocol to achieve the exploration of chemical space for selected battery systems and in a longer perspective for battery systems of an arbitrary chemistry	30 - UNIBAS	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	36
D2.4	Protocol for SEI composition and degradation prediction	11 - CTH	Report	Public	33
D2.5	Initial protocols for experimental spectra prediction	15 - CNR	Report	Public	20

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Description of deliverables

D2.1: Initial QM data sets for ML-training and analysis (UU, M12)
D2.2: 1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system (UCAM, M18)
D2.3: Full protocol to achieve the exploration of chemical space for selected battery systems and in a longer perspective for battery systems of an arbitrary chemistry (UBAS, M36)
D2.4: Protocol for SEI composition and degradation prediction (CTH, M33)
D2.5: Initial protocols for experimental spectra prediction (CNR, M20)

D2.1 : Initial QM data sets for ML-training and analysis [12]

The initial QM (Quantum Mechanical) data sets for ML-training and analysis is released together with a short user-guide/report.

D2.2 : 1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system [18]

Completion of 1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system. The release is accompanied with a short descriptive report.

D2.3 : Full protocol to achieve the exploration of chemical space for selected battery systems and in a longer perspective for battery systems of an arbitrary chemistry [36]

Release of full pull protocol to achieve the exploration of chemical space for selected battery systems, and in a longer perspective for battery systems of an arbitrary chemistry.

D2.4 : Protocol for SEI composition and degradation prediction [33]

Publication of protocol for computational prediction of SEI composition and degradation.

D2.5 : Initial protocols for experimental spectra prediction [20]

Release of initial protocols for calculational prediction of experimental spectra.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS1	M2.1: Delivery of full protocol to achieve the exploration of chemical space for selected battery systems	2 - UU	12	The protocol is delivered from full QM data set and force field available. The delivery on time of D2.3 is the mean of verification. Associated risk R2.1.

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Work package number [9]	WP3	Lead beneficiary [10]	3 - KIT
Work package title	Multiscale Modelling		
Start month	1	End month	36

Objectives

Battery performance and lifetime are determined by many processes that occur on vastly different time and length scales. Multi-scale modelling techniques are currently being developed, for example, to optimize real and virtual electrode microstructures [99], study the effects the fabrication process on cell performance [100], electrode surface film growth [101] and aging and degradation assessment [102].
In this WP we will develop and validate multi-scale simulations that utilize a number of different models and conceptual approaches that will contribute significantly to establishing the battery interface genome (WP11). Mesoscale and continuum modelling can be used to explore rare events, cell function and long-term degradation at the device level.
We will develop a comprehensive model of the SEI/CEI, which remains a significant challenge that will be addressed by the development of new scale bridging models by the partners in this WP. In particular, the development of mesoscale models that incorporate material specific information is key to describe the complexities of the SEI/CEI accurately. Given the long time-scales involved, the development of advanced coarse-graining simulation techniques is a key challenge, as well as their harmonization with continuum modelling.

References:
[99] Feinauer J., et al. J. Comput. Sci., 31, 172–184 (2019)
[100] Ngandjong A. C. et al. JPC. Lett., 8, 5966 (2017)
[101] Röder F. et al. J. Electrochem. Soc., 164, E3335(2017)
[102] Kupper C. & Bessler, W.G. J. Electrochem. Soc.,164, A304-320 (2017)

Description of work and role of partners

WP3 - Multiscale Modelling [Months: 1-36]
KIT, DTU, UU, CNRS, WWU, CEA, NIC, PDT, CSIC, CNR, CID, BASF, FZJ, SAFT
Task 3.1: Development and validation of multiscale modelling frameworks
Task leader: PDT; Partners involved: DTU, UU, KIT, CNRS, CEA, NIC, CNR, CID, FZJ; M1-M18
Atomistic simulations generate the picture of the complex reactions on the very local and limited surfaces of electrodes. First-principles schemes are used to understand the electronic properties that control structure and stability, through approximations at and beyond the DFT level (UU, KIT, CNR). To render the formation of SEI/CEI on the whole electrode surfaces area, it is necessary to develop accurate models for realistic electrodes starting at the atomistic scale (DTU, KIT, CNRS, PDT), including chemical reactions (FZJ). Such electronic and atomistic models can be combined to screen the (theoretical) suitability of new materials [103] and predict important parameters describing thermodynamics [104], chemical reaction kinetics [105], structural properties [106], and transport phenomena [37] in batteries. We will take up the results of WP2 at the atomistic scale and forward the resulting mesoscopic result to models on higher scales. Models can be sequentially linked or iteratively coupled, for example passing output parameters from material models as input parameters in battery electrode and cell models and possible feedback backwards. More advanced links can be also generated via appropriate hybrid-simulation techniques between DFT, MD, and Monte Carlo (MC)[106] or via the transfer of free-energy information from the atomistic to the continuum scale [107]. All partners in this WP will participate in the generation of such models at the scales corresponding to their indicated primary expertise. The framework will carry atomistic information (FZJ, KIT) towards higher scales (PDT, CEA, CID, NIC) to realize an SEI/CEI morphology model [108]. The key focus of this task is to further the development of hybrid and mesoscale models (PDT, CEA, FZJ, KIT), such as DPD, coarse grained MD and reactive FFs, phase field modelling, cluster expansion and kMC [109] (FZJ, KIT, DTU) and consistent upscaling of these models to the macroscopic level by homogenizing the derived mesoscale models into a P2D continuum model (CID, NIC, CNRS).
This framework will ensure more consistent and time efficient exploration of the vast design space thereby enabling virtual electrode design and optimization, while preserving consistency to lower scales. This novel multiscale modelling framework will, therefore, efficiently support closed-loop autonomous materials findings and interphase engineering.

Task 3.2: Verification and Validation of Scale-Bridging Protocols for SEI/CEI formation
Task leader: CEA; Partners involved: ALL; M1-M36
In this task, all partners will collaborate to iteratively validate and verify the models developed in Task 3.1. Key questions are the influence of the surface morphology or locally inhomogeneous electric fields on the formation of, e.g., dendritic

structures. Explicit modelling of multiple charge/discharge cycles will provide insights into ageing phenomena. We will also investigate electrochemical and mechanical degradation mechanisms (including SEI growth, CEI growth and volumetric expansion and contraction or mechanical changes). CEA will collect available data on the systems chosen for this project, e.g., LNO, specify the data required for verification, validation and uncertainty quantification and perform the exercise of V&V with available data (using output of Task 3.1) with input from WWU, BASF and SAFT. The modelling groups (DTU, UU, KIT, CNRS, NIC, PDT, CID, CNR, and FZJ) will iteratively improve the model based on experimental input. The output will be a partial V&V with information on missing experimental data and missing models. First principles computational approaches, which can now treat structures of unprecedented size for ab initio thanks to frontier HPC and code developments at the (pre-)exascale, will be applied to a few selected sub-systems as consistent benchmarks for the multiscale schemes (by CNR and CSIC). They will also allow the computation of spectra for comparison with experiment (by CNR). The developed workflow for materials will also be validated in an industrial R&D environment. We will address the challenges of uncertainty quantification stemming from the intrinsic variability of the SEI/CEI morphology.

Task 3.3: AI enhanced models
Task leader: KIT; Partners involved: DTU, UU, CNRS, CEA, PDT; M1-M36
Because of approximations involved in all models, straightforward parameter passing propagates errors that tend to increase along the simulation chain. Here, we will develop of systematic calibration techniques in model coupling and linking that reduce such errors by optimizing the most uncertain model parameters (DTU, UU, KIT, CNRS, PDT). These partners will also develop novel modules based on ML/AI approaches, that surrogate the information passed between models and systematically design them to reduce the errors. The modelling partners will continuously improve the models based on input from Task 3.4 The combination of these two strategies will deliver breakthroughs in the accuracy of multiscale simulations and thereby of their predictive value. These models will be validated experimentally by data gathered by CEA, and the activity works in conjunction with WP10, where AI accelerated materials discovery is pursued from an experimental direction and will be closely linked to WP11 (Task 11.3) on hierarchical latent space models.

Task 3.4: Verification and Validation of Models for HTS experiments
Task leader: WWU; Partners involved: DTU, NIC, KIT, SAFT; M12-M32
In this task we address the objective to integrate computational and experimental workflows by systematic incorporation of data from high-throughput experiments in WP6 and procedures from WP9. Model integration will be performed by DTU, NIC, and KIT, while the link to HTS data will be provided by WWU, KIT. Such integrated models are key to the development of autonomous facilities, in particular for application areas where only sparse data is available. Filtering relevant information from high-throughput experiments via AI approaches, e.g. about specific positive correlations of different electrolyte components, may provide important challenges for theoretical work. In a forward-backward loop the theoretical analysis may then yield suggestions for improved electrolyte compositions.

Task 3.5: Workflow demonstrators
Task leader: KIT; Partners involved: DTU, UU, CNRS, NIC, PDT, CNR, CID, FZJ; M12-M36
Presently, multiscale models are often constructed ad-hoc in teams of experts that cover all the relevant phenomena, which severely limits their complexity and transferability. Here, we will exploit computational infrastructures developed in WP9 to formalize the development of multiscale workflows for key demonstrator projects, e.g. the BIG-MAP App-store (KD9). This effort will be coordinated by KIT with all partners providing modules/apps based on the modelling efforts of the other tasks in this WP. There workflows will be part of an emerging collaborative virtual environment in which simulations and data can be shared, first among the partners of this consortium, but later among the entire Battery2030+ initiative and the community at large. Development of these components will eventually lead to a digital representation of the Battery Interface Genome. This task is performed in close collaboration with Task 11.3.

References:
[103] Husch T. & Korth, M. Phys. Chem. Chem. Phys. 17, 22596 (2015)
[104] Chang K. et al. Chem. Mater. 24, 97 (2012)
[105] Van der Ven, A., Bhattacharya, J. & Belak, A. A. Acc. Chem. Res. 46, 1216 (2013)
[106] Takenaka N. et al. J. Phys. Chem. C, 118, 10874-10882 (2014)
[37]Jäckle, M. et al. Energy Environ. Sci. 11, 3400–3407 (2018)
[107] A. Latz & J. Zausch, Beilstein J. Nanotech., 6, 987-1007 (2015); Zelič K. & Katrašnik T. J. Electrochem. Soc., 166, A3242-A3249 (2019); Zelič K. & Katrašnik T. Sci Rep., 9, 2123 (2019)
[108] Wang, A. et al. Comp. Mat., 4, 1-24, (2018)
[109] Bhattacharyya et al., Nat. Comm. 10, 3451(2019)

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Participation per Partner	
Partner number and short name	**WP3 effort**
1 - DTU	12.00
2 - UU	24.00
3 - KIT	53.00
4 - CNRS	0.00
UPJV	14.00
5 - WWU	23.00
6 - CEA	8.00
7 - NIC	27.00
9 - PDT	35.00
13 - CSIC	12.00
15 - CNR	24.00
24 - CID	8.00
28 - BASF	3.00
33 - FZJ	12.00
34 - SAFT	0.50
Total	255.50

List of deliverables					
Deliverable Number[14]	**Deliverable Title**	**Lead beneficiary**	**Type[15]**	**Dissemination level[16]**	**Due Date (in months)[17]**
D3.1	Validated mesoscale models for SEI/CEI morphology	9 - PDT	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D3.2	Verification of scale bridging models against SEI/CEI experiment	6 - CEA	Report	Confidential, only for members of the consortium (including the Commission Services)	24
D3.3	Computational Framework for AI-enhanced models	3 - KIT	Other	Confidential, only for members of the consortium (including the Commission Services)	18
D3.4	Incorporation of Multiscale-Model into hybrid models based on HTS data	7 - NIC	Report	Confidential, only for members of the consortium (including the Commission Services)	32

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List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D3.5	Workflow demonstrator	3 - KIT	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	32

Description of deliverables

D3.1: Mesoscale models for SEI/CEI morphology (PDT, M12)
D3.2: Verification of scale bridging models against SEI/CEI experiment (CEA, M32)
D3.3: Computational Framework for AI-enhanced models (KIT, M18)
D3.4: Demonstration of model improvement by incorporation of AI-enhanced models (DTU, M36)
D3.5: Incorporation of Multiscale-Model into hybrid models based on HTS data (NIC, M32)
D3.6: Workflow demonstrator (KIT, M32)
D3.7: Transferable workflows for SEI morphology based on Task 3.1 and 3.5 (FZJ, M36)

D3.1 : Validated mesoscale models for SEI/CEI morphology [12]

Submission of report/paper on validated mesoscale models for SEI/CEI morphology.

D3.2 : Verification of scale bridging models against SEI/CEI experiment [24]

Verification of scale bridging models against SEI/CEI experiment has been performed and documented.

D3.3 : Computational Framework for AI-enhanced models [18]

Computational Framework for AI-enhanced models is made available to the partners.

D3.4 : Incorporation of Multiscale-Model into hybrid models based on HTS data [32]

Incorporation of Multiscale-Model into hybrid physics and data-driven models based on HTS (High Throughput Screening) data.

D3.5 : Workflow demonstrator [32]

Demonstration of autonomous workflow for multi scale simulations to consortium.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS2	M3.1: Incorporation of an AI-enhanced multi-scale model into the workflows of Task 3.1	3 - KIT	24	The correct incorporation of the AI-enhanced model is validated by the ability to run simulations in production mode. Associated risk R3.1.
MS3	M3.2: Integration of multi-scale workflow	3 - KIT	32	The workflow is integrated in BIG-MAP App-store into WP9. Associated risk R3.2.
MS16	M10.2: Demonstrate Figure Of Merit (FOM) extraction	3 - KIT	24	The FOM extraction are successful for selected analyses from WP3/WP6 robots using modular analysis package. Associated risk R10.2.

Schedule of relevant Milestones				
Milestone number[18]	**Milestone title**	**Lead beneficiary**	**Due Date (in months)**	**Means of verification**
MS18	M11.2: Concept of uncertainty-guided hybrid data-driven and physical model demonstrated	1 - DTU	32	Delivery of the 1st generation of hybrid physics- and data-driven model of battery interfaces. Associated risk R11.2.

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Work package number [9]	WP4	Lead beneficiary [10]	10 - Fraunhofer
Work package title	Modular Synthesis Robotics		
Start month	1	End month	36

Objectives

The main aim of this work package is to develop an open-source framework of hardware and software modules that allows heterogeneous hardware such as peristaltic pumps, pipetting robots, shakers, cooling units, conveyer belts, etc. to be seamlessly integrated to automate specific synthesis processes. The developed framework aims to implement optimized molecules and materials for protective coatings that are the output of the cross-section WP10 (AI-accelerated Materials Discovery). As part of an integration and demonstration effort the framework will target two very different core processes namely (low-temperature) organic syntheses and (high-temperature) inorganic syntheses as protective coatings for active anode and cathode particles. The measurable objective of WP4 is to have two semi-automated syntheses systems ready, relying both on expert knowledge and automated processes. The software/hardware connectors available are to interface within the other WPs, specifically WP6 and WP10.

Description of work and role of partners

WP4 - Modular Synthesis Robotics [Months: 1-36]
Fraunhofer, CEA, NIC, WUT, UT, ULIV, SOLB, ITU, FZJ
Task 4.1: Specifications
Task leader: ITU; Partners involved: All WP partners; M1-M6
The first task is to specify the syntheses and processing steps that the framework should be able to handle (All). The specifications will consider the expectations and requirements from the internal stakeholders (project partners as well as WP5, WP6, WP9, WP10), especially the definition of material classes and interfaces to AI materials discovery (WP10) as decision-making authority (provider of the optimized molecules as protective coatings) and handling of data (WP9). Subsequently, the processes will be broken down into single steps (e.g. pumping, weighting, stirring, solvent extraction etc.) and mapped to existing hardware modules (ITU, UT, FRAUNHOFER, ULIV). For each step, critical parameters and tolerance windows via a sensitivity analysis will be defined to ensure a robust process, good process control and safe operation with chemical and mechanical hazards (ULIV, FRAUNHOFER). Soft and hardware specifications will allow a decentralized construction of the different hardware and software modules in Task 4.2 and the integration and validation in one location (Task 4.3). Data lineage and provenance will be co-specified with WP5, WP6, WP9 and WP10 (All).
For the organic and the inorganic syntheses under inert environment (Schlenk-technique for organic and inert housing for inorganic systems, respectively), an automated systems will be developed based on equipment available at ULIV and FRAUNHOFER (Task 4.2). The robotic data handling protocols will allow variation of key process variables including reaction time, temperature and atmosphere.

Task 4.2: Hardware and software design
Task leader: UT; Partners involved: FRAUNHOFER, ULIV, ITU; M6-M30
This task is dedicated to the design and construction of the software layers of the framework to be able to integrate the heterogeneous hardware modules. Existing solutions (ROS, LCM, LIMS) for a robotic middle layer and standardized communication protocols will be evaluated to ensure interoperability and data transfer with connected work packages WP6, WP9 and WP10.
The modular robot system for the multistep synthesis of (hybrid) organic products in one reaction chamber will be constructed in a fume hood and with standard lab-equipment (FRAUNHOFER, ITU, UT). For the demonstration of the coatings either intermediate products (e.g. silanes) or products (e.g. polymers) can be utilized. As a starting point for the construction, an established polyether-based hybrid-polymer is proposed for the later optimization via computer aided characterization of the intermediated products (FRAUNHOFER, ITU). The system will be modularly adaptable to the requirements of a multitude of specific syntheses (e.g. specific purification setups) in a way that it can for instance provide protective coatings for the cathode as well as coatings for aqueous processing of the Ni-rich NMC/NIO electrode materials without metal-leaching.
The coating of inorganic materials will be demonstrated by adaptation of existing hardware (Formulation Engine, Labman Automation) and extensive experience [110] to enable coating of benchmark materials like alumina and silica, onto the control NMC/NIO cathode powder (ULIV, UT, ITU). Processes utilized are chemical solution, deposition from the hydrolysis and polycondensation of liquid precursors (e.g. aluminum sec-butoxide, aluminum ethoxide) and chemical impregnation of vaporized solid precursors. Appropriate inert atmosphere handling and the integration of

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calcination steps will be demonstrated in this enabling activity. The robotic protocols will enable investigation of multilayer coatings where distinct precursors are used successively.

Task 4.3: Integration and validation
Task leader: FRAUNHOFER; Partners involved: ULIV, UT, ITU, NIC; M12-M36
In this task, the hardware modules will be combined and integrated with the software modules from Task 4.2. Sensors for on-line and connectors for off-line characterization for every process step will be installed and the connection to the central AI optimizer established (demonstrated by external control of motors, pumps etc. via Task 10.4, WP10). After successful installation of the different layers of operation, viability of the hardware control will be demonstrated by two stand-alone syntheses each for the inorganic and the organic route as specified in Task 4.1. The intermediate or polymer material will then be coated manually via established routes (NIC, FRAUNHOFER). The inorganic film will be directly applied via sol-gel or co-precipitation on the particle (ULIV). The characterization and comparative study of the manually and automatically prepared protective coatings in will validate the automated syntheses (NIC, FRAUNHOFER, ULIV). By means of ML on NMR and Raman data, optimized syntheses will be proposed (WP10, Task 10.1) and tested (ITU, ULIV, FRAUNHOFER).

Task 4.4: Synthesis of components for organic protective coatings
Task leader: NIC; Partners involved: FRAUNHOFER, WUT, SOLB, FZJ; M6-M30
This task covers syntheses of components for organic protective coatings and electrolytes. At least two selected molecules defined in Task 10.4 as potential candidates for protective coatings will be synthesized (NIC). Molecules giving promising results will be upscaled and applied as protective coating on the cathode powder and tested (NIC, FZJ, FRAUNHOFER). Results will be feed back to the materials funnel, WP10, Task 10.4 (NIC, FZJ, FRAUNHOFER). Another electrolyte component, namely three different types of conductive salts based on Hückel anions, will be synthesized in well scalable single-step, one-pot syntheses (WUT). In addition, at least two sulphur based SEI forming additives will be synthesized (WUT). Promising electrolyte components will be upscaled to g (additives) or possibly kg scale (salts) and transferred to WP6, Task 6.2 for extensive screening of different electrolyte formulations to improve cell performance (conductivity and coulombic efficiency) (WUT, FZJ, FRAUNHOFER, SOLB).

Task 4.5 Combinatorial synthesis and application of inorganic coatings
Task leader: CEA; Partners involved: UMI, FZJ; M6-M30
This task is dedicated to the development of a generic approach for engineering efficient electrode coatings, using a PVD method. Specific magnetron sputtering apparatus at CEA will be utilized to enable the homogeneous or the deliberately heterogeneous deposition of thin films with complex compositions on a single substrate (typically Si, fused silica or alumina 4" wafers) for the generation of SEI/CEI libraries either on an inert substrate or on an electrode material (CEA). The latter will be prepared as a homogeneous thin film from target materials provided by UMI, with a priority for Ni-rich NMC (CEA, UMI). SEI/CEI material libraries will be generated using fast sequential deposition of single components from multiple targets, combined with their spatially-controlled mixing (CEA). Subsequent ultrafast annealing will be possibly used to generate a controlled interphase between the coating and the electrode. Automated high throughput assessment of the physical, chemical and electrochemical properties of pure coatings and coated electrodes will be carried out in WP6, Task 6.5 (CEA).

References:
[110] Boldrin P. et al. Chemical Science, 6, 935-944 (2016).

Participation per Partner

Partner number and short name	WP4 effort
6 - CEA	11.00
7 - NIC	12.00
10 - Fraunhofer	40.70
12 - WUT	47.00
19 - UT	24.00
20 - ULIV	42.20
27 - SOLB	5.00

Partner number and short name	WP4 effort
31 - ITU	41.00
33 - FZJ	12.00
Total	234.90

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D4.1	Specification (flow chart) of hardware and software architecture	31 - ITU	Report	Public	6
D4.2	Robotic system for organic synthesis installed including sensors	10 - Fraunhofer	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	30
D4.3	Robotic system for inorganic synthesis installed including sensors	20 - ULIV	Demonstrator	Confidential, only for members of the consortium (including the Commission Services)	30
D4.4	Report on synthesis and upscale of molecules for SEI formation and electrolyte components	7 - NIC	Report	Confidential, only for members of the consortium (including the Commission Services)	30
D4.5	Report on inorganic coatings prepared by combinatorial syntheses	6 - CEA	Report	Public	30
D4.6	Demonstration of automated synthesis procedure	10 - Fraunhofer	Demonstrator	Public	36
D4.7	Design of robotic system for organic synthesis completed	10 - Fraunhofer	Report	Public	18
D4.8	Design of robotic system for inorganic synthesis completed	20 - ULIV	Report	Public	18

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Description of deliverables

D4.1: Specification (flow chart) of hardware and software architecture (ITU, M6)
D4.2: Robotic system for organic synthesis installed including sensors (FRAUNHOFER, M30)
D4.3: Robotic system for inorganic synthesis installed including sensors (ULIV, M30)
D4.4: Report on synthesis and upscale of molecules for SEI formation and electrolyte components (NIC, M30)
D4.5: Report on inorganic coatings prepared by combinatorial syntheses (CEA; M30)
D4.6: Demonstration of automated synthesis procedure (FRAUNHOFER, M36)

D4.1 : Specification (flow chart) of hardware and software architecture [6]

Report with specification (flow chart) of hardware and software architecture submitted.

D4.2 : Robotic system for organic synthesis installed including sensors [30]
Protoype robotic system for organic synthesis installed including sensors developed.

D4.3 : Robotic system for inorganic synthesis installed including sensors [30]
Prototype robotic system for inorganic synthesis installed including sensors developed.

D4.4 : Report on synthesis and upscale of molecules for SEI formation and electrolyte components [30]
Report/paper submitted on synthesis and upscale of molecules for SEI formation and electrolyte components.

D4.5 : Report on inorganic coatings prepared by combinatorial syntheses [30]
Report/paper submitted on inorganic coatings prepared by combinatorial syntheses.

D4.6 : Demonstration of automated synthesis procedure [36]
Demonstration of automated synthesis procedure completed.

D4.7 : Design of robotic system for organic synthesis completed [18]
Full design of robotic system for organic synthesis completed.

D4.8 : Design of robotic system for inorganic synthesis completed [18]
Full design of robotic system for inorganic synthesis completed.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS4	M4.1: Specifications are defined	10 - Fraunhofer	6	Material classes and interfaces to AI materials discovery, decision-making authority and handling of data are all defined and available at M6. Associated risk R4.1.
MS5	M4.2: Hardware integrated and software architecture developed	10 - Fraunhofer	30	The integration of hardware and development of architecture is validated by the installation of robotic system for synthesis including sensors (D4.2). Associated risk R4.2.

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Work package number [9]	WP5	Lead beneficiary [10]	6 - CEA
Work package title	Characterization		
Start month	1	End month	36

Objectives

The main objective of WP5 is to develop synergies to initiate a pilot action towards the implementation of a European multi-modal experimental platform using standardized cells/protocols/metadata/data collection, treatment and analysis. In this WP, we aim at validating the concept and demonstrate its feasibility on a selected chemistry using a subset of lab-scale and LSF techniques.
The data will be acquired using the standards and protocols defined in WP7 and WP8. The extracted data specified in the form defined by WP9 and labelled in terms of fidelity level will be transferred to central BIG-MAP, e.g. delivered to the WPs taking care of handling, storage, database and modelling.

Description of work and role of partners

WP5 - Characterization [Months: 1-36]
CEA, DTU, UU, CNRS, NIC, CTH, CSIC, TUD, UCAM, UOXF, ESRF, ILL, SOLEIL, UMI, SAFT
Task 5.1: Benchmark
Task leader: TUD; Partners involved: CEA, UU, ESRF, SOLEIL, ILL, CNRS, CTH, Oxford, UCAM, CSIC, NIC, UMI, SOLB, SAFT; M1-M30
The objective is to build an experimental matrix containing the information required for establishing the WP5 workflow on the case study (selected chemistry). The matrix will allow the exhaustive report of observables vs techniques. The criteria and parameters to establish the matrix are first to be defined (scales, resolutions, operando mode, availability, maturity, reactivity, fidelity, etc.) in relation to the BIG-MAP central objective. The observables (quantities extracted from data) will be identified and organized according to WP7 and WP8 and in tight relation with the modelling/numerical activities. Both lab-scale and LSF techniques will be considered. Both methods and observables for screening vs high fidelity data will be distinguished.
First, the criteria and parameters to organize the experimental matrix will be defined by TUD, UU, CTH, Oxford and UCAM. The experimental observables will be identified and classified by CNRS and CEA. The experimental techniques will be identified and classified by CNRS, CEA, ESRF, SOLEIL and ILL. The output is the experimental matrix (generation1: state-of-the art, generation2: BIG-MAP final matrix) that will be assembled by TUD and CEA (with support from CSIC, NIC, UMI, SAFT, SOLB). The task will be refined along the project to implement the achievements and findings obtained through the WP and other related WPs.

Task 5.2: Workflow
Task leader: CEA; Partners involved: UU, DTU, TUD, ESRF, SOLEIL, ILL, CNRS, CTH; M1-M36
The objective is to set-up the WP5 characterization loop/sequences to be performed within the BIG-MAP to acquire and deliver data using the standardized methodology/format/protocols defined in WP7 and WP8, aided by AI modules (WP10) and modelling (WP2, WP3 and WP11). This will be defined in tight relation to WP9 (Interoperability & Infrastructures). Both model and real interfaces may be probed by the selected techniques. The workflow will be dynamically refined along the project duration to integrate progress in the matrix definition as well as numerical & experimental outputs. The experiments will be organized in Tier 1 (first priority techniques, implemented M6-M30) and Tier 2 (second round techniques implemented M20-M36 depending on the results of Tier 1 experiments and modelling inputs).
SOLEIL, ESRF and ILL (with support from all WP5 partners) will identify a few key techniques and key experiments to be performed. The generation 1 state-of-the art matrix of Task 5.1 will serve as the basis to select the techniques to be implemented in WP5-Tier1 experiments. Different scenarios may be proposed related to families of techniques (e.g. X-ray tomography and neutron imaging, absorption/vibrational spectroscopy, or atomic scale/nanoscale scattering) and one will be implemented to validate the methodology and establish a demonstrator (KD4). Following the identification phase, the workflow will be constructed by ESRF, ILL and SOLEIL, to define the timeline and order of implementation of data acquisition for high-throughput and high-fidelity data. In particular, coordination between the various sites and partners and beam time schedule will be determined in tight connection to the loop demonstrators / infrastructure integration plan of WP9. The definition of workflow will take into account the optimization of the fidelity cost. The workflow demonstrator describing the experimental plan/methodology will be set by CEA, CNRS, TUD, UU, CTH and DTU. Consistency with other WPs will be insured to deliver the proof-of-concept BIG-MAP experimental workflow.

At the end of the task, perspectives and future vision towards the European multi-modal platform will be defined by CEA, DTU and UU.

Task 5.3: Data acquisition & visualization
Task leader: ESRF; Partners involved: CEA, UU, TUD, SOLEIL, ILL, CNRS, CTH, Oxford, UCAM, CSIC, UMI, SOLB, SAFT; M6-M36
The objective is to design, prepare and perform the selected experiments according to the defined order of implementation and experimental plan prepared in Task 5.2, in tight relation with the materials providers, as well as WP7, WP8 and WP9. The final result of this task will be the practical validation of the WP5 workflow on a selected chemistry using a sub-set of key techniques. For instance, sequential lab XCT, neutron imaging coupled to low resolution X-ray imaging, and synchrotron 3D high resolution tomography, could be a candidate set of techniques.
The first step is the harmonization of electrochemical cells to guarantee interoperability among the different instruments (CEA, with support of all WP5 partners). In-Lab experiments (high throughput screening and high fidelity) will be realized to probe the desired electrochemical, chemical, electronic, structural and morphological properties at multiple scale level (materials, interfaces, components and cells) according to the workflow (UU, CTH, Oxford, UCAM, CSIC, CEA, CNRS). The LSF experiments (screening, high quality) selected in the workflow will be performed (ESRF, SOLEIL, ILL and TUD). CNRS, SOLEIL, ESRF, ILL and CEA will be in charge of developing Automated (standardized) visualization and pre-treatment, possibly on-the-fly.

Task 5.4: Data Analysis
Task leader: ILL; Partners involved: CEA, UU, DTU, TUD, ESRF, SOLEIL, CNRS, CTH, Oxford, UCAM, CSIC, UMI, SOLB, SAFT; M8-M36
The objective is to perform data analysis to extract the main observables according to Task 5.1-5.2, using cells developed in Task 5.3 and automated analysis-modules developed in WP10, and deliver the analysed data/output quantities in the format defined by WP9. The task will be developed in tight relation with WP8, WP9, WP10, WP11 and almost all modelling tasks (WP2). First, the required AI modules and modelling inputs will be identified (ILL, ESRF, SOLEIL, CTH, UU, DTU). ESRF, SOLEIL and ILL will organize the implementation of data analysis, automatization and standardisation, with support from all partners. CEA will realize the practical application of novel data analysis tools on the chemistry selected for the key demonstrator (KD4). An appropriate data exploitation procedure for big data/bad data handling and managing will be constructed by ILL, ESRF, SOLEIL, CNRS, DTU and CEA in tight collaboration with related WPs.

Participation per Partner

Partner number and short name	WP5 effort
1 - DTU	24.00
2 - UU	24.00
4 - CNRS	39.00
6 - CEA	48.00
7 - NIC	3.00
11 - CTH	27.00
13 - CSIC	6.00
14 - TUD	31.00
17 - UCAM	19.30
18 - UOXF	15.00
21 - ESRF	12.00
22 - ILL	23.00
23 - SOLEIL	15.00
26 - UMI	2.00

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Partner number and short name	WP5 effort
34 - SAFT	5.50
Total	293.80

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D5.1	State-of-the art experimental matrix, tier 1 experimental plan and workflow	14 - TUD	Report	Public	6
D5.2	Global BIG-MAP experimental matrix, proof-of-concept of BIG-MAP experimental workflow and definition of perspectives and future vision towards the European multimodal platform	6 - CEA	Report	Public	36
D5.3	Demonstration of the capability to run coordinated multi-techniques experiments to acquire multi-scale data, and practical application to a selected chemistry	21 - ESRF	Demonstrator	Public	32
D5.4	Report on lab-scale and large-scale facilities automated and standardized data analysis	22 - ILL	Report	Public	36
D5.5	Design of workflow for a European experimental multimodal platform completed	6 - CEA	Report	Public	18

Description of deliverables

D5.1: State-of-the art experimental matrix, tier 1 experimental plan and workflow (TUD, M6)
D5.2: Global BIG-MAP experimental matrix, proof-of-concept of BIG-MAP experimental workflow and definition of perspectives and future vision towards the European multi-modal platform (CEA, M36)
D5.3: Demonstration of the capability to run coordinated multi-techniques experiments to acquire multi-scale data, and practical application to a selected chemistry (ESRF, M32)
D5.4: Report on lab-scale and large-scale facilities automated and standardized data analysis (ILL, M36)

D5.1 : State-of-the art experimental matrix, tier 1 experimental plan and workflow [6]

Report on state-of-the art experimental matrix, tier 1 experimental plan and workflow submitted.

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D5.2 : Global BIG-MAP experimental matrix, proof-of-concept of BIG-MAP experimental workflow and definition of perspectives and future vision towards the European multimodal platform [36]

Report submitted on a global BIG-MAP experimental matrix, proof-of-concept of BIG-MAP experimental workflow and definition of perspectives and future vision towards the European multimodal platform.

D5.3 : Demonstration of the capability to run coordinated multi-techniques experiments to acquire multi-scale data, and practical application to a selected chemistry [32]

Completion of a demonstration of the capability to run coordinated multi-techniques experiments to acquire multi-scale data, and practical application to a selected chemistry.

D5.4 : Report on lab-scale and large-scale facilities automated and standardized data analysis [36]

Report/paper submitted on lab-scale and large-scale facilities automated and standardized data analysis.

D5.5 : Design of workflow for a European experimental multimodal platform completed [18]

Design of workflow for a European experimental multimodal platform completed.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS6	M5.1: State-of-the-art experimental matrix completed	6 - CEA	6	Confirmation that the state-of-the-art is delivering all available parameters available in the literature for the matrix: scales, resolutions, operando mode, availability, etc. Associated risk R5.1.
MS7	M5.2: Technical implementation of the Demonstrator workflow (KD4)	6 - CEA	12	Framework for the running of coordinated multi-techniques experiments to acquire multi-scale data is operational. Associated risk R5.2.

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Work package number [9]	WP6	Lead beneficiary [10]	33 - FZJ
Work package title	HTS and Testing		
Start month	1	End month	36

Objectives

WP6 will establish a chemistry neutral and versatile materials characterization as well as performance evaluation module within BIG-MAP, with a focus on advanced electrolyte formulations for lithium and post-lithium batteries. Through strong interaction and complementarity, a new degree of integration in the high throughput formulation-characterization-performance evaluation chain across time and length scales will be achieved. This will be demonstrated during the ramp-up phase utilizing liquid electrolytes and compatible electrode materials with proven capabilities. Apart from breaking new ground on the methodology, the abundance of in-depth data will be used to build the BIG. Characterization of electrolyte/electrode interfaces and interphases, the key enablers for long battery lifetime, will be performed along the entire materials lifecycle, including in situ measurements in a three-electrode setup and long-term performance evaluation (KD5). The herein proposed high throughput screening approach will serve the community through a tiered screening pipeline, accelerating the identification of lead electrolyte candidates for selected cell chemistry application(s), and the generation of abundant pertinent interphase/interface/device data across the entire lifetime of the battery. Having demonstrated the capability of superseding throughput and integration over existing high throughput materials discovery pipelines for liquid electrolyte formulation studies, the module will demonstrate its extendibility through sub-module adaptation towards other electrolyte classes and the established methodology opened to further research categories of interest.

Description of work and role of partners

WP6 - HTS and Testing [Months: 1-36]
FZJ, KIT, CEA, Fraunhofer, WUT, CID, UMI, SOLB, BASF, NVOLT, SAFT
Task 6.1: Preparation and characterization of "feeding" units for the HTS assays
Task leaders: BASF; Partners involved: SOLB, UMI, CID, NVOLT, SAFT, KIT, FZJ, CEA, FRAUNHOFER; M1-M36
Within this task, the materials providers will ensure a reliable supply of liquid electrolyte components and electrode materials including reference data sets for material properties and electrochemical performance, required for the HTS assays. Liquid electrolyte components comprising selected commercial and precommercial conducting lithium salts, solvents/co-solvents and functional additives will be provided by SOLB. The Ni-rich NMC-811 provided by UMI and the lithium nickel oxide (LNO), provided by BASF, will be used as cathode active materials. Material synthesis (on <100 g scale) will be optimized with respect to initial discharge capacity and cycle life as well as robustness of the synthesis, scalable up to >1 kg. Materials will be characterized by means of electrochemical testing (different cell setups), elemental analysis, electron microscopy and X-ray diffraction. Depending on the progress in the materials discovery, a modified material composition with slightly diluted Ni content e.g. LiNi1-x-MxO2 (M e.g. Co, Mn, etc.) can be synthesized and provided as well. Electrode sheets of aforementioned materials will be additionally provided in a small quantity. The production of electrodes and advanced generation cell prototypes will be conducted by CID, BASF, UMI, NVOLT and SAFT. The initial process parameters will be selected based on previous know-how and iteratively updated using the models from WP10. Similar selection will be conducted for anode materials based on graphite and graphite/silicon commercially available materials, manufactured by CID. The resulting positive and negative electrodes will be characterized regarding their electrical conductivity, adhesion strength, pore size distribution and electrochemical performance (small test cells) (BASF, KIT, FZJ, CEA, FRAUNHOFER).

Task 6.2: Formulation and characterization of advanced electrolyte components for the HTS assays
Task leader: WUT; Partners involved: CID, KIT, FZJ, CEA, FRAUNHOFER; M1-M36
The expertise and know-how within this task is related to the smartly tailored formulation of liquid electrolyte components, namely conducting salts and functional additives/co-solvents for lithium and post-lithium chemistries (WUT) relevant for the electrolyte formulation, resulting cell chemistries and diverse characterizations on the electrolyte and cell level (CID, KIT, FZJ, CEA, FRAUNHOFER). The proprietary conducting salts are based on weakly-coordinating anions that weaken the interactions between anion and cation in the structure, thus resulting in increased ionic conductivity and cation transference number values, lower tendency towards formation of associates and high tolerance to moisture. These conducting salts containing novel, proprietary anions, are in addition functional as SEI modifiers and moisture absorbent/inside desiccants, present in electrolyte as single additive or in a mixture. The formulation aspects will additionally be related to new sulfur-containing aliphatic aromatic functional additives as well

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as to the fluorine-free and multivalent anions. The overall approach will comprise optimization aspects and preliminary compatibility studies in a close alliance with WP2, WP4 and WP10.

Task 6.3: HTS analysis via selected methods
Task leaders: KIT; Partners involved: WUT, FZJ, BASF, CID; M1-M36
The capabilities and knowledge centred on the combinatorial synthesis, high throughput characterization, automated orchestration, and materials informatics (KIT/CELEST) will be expanded by a new method in battery research: the scanning droplet cell (SDC), which can rapidly create batteries on the millimeter scale in a sequential manner. Through a specially engineered measurement, tip hundreds to thousands of small post-Li battery cells will be formed, thus allowing for rapid evaluation of electrode composition, electrochemical protocols, electrolyte formulation and processing variation. As only the counter (in principle exchangeable) and reference electrode (flushable) are reused, the SDC offers the unique opportunity to directly investigate the SEI ex situ. For ex situ characterization, a full-fledged high throughput analysis suite with a dedicated XPS system with UPS, Auger, SEM and an Ar-cluster sputter source is available, as well as ATR/DRIFTS and Raman mapping robots. The SDC is envisioned to be equipped with an in situ Raman spectrometer allowing for rapid sequential in situ measurements using the developed automated analysis tools. All equipment is envisioned to be autonomously orchestrable with minimal expert mediation (in tight relation with WP4, WP8 and WP10). Besides automated equipment, several robotic arms will allow for rapid sample ex- and interchange. Custom electrolyte materials for the SDC (KIT) will be synthesized at WUT (in agreement to specifications set by KIT and BASF), electrode materials in small quantities will be contributed by BASF. Results from SDC will be communicated to FZJ and CID where long term tests will be conducted. A joint demonstrator between this and Task 6.4 will be built for the AI accelerated optimization of SEI resistance at KIT and FZJ.

Task 6.4: HTS in electrolyte formulation, cell assembly and “filtration” measurements
Task leader: FZJ; Partners involved: WUT, SOLB, BASF, CID, KIT, CEA, FRAUNHOFER; M1-M36
The developed and well-established HTS approach comprises fast and systematic, fully automated formulation of liquid electrolytes (wide variety of electrolyte components including conducting salts, solvents/co-solvents and functional additives (WUT), cell assembly in two (coin cell) and three (EL-CELL®) electrode setup, as well as preselected physicochemical (determination of viscosity, transference number and refractive index) and electrochemical measurements (EIS, LSV, CV, galvanostatic cycling experiments) on a electrolyte and cell level, serving as a filtration effect towards identifying affordable, electrochemically and thermally outperforming lead electrolyte candidates for a specific application in a given cell chemistry. The entire value chain, governed by the laboratory information management system (LIMS), enables prediction of vital electrolyte properties and establishment of structure-property-reactivity-performance relationships, based on the synergy of experimental data pool, ML, and AI (in synergy with WP4). AI-based analysis of available HTS-data (WP2, WP8 and WP10) may also be used to direct the search for new combinations of electrolyte formulations, either in terms of concentrations or even different components in order to optimize relevant properties.
The obtained results will be communicated with KIT such that synchronized experiments focused on interfacial (KIT, FZJ) and cell level effects (FZJ, KIT, SAFT, CID) can be studied. In collaboration with WP10, KIT and FZJ will conduct joint AI accelerated electrolyte formulation experiments for optimization of SEI resistance (KD5).

Task 6.5: HTS of inorganic protective coatings
Task leader: CEA; Partners involved: WUT, FZJ, FRAUNHOFER, CID, KIT; M1-M36
Development of a specific HTS approach adapted to electrode materials and Li-ion conducting protective coatings prepared by combinatorial sputtering method (WP4, Task 4.5), with the aim to identify appropriate surface modifications of high energy density cathode materials, possibly of anode materials, able to enhance the performance of the considered cathode/anode materials in liquid electrolyte-based battery cells (FZJ, KIT, CID, WUT, FRAUNHOFER). This task will aim at obtaining a combined mapping of geometrical, electrochemical and chemical features of the coating libraries generated on 4’’ wafers. CEA will carry out fast galvanostatic cycling tests and EIS measurements using 64-well cells, whereas thickness mapping will be carried out by mechanical profilometry. Additionally, CEA will perform surface chemical screening on aforementioned large scale electrodes using EDX, XPS, AES and HAXPES methods in order to automatically evaluate the SEI distribution driven by electrolyte or surface composition changes. Statistical methods using, e.g., Principal Component Analysis (PCA) will be developed. Advanced characterization by means of HR-STEM will provide complementary insights on materials evolution.

Participation per Partner

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Partner number and short name	WP6 effort
3 - KIT	14.00
6 - CEA	11.00
10 - Fraunhofer	9.30
12 - WUT	24.00
24 - CID	36.00
26 - UMI	6.00
27 - SOLB	4.00
28 - BASF	11.00
29 - NVOLT	12.00
33 - FZJ	89.00
34 - SAFT	12.00
Total	228.30

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D6.1	Set up "feeding" units for the HTS assays at FZJ comprising advanced functional electrolyte components from Solvay and WUT (commercially available and newly synthesized) and compatible electrode materials	28 - BASF	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D6.2	Develop materials experiment embeddings for advanced functional liquid electrolytes in lithium-based battery cells containing compatible electrodes with proven capabilities	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D6.3	1st Deployment of HTS experimentally obtained raw results and subsequent analyses for data lineage tracking	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D6.4	Advanced direct SEI investigations for chemistry neutral lithium-based batteries by integrated	3 - KIT	Report	Public	24

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List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
	high throughput electrochemistry with ex situ high throughput spectroscopy				
D6.5	Generate high quality, abundant pertinent interphase/interface/ device data across the entire lifetime of the battery cell	33 - FZJ	Report	Confidential, only for members of the consortium (including the Commission Services)	36

Description of deliverables

D6.1: Set up "feeding" units for the HTS assays at FZJ comprising advanced functional electrolyte components from Solvay and WUT (commercially available and newly synthesized) and compatible electrode materials (BASF, M12)
D6.2: Develop materials experiment embeddings for advanced functional liquid electrolytes in lithium-based battery cells containing compatible electrodes with proven capabilities (FZJ, M12)
D6.3: 1st deployment of HTS experimentally obtained raw results and analyses for data lineage tracking (FZJ M18)
D6.4: Advance direct SEI investigations to for chemistry neutral lithium-based batteries by integrated high throughput electrochemistry with ex situ high throughput spectroscopy (KIT, M24)
D6.5: Generate high quality, abundant pertinent interphase/interface/device data across the entire lifetime of the battery cell (FZJ, M36)

D6.1 : Set up "feeding" units for the HTS assays at FZJ comprising advanced functional electrolyte components from Solvay and WUT (commercially available and newly synthesized) and compatible electrode materials [12]

Set up of "feeding" units completed for the HTS assays at FZJ comprising advanced functional electrolyte components from Solvay and WUT (commercially available and newly synthesized) and compatible electrode materials.

D6.2 : Develop materials experiment embeddings for advanced functional liquid electrolytes in lithium-based battery cells containing compatible electrodes with proven capabilities [12]

Report submitted on the development of materials experiment embeddings for advanced functional liquid electrolytes in lithium-based battery cells containing compatible electrodes with proven capabilities.

D6.3 : 1st Deployment of HTS experimentally obtained raw results and subsequent analyses for data lineage tracking [18]

1st Deployment of HTS experimentally obtained raw results and subsequent analyses for data lineage tracking.

D6.4 : Advanced direct SEI investigations for chemistry neutral lithium-based batteries by integrated high throughput electrochemistry with ex situ high throughput spectroscopy [24]

Report/paper submitted on the use of advanced direct SEI investigations for chemistry neutral lithium-based batteries by integrated high throughput electrochemistry with ex situ high throughput spectroscopy.

D6.5 : Generate high quality, abundant pertinent interphase/interface/device data across the entire lifetime of the battery cell [36]

Report submitted on the generation of high quality, abundant pertinent interphase/interface/device data across the entire lifetime of the battery cell.

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Schedule of relevant Milestones				
Milestone number[18]	**Milestone title**	**Lead beneficiary**	**Due Date (in months)**	**Means of verification**
MS8	M6.1: Establish and validate HTS assay and testing methodology for liquid electrolyte-based lithium batteries	33 - FZJ	12	The methodology enable optimization in electrolyte formulation, preparation of inorganic coatings, selected characterization and analysis. Associated risk R6.1.
MS9	M6.2: Establish interface between the HTS systems and AI orchestration	33 - FZJ	18	The HTS is deployed experimentally including AI orchestration to obtain raw results to enable analyses for data lineage tracking. Associated risk R6.2.
MS10	M6.3: Critical review of the different methodologies and proposed evolution directions	33 - FZJ	24	The SEI/CEI investigations enable decisions on the optimum high throughput electrochemistry for neutral lithium-based chemistry. Associated risk R6.3.
MS16	M10.2: Demonstrate Figure Of Merit (FOM) extraction	3 - KIT	24	The FOM extraction are successful for selected analyses from WP3/WP6 robots using modular analysis package. Associated risk R10.2.

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Work package number [9]	WP7	Lead beneficiary [10]	8 - SINTEF
Work package title	Battery Interface Ontology		
Start month	1	End month	36

Objectives

WP7 will develop a battery interface ontology (BIO) that ensures interoperability between multiple scales, techniques and domains in the battery discovery process. The BIO will facilitate the work of battery experts in different fields to convert real-life observations to a common digital representation. The result will support the creation of a database utilizing a descriptive, formalized, scheme to improve the reproducibility of experiments and simulations.
Successful development of the BIO requires a close collaboration with other cross-cutting initiatives and competence pillars in BIG-MAP. To ensure interoperability, it is crucial that common requirements, standards, and interfaces are established early and maintained throughout the project and beyond. To achieve this, the BIO will collaborate with WP8 (Standardization and Protocols) and WP9 (Infrastructure and Interoperability). The BIO should be developed early in the project so that it can be applied to support the activities of the other WPs, notably WP10 (AI-accelerated Materials Discovery) and WP11 (Battery Interface Genome). The BIO will also involve a close collaboration with WP3 (Multi-scale Modelling).

Description of work and role of partners

WP7 - Battery Interface Ontology [Months: 1-36]
SINTEF, DTU, NIC, WUT, CSIC, EPFL
Task 7.1: Establish ontology standards to support interoperability and dissemination
Task leader: WUT; Partners involved: SINTEF, DTU, EPFL; M1-M36
This task shall identify and formalize the critical information needed to support the interoperability of the BIO framework with other BIG-MAP WPs specifically and the European modelling community generally. Common data structures including descriptions of data provenance and quantifiers of uncertainty shall be agreed and aligned with WP9. There will be constant exchange between the ontology, the AI platform, project database, and others. Within this task, collaboration with the EMMO will support the integration of the BIO into European modelling communities and facilitate exchange with industry and academia. This task spans the length of the project to ensure that the agreed standards are maintained or modified as needed. A report on the ontology standards and development strategy will be delivered in M3 (D7.1).
WUT will be responsible for coordinating common data structures with other BIG-MAP nodes, most notably WP8 and WP9. SINTEF, DTU, and EPFL will be responsible for ensuring the resulting standards are compatible with European modelling and ontology activities.

Task 7.2: Design a general battery ontology
Task leader: SINTEF; Partners involved: WUT, DTU, EPFL, CSIC; M1-M18
This task will design and implement an ontology for batteries in general. This will categorize and describe the different relevant models, characterization, and workflows needed to describe a generic battery. The ontology will support the description of cell architecture, processes for the transport of mass, charge and heat, and electrochemical cell reactions. The ontology will be implemented in OWL, a language commonly used to describe ontologies that also allows for machine reasoning. The task will first establish the battery taxonomy by identifying and defining the classes (concepts) required to describe the battery and grouping them into a taxonomic (class-subclass) structure. The taxonomy will then be populated with relations to create the ontology. The initial version will be implemented in OWL is delivered in M6 for other WPs to begin understanding and implementing the framework (D7.2, KD6). SINTEF will be responsible for developing the ontology structure and implementation. WUT, DTU, CSIC, and EPFL will develop the battery-specific classes needed to describe the system.

Task 7.3: Design the battery interface ontology (BIO)
Task leader: SINTEF; Partners involved: WUT, DTU, EPFL, NIC; M3-M36
This task will build upon the general battery ontology created in Task 7.2 to create an ontology specifically for battery interfaces. The BIO will support the description and characterization of key aspects governing battery interface performance including the formation of interphase layers, passivating layers, active material dissolution, and charge transfer reactions, etc. The BIO will be implemented in OWL and fit seamlessly within the general battery ontology from Task 7.2. To support the activities occurring in other cross-cutting initiatives and competence pillars, the BIO must be operational in the first half of the project. This will be accomplished by a stable release in M18 (D7.3). The published

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taxonda and standards will be prepared for integration into the EMMO by M36 (D7.5). SINTEF will be responsible for developing the ontology structure and implementation. WUT, DTU, CSIC, and EPFL will develop the classes needed to describe battery interfaces.

Task 7.4: Implement the ontology to describe specific case studies
Task leader: EPFL; Partners involved: SINTEF, WUT, DTU; M9-M36
In this task, the BIO framework developed in Tasks 7.2 and 7.3 will be applied to create case studies, describing instances of battery interfaces. This will provide a framework for processing experimental and simulation data and support the BIG-MAP platform. This task will begin after the initial BIO version is delivered. The task will create case studies of the critical battery interfaces identified in the project. A report describing the implementation and findings will be delivered in M24 (D7.4). EPFL will be responsible for leading the implementation of the ontology to describe specific case studies, in line with EPFL's role in WP9. SINTEF will adapt the ontology as needed. WUT, NIC, and DTU will support the development of case-specific classes.

Participation per Partner

Partner number and short name	WP7 effort
1 - DTU	12.00
7 - NIC	5.00
8 - SINTEF	23.00
12 - WUT	12.00
13 - CSIC	6.00
16 - EPFL	18.00
Total	76.00

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D7.1	Report on ontology standards and development strategy	12 - WUT	Report	Public	3
D7.2	Initial version of battery ontology	8 - SINTEF	Report	Public	6
D7.3	First stable release of battery interface ontology	8 - SINTEF	Report	Public	18
D7.4	Report on battery interface ontology case study	16 - EPFL	Report	Public	24
D7.5	Battery Interface Ontology published according to standards in the European modelling community	8 - SINTEF	Report	Public	36

Description of deliverables

D7.1: Report on ontology standards and development strategy (WUT, M3)

D7.2: Initial version of battery ontology (SINTEF, M6)
D7.3: First stable release of battery interface ontology (SINTEF, M18)
D7.4: Report on battery interface ontology case study (EPFL, M24)
D7.5: Published according to standards in the European modelling community (SINTEF, M36)

D7.1 : Report on ontology standards and development strategy [3]

Report/paper submitted on ontology standards and development strategy.

D7.2 : Initial version of battery ontology [6]

Initial version of battery ontology submitted.

D7.3 : First stable release of battery interface ontology [18]

First stable release of battery interface ontology.

D7.4 : Report on battery interface ontology case study [24]

Report/paper submitted on a battery interface ontology case study.

D7.5 : Battery Interface Ontology published according to standards in the European modelling community [36]

The Battery Interface Ontology (BIO) has been published according to standards in the European modelling community.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS11	M7.1: Consistent representative description of battery interface ontology	8 - SINTEF	6	A survey sent to relevant WP members to determine if the BIO is being adopted and provides value. Associated risk R7.1.
MS12	M7.2: Integration with BIG-MAP AI and database platforms	8 - SINTEF	21	Successful operation of a case study of the critical battery interfaces identified in the project. Associated risk R7.2.

DRAFT

Work package number [9]	WP8	Lead beneficiary [10]	4 - CNRS
Work package title	Standards and Protocols		
Start month	1	End month	36

Objectives

Owing to the importance of standardization and protocols, the timeline for WP8 is very critical and its success will rely on the early definition of a set of protocols and standards and their rapid implementation for each experimental and modelling/simulation WP. Furthermore, working groups including key persons from downstream (data generation in WP2, WP3 and WP5), as well as upstream WPs (WP9 and WP11) will be created in order to established feedback loops and allow for the constant refinement of the pre-defined standards and protocols during the course of the project (36 months). WP8 is therefore organized in 4 tasks: selection and refinements of pre-existing initiatives, creation of working groups and workflows, implementation of these standards and protocols, creation of common European platforms for materials and battery testing. Furthermore, the list of metadata as well as protocols will be made available to the community on the project website.

Description of work and role of partners

WP8 - Standards and Protocols [Months: 1-36]
CNRS, UU, UCAM, UOXF, ESRF, ILL, SOLEIL, BASF
Task 8.1: Selection and refinement of pre-existing initiatives regarding standards and protocols
Task leader: CNRS; Partners involved: SOLEIL, ILL, ESRF, UU, OXFORD, UCAM, BASF; M1-M6
The objective of this task is to make a pertinent selection of established initiatives regarding standardization of experimental data (in-house and LSF) as well as simulation and modelling data. The overarching goal is to identify data formats that ensure maximal compatibility on a general consensus, including the extension of metadata tracking. Pre-existing initiatives with which coordination actions will be established entail industrial standards like NEXUS/ HDF5, but also academic implementations PANOSC, MODA, EMMC as well as initiatives from the thematic group New and Emerging Battery Technologies from ETIP, Batteries Europe, the DEFACTO H2020 project, the NFTA action on metadata for materials, The Materials Project and others. For the selection, one working group for each type of experimental and modelling/simulation data will be established, which will include key persons from each corresponding WP2, WP3 and WP5, as well as from WP9 and WP11 (CNRS, SOLEIL, ESRF, UCAM, OXFORD, BASF). Afterwards, protocols and standards will be refined to address the specific need for BIG-MAP (UU, CNRS, SOLEIL). Downstream processing protocols will define the format of both the output data (results) and the supplementary metadata required to interpret the results. A formal data and metadata format and content for each type of measurements will be developed in collaboration with WP5 and WP2/WP3, such that the equivalence of data and metadata coming from different experiments will be assured (SOLEIL, CNRS, UU, ILL). Data resulting from upstream AI results and battery fabrication procedures must be prepared to allow for experimental questions and measurement protocols to be extracted. For example a common nomenclature/format for sample and data identification (e.g. sample name, sample origin, sample type, sample chemical composition, production protocol, required characterization method, data and metadata name, data source and location, data archival, etc.) will be defined in collaboration with WP7 and applied at all characterization centres, forming a DOI for each sample that will allow for automatic data analysis protocols to be followed.

Task 8.2: Creation of working groups and workflow
Task leader: SOLEIL; Partners involved: CNRS, ILL, ESRF, UU, OXFORD, UCAM, BASF; M6-M36
Once the initial standards and protocols are established, extended working groups will be permanently defined (CNRS, SOLEIL). These groups will gather key persons from the WPs in which data are collected, as well as from WP9 and WP11, all together with partners from WP8. Doing so, feedback loops will be created in order to permanently refined the standards and protocols and ensure their compatibility with BIG-MAP (CNRS, SOLEIL, ESRF, ILL, OXFORD, UU, UCAM, BASF).

Task 8.3: Implementation of these standards and protocols
Task leader: CNRS; Partners involved: SOLEIL, ILL, ESRF, UU, OXFORD, UCAM; M6-M36
Once the standards and protocols established for the data acquisition and sharing, they will be implemented into each WP (CNRS, SOLEIL, UU, SOLEIL). For that, each partner involved in the WPs will receive the standards and protocols as well as the list of keywords and metadata that must be collected and shared. These tools will be automated and made available and easily accessible to the community via the project website and app-store before to be made available to

the whole community (SOLEIL, UCAM, OXFORD). IT tests will be performed, with each partner adding data that will be tested online and approved by the WP8 working groups (CNRS, UCAM). Each key person identified in the WPs where data is generated will be in charge to ensure that standards and protocols are respected, as well as to inform the working groups creating in Task 8.2 of any difficulty encountered.

Task 8.4: Organization of European platforms for battery testing
Task leader: CNRS; Partners involved: SOLEIL, UU; M24-M36
Having established the standards and protocols that will support the creation of the Battery Interface Genome (WP11), these standards and protocols will be extended to the creation of a European certification for battery performances that will allow research laboratories to certify their results (CNRS, UU, SOLEIL). For that, already existing upscaling pre-industrialization platforms will be made open (CNRS/RS2E platform for instance), and protocols in terms of cell assembly and battery testing established in Task 8.1 will be used. Furthermore, these standards can be transferred to the relevant standardization committees such as CENELEC/TC 21X, IEC/TC 21 or ISO/TC 22/SC 37. Creating such platforms will allow not only for partners of the consortium to validate their findings, but also to partners outside of the consortium to obtain a European certification platform that will be recognized by the different stakeholders of the BIG-MAP (CNRS, UU).

Participation per Partner

Partner number and short name	WP8 effort
2 - UU	12.00
4 - CNRS	93.00
17 - UCAM	12.00
18 - UOXF	15.00
21 - ESRF	11.00
22 - ILL	12.00
23 - SOLEIL	12.00
28 - BASF	1.50
Total	168.50

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D8.1	Initial templates for standards and protocols completed	4 - CNRS	Report	Confidential, only for members of the consortium (including the Commission Services)	6
D8.2	DOI format for samples exchange made available online for the whole consortium	4 - CNRS	Other	Confidential, only for members of the consortium (including the Commission Services)	6
D8.3	Release of updated standards and protocols following the working group meeting at M6	1 - DTU	Report	Confidential, only for members of the consortium (including	6

DRAFT

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
				the Commission Services)	
D8.4	Update of standards and protocols following the working group meeting at M18	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D8.5	Update of standards and protocols following the working group meeting at M30	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	30
D8.6	Online data analysis tools made available to the consortium	4 - CNRS	Other	Confidential, only for members of the consortium (including the Commission Services)	12
D8.7	Online data analysis tools made available to the whole community	4 - CNRS	Websites, patents filling, etc.	Public	36
D8.8	First European platform open to researchers/ industries outside of the consortium where batteries can be tested following the tests protocols defined in BIG-MAP	4 - CNRS	Websites, patents filling, etc.	Public	36

Description of deliverables

D8.1: Templates for standards and protocols (CNRS, M6)
D8.2: DOI format for samples exchange made available online for the whole consortium (CNRS, M6)
D8.3: Update of standards and protocols following the working group meeting at M6 (SOLEIL, M6)
D8.4: Update of standards and protocols following the working group meeting at M18 (SOLEIL, M18)
D8.5: Update of standards and protocols following the working group meeting at M30 (SOLEIL, M30)
D8.6: Report for meeting of each working groups (SOLEIL, M12)
D8.7: Online tools made available to the whole community (CNRS, M36)
D8.8: First European platform open to researchers/industries outside of the consortium where batteries can be tested following the tests protocols defined in the BIG-MAP (CNRS, M36)

D8.1 : Initial templates for standards and protocols completed [6]

The initial templates for standards and protocols has been submitted.

D8.2 : DOI format for samples exchange made available online for the whole consortium [6]

DOI format for samples exchange made available online for the whole consortium.

D8.3 : Release of updated standards and protocols following the working group meeting at M6 [6]

Release of updated standards and protocols following the working group meeting at M6.

D8.4 : Update of standards and protocols following the working group meeting at M18 [18]

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Update of standards and protocols following the working group meeting at M18.

D8.5 : Update of standards and protocols following the working group meeting at M30 [30]

Update of standards and protocols following the working group meeting at M30.

D8.6 : Online data analysis tools made available to the consortium [12]

Online data analysis tools made available to the consortium.

D8.7 : Online data analysis tools made available to the whole community [36]

Online data analysis tools made available to the whole community.

D8.8 : First European platform open to researchers/industries outside of the consortium where batteries can be tested following the tests protocols defined in BIG-MAP [36]

First European platform open to researchers/industries outside of the consortium where batteries can be tested following the tests protocols defined in BIG-MAP.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS13	M8.1: Creation of standards	4 - CNRS	6	The parameters for standards are battery cycling, characterization (large- and laboratory scale), and modelling at several scales made available online for the battery community. Associated risk R8.1.

DRAFT

Work package number [9]	WP9	Lead beneficiary [10]	16 - EPFL
Work package title	Infrastructure and Interoperability		
Start month	1	End month	36

Objectives

The goal of WP9 is to develop the infrastructure and the capabilities (software infrastructure, simulation control, experimental control, and data interoperability) leading to automated simulations and experiments, to access these capabilities and data, and to have simulations and experiments communicate to each other, demonstrating the capability of a simulation to request the execution of an experiment, and for an experiment to request the execution of a simulation. This goal is achieved through the completion of the five tasks outlined below. In addition, this WP will closely interact with WP2 and WP3, for sample definition and reproducibility, with WP5 for sample characterization, with WP7 and WP8 for standards for data and interfaces, with WP2, for automatic generation of neural networks, and with WP11 for data fidelity and complex deep learning simulation tools.

Description of work and role of partners

WP9 - Infrastructure and Interoperability [Months: 1-36]
EPFL, DTU, UU, KIT, CEA, CTH, TUD, CNR, ESRF, ILL, SOLEIL, SOLB, 3DS
Task 9.1: Robust and reliable workflows for automated simulations
Task leader: EPFL; Partners involved: CNR, UU, KIT, DTU, 3DS; M1-M36
This task will focus on the development of the workflows for automated calculations ("turnkey solutions") to allow for the determination of, e.g., the crystal structure of parts of a battery system at both zero and finite temperature. Examples include an atomistic model of a bulk electrolyte; a more complex example would be a model of the SEI (EPFL, UU, DTU, 3DS) and the calculation of relevant properties (CNR, EPFL), e.g., vibrational spectra (Raman, infrared, UVvis absorption), predicted X-ray or neutrons diffraction patterns; the latter such that they be comparable to experimental results from LSFs (e.g. spectroscopy, tomography, neutron depth profiling/imaging) in WP5. The resulting open source apps and workflows will be made available to the community in the BIG-MAP App-store in collaboration with other EU initiatives, such as the Market Place initiatives.

Task 9.2: Integration of the computational platforms
Task leader: EPFL; Partners involved: DTU, KIT, 3DS; M1-M36
AiiDA and ASE will act as the open-source software infrastructure to develop workflow tools and simulation services, to interoperate with open or proprietary codes and to store simulation data. Partners will develop robust workflows for the different quantum, atomistic, finite-element, and/or continuum simulations engines (from VASP to GPAW to Quantum ESPRESSO to 3DEXPERIENCE Platform). SimStack, which uses AiiDA as a computational backend, will provide remote access to proprietary data sets and simulation protocols. Integration of AiiDA and ASE will be performed by EPFL, DTU and the connection to the 3DEXPERIENCE Platform will be performed by 3DS; while the integration of SimStack will be performed by KIT and EPFL.

Task 9.3: Development of a software framework for data management, linkage and protection
Task leader: KIT; Partners involved: CTH, DTU, EPFL, CEA, SOLB; M1-M18
This task will establish a data management framework for BIG-MAP for data generated in experiments, in close collaboration with Task 9.2 on simulations (KIT, CTH, DTU, EPFL). The overarching goal is to adapt existing software frameworks like AiiDA and closely collaborate with external (national and international) initiatives like "Material Digital" (BMBF, Germany). The resulting framework should enable participants to make proprietary data available to defined groups in the community without the need to deposit the raw data into publicly accessible databases. In this task demonstrators for such access protocols shall be developed. This task aims to deploy a software framework for data management in materials research based on the AiiDA framework. Adaptions for experiments will mostly involve in the deployment of nodes that accept multiple runs and deal with common many-to-many associations in materials experimentation. To allow for facile data exchange with IP awareness there will be a hybrid data storage approach. Users may either store data on-premises or in the cloud and decide if the entire raw or only analysed data is shared, and there will be an interface for starting a simulation or experiment based on altered parameters from lineage tracking externally given access rights.
Task 9.4: Deployment of a cloud platform for automated simulations and data access
Task leader: EPFL; Partners involved: DTU, KIT; M1-M36

Development and deployment of a cloud computing platform to perform simulations/characterization, where the workflows developed are preinstalled and ready to be used (EPFL, KIT, DTU). This platform allows researchers to transparently connect to HPC resources, run workflows in the cloud and automatically track the provenance. The connection with the experimental platforms will also allow users to automate simulations started from the lineage tracked in experiments, and will serve as the platform for the demonstrators of Task 9.5. The UI will be based on Jupyter, Jupyter Lab and/or SimStack, together with the app-mode plugin to have an app-like interface to workflows and simulations. The infrastructure will be a) deployed on a central server, and to be accessed by the members of the BIG-MAP consortium, as a central simulation hub for the project/Battery2030+; and b) deployment will be automated via ansible scripts to automate the installation and re-deployment of the whole infrastructure in a different computer centre (e.g. on bare-metal machines, using a virtualization technology like OpenStack, or on an autoscaling kubernetes cluster supporting an arbitrarily large number of users). The goal is to make it straightforward to redeploy the same infrastructure in each institution part of BIG-MAP and to make these platforms interoperable. Such a platform will accelerate interaction between theory and experiments and discovery of novel well as centralize data stewardship and management, guarantee reproducibility, remove the bottlenecks for researchers related to installation and infrastructure management, and facilitate access to data and HPC/HTC resources, as well as understanding and analysis of data.

Task 9.5: Integration of automated experiments and automated simulations
Task leader: CTH; Partners involved: 3DS, SOLEIL, ILL, ESRF, TUD, SOLB, CEA; M1-M18
This task is focused on the key demonstrator (KD8) of a feedback loop between experiments and computation. Core deliverables of the project will be demonstrators of automated capabilities to perform a simulation on demand – for a simulation to request an experiment, and for an experiment to request a simulation, towards a complete integration with lab- and large-scale facilities (WP5 and WP10). This task will start with the definition of simulation and experimental platforms for the integration in the demonstrator (CTH, TUD, 3DS, SOLEIL, ILL, ESRF), and proceeds with the development of interface for data management between simulation and experimental platforms (3DS, CTH, TUD, SOLEIL, CEA) up to the validation of demonstrator (CTH, TUD, 3DS, SOLEIL, ILL, ESRF, SOLB).

Participation per Partner

Partner number and short name	WP9 effort
1 - DTU	12.00
2 - UU	12.00
3 - KIT	14.00
6 - CEA	1.00
11 - CTH	9.00
14 - TUD	6.00
15 - CNR	12.00
16 - EPFL	42.00
21 - ESRF	6.00
22 - ILL	6.00
23 - SOLEIL	14.00
27 - SOLB	3.00
32 - 3DS	23.00
Total	160.00

DRAFT

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D9.1	Prototype of the BIG-MAP App-store	3 - KIT	Websites, patents filling, etc.	Public	6
D9.2	Automated workflows linking experiments and modelling for representative samples of battery materials	16 - EPFL	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D9.3	Integrated AiiDA, ASE, SimStack platform	16 - EPFL	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D9.4	Proprietary data management framework capable of ingesting data from materials experiments (e.g. data from high-throughput experimentation, or a materials library)	3 - KIT	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D9.5	Updated BIG-MAP App-store	16 - EPFL	ORDP: Open Research Data Pilot	Public	36
D9.6	Demonstrator of a simulation run by an experiment, and an experiment run by a simulation	11 - CTH	Demonstrator	Public	36

Description of deliverables

D9.1: Prototype of the BIG-MAP App-store (KIT, M6)
D9.2: Automated workflows linking experiments and modelling for representative samples of battery materials (EPFL, M18)
D9.3: Integrated AiiDA, ASE, SimStack platforms (EPFL, M18)
D9.4: Proprietary data management framework capable of ingesting data from materials experiments (e.g. data from high-throughput experimentation, or a materials library) (KIT, M24)
D9.5: Updated BIG-MAP App-store (EPFL, M36)
D9.6: Demonstrator of a simulation run by an experiment, and an experiment run by a simulation (CTH, M36)

D9.1 : Prototype of the BIG-MAP App-store [6]

Prototype of the BIG-MAP App-store developed.

D9.2 : Automated workflows linking experiments and modelling for representative samples of battery materials [18]

Report/paper submitted on automated workflows linking experiments and modelling for representative samples of battery materials.

D9.3 : Integrated AiiDA, ASE, SimStack platform [18]

Report/paper submitted on integrated AiiDA, ASE, SimStack platform.

DRAFT

D9.4 : Proprietary data management framework capable of ingesting data from materials experiments (e.g. data from high-throughput experimentation, or a materials library) [24]

Proprietary data management framework capable of ingesting data from materials experiments (e.g. data from high-throughput experimentation, or a materials library).

D9.5 : Updated BIG-MAP App-store [36]

Launch of updated BIG-MAP App-store, including tools providing access to Open Data from the project deposited in the Materials Cloud repository.

D9.6 : Demonstrator of a simulation run by an experiment, and an experiment run by a simulation [36]

Demonstrator of a simulation run by an experiment, and an experiment run by a simulation.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS3	M3.2: Integration of multi-scale workflow	3 - KIT	32	The workflow is integrated in BIG-MAP App-store into WP9. Associated risk R3.2.
MS14	M9.1: Successful delivery of automated integrated workflow	16 - EPFL	18	The workflow enable the creation of microscopic representative sample of battery materials. Associated risk R9.1.

DRAFT

Work package number [9]	WP10	Lead beneficiary [10]	3 - KIT
Work package title	AI Accelerated Materials Discovery		
Start month	1	End month	36

Objectives

This work package seeks to implement a sub-framework to accelerate materials discovery and optimization both in experiments and in silico through close collaboration with various connected WPs. This cross-cutting initiative mainly provides the technology and implementation of sequential (active) learning methods, automated analysis and reasoning to accelerate materials experiments (WP6), synthesis routes, and simulations (WP2 and WP3). To minimize uncertainty in building the battery interphase genome (BIG), WP11 will directly interface with the expertise in ML/DL methods.
AI-accelerated materials discovery, in close collaboration with WP2, WP3, WP9 and WP11, is envisioned to be primarily enabled through active learning (Task 10.1) that is utilized as an accelerator to identify the optimal conditions for the next experiment/simulation to run. This requires a latent space representation of materials and experimental results that will be mainly developed in WP11 and deployed in this work package as Task 10.3. Latent space representations in turn require automated analysis of experimental results (Task 10.2). To accelerate discovery in a semi-autonomous mode and to unravel new insights, select ML models will be analysed (Task 10.3) such that researchers can extract new insights. A first demonstration of an automated reasoning agent (Task 10.4) will be demonstrated in a self-calibrating tiered screening pipeline. Communication across different modules, tasks and groups will require a partially centralized data management framework as developed in WP9. Data management and lineage tools will be developed in WP9 and deployed in this work package to enable reproducible ML in materials science.

Description of work and role of partners

WP10 - AI Accelerated Materials Discovery [Months: 1-36]
KIT, DTU, Fraunhofer, ULIV, CID, UMI, SOLB, BASF, NVOLT, ITU, FZJ
Task 10.1: Accelerating experiments with active learning
Task leader: KIT; Partners involved: ULIV, ITU, BASF, NVOLT, FRAUNHOFER, FZJ; M1-M18
The aim of this task is to develop and implement AI/ML algorithms to efficiently sample the chemical search-space thorough iterative guidance. The approach to be developed principally by KIT, with contributions from ULIV and ITU, is based on the active learning paradigm, whereby the predictions and uncertainties from a model, serve as the input to define an acquisition function. The development and deployment of these models happens in close collaboration with WP2 and WP11, especially Task 2.3 and Task 11.4. The goal is to improve material and model performance in the long run, i.e., learning from and guiding the experiments. Experimental guidance will happen through collaboration with WP4 and WP6 through interfaces developed in WP9. This task therefore implements learning methods to select the optimal subsequent experiment or simulation to run. This task will survey different viable ML algorithms to construct an acquisition function and determine viable research modes. Active learning will be deployed to characterization robots (KIT, FZJ) and synthesis robots (FRAUNHOFER), but also linked to atomic scale simulation methods as an accelerator (WP2). Participants will demonstrate the capability of active learning to accelerate select research tasks. Within this task uncertainty calibration will be used to differentiate aleatoric and epistemic uncertainty. As demonstrators several high-throughput instruments will be accelerated or methods deployed (BASF, NVOLT) and synthesis paths optimized.

Task 10.2: An automated data analysis framework
Task leader: ULIV; Partners involved: KIT, BASF, DTU, FZJ, NVOLT; M1-M24
To enable all of the above tasks there is a critical need for an automated data analysis framework. This analysis framework is led by ULIV with contributions from KIT needs to be able to perform routine analyses (performed by KIT, BASF, NVOLT, FZJ, ULIV) of battery related research data and generate figures of merit (FOM) with provenance tracking. As algorithms will evolve over time, this task seeks to deploy an analysis framework that can function on demand and re-analyse relevant data with minimal user input. For the ramp up phase, this task will focus on FOM extraction and easy to implement experiment embeddings with similar functional capabilities like CombIGOR, JCAPDataProcess but the automation level of Crystal.AI. This task will closely corporate with WP6 to remove potential bottlenecks in the data analysis from high-throughput synthesis, characterization, and performance evaluation. There is also a critical need to align data sharing standards with WP4 and deploy data lineage tracking as well as a strong collaboration with WP5, WP6 and WP9. As a demonstrator pertinent spectroscopic and electrochemical data will be automatically analysed to be used in experiment embeddings. Development will be aligned to simulation efforts by DTU and partners in Tasks 2.5, 5.4 and 9.5.

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Task 10.3: Transfer learning and new fundamental insights
Task leader: DTU; Partners involved: KIT, ULIV, CID, KIT; M1-M24
This task will deploy the dynamic interface descriptors identified by DTU and partners in WP11 (Task 11.1). The task is co-led by KIT with contributions from ULIV to deploy the descriptors in the experimental (CID) and simulation (KIT, DTU) model systems. The focus is hereby on the implementation, i.e., the deployment of an software interface for the interlinking of latent spaces across simulations and experiments into the active learning algorithms, validation and feedback scheme. The goal is to aid the ML model building and accelerate explainable AI by supplying pertinent information through transfer learning. This task will therefore also critically verify embeddings for materials, formulations, and experiments.

Task 10.4: Automatic reasoning and materials funnel
Task leader: KIT; Partners involved: UMI, BASF, SOLB, DTU, FZJ, FRAUNHOFER, NVOLT; M1-M36
A KIT lead materials funnel (tiered screening pipeline) within BIG-MAP will bundle several WPs (WP2, WP3, WP4, WP5 and WP6), in the identification of top performing electrolyte formulations and the resulting interphase synthesis. Within a material funnel, a series of tiers exist that evaluate a materials or device performance. Within each tier a set of criteria exists that decide whether a material succeeds to the next tier. This task would aid in the construction of a materials funnel by focusing on the organizational aspect, i.e., by deciding the criteria to be met at each tier. After an initial pass, this task would adjust rules in an interactive way and thus be "self-calibrating" similar to a gradient booster. A demonstrator of this task is the organization of a small tiered screening pipeline for electrolyte components. The tiered screening pipeline acts as a fallback demonstrator ingesting data from WP2 and WP3 (DTU) to guide electrolyte formulation (FRAUNHOFER, SOLB) select electrodes (BASF) and perform subsequent experiments (KIT, FZJ) with possible deployment to NVOLT to evaluate the entire value chain of BIG-MAP.

Participation per Partner

Partner number and short name	WP10 effort
1 - DTU	24.00
3 - KIT	57.00
10 - Fraunhofer	3.00
20 - ULIV	38.00
24 - CID	12.00
26 - UMI	4.00
27 - SOLB	5.00
28 - BASF	3.00
29 - NVOLT	8.00
31 - ITU	4.00
33 - FZJ	12.00
Total	170.00

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D10.1	Active learning package/ module demonstrated to work on pre-	3 - KIT	Demonstrator	Public	18

DRAFT

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
	generated simulation or experimental data sets				
D10.2	Modular package for analysis of pertinent spectroscopic data and electrochemistry	20 - ULIV	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D10.3	Demonstration of linking active learning accelerated HTS and simulations	1 - DTU	Report	Confidential, only for members of the consortium (including the Commission Services)	18
D10.4	Tiered theory and experiment screening pipeline as first test case for automatic reasoning calibration	3 - KIT	Report	Public	36

Description of deliverables

D10.1: Active learning Package/Module working on pre-generated simulation or experimental data sets (KIT, M18)
D10.2: Modular package for analysis of pertinent spectroscopic data and electrochemistry (ULIV, M24)
D10.3: Demonstration of linking active learning accelerated HTS and simulations (DTU, M24)
D10.4: Tiered theory and experiment screening pipeline as first test case for automatic reasoning calibration (KIT, M36)

D10.1 : Active learning package/module demonstrated to work on pre-generated simulation or experimental data sets [18]

Active learning package/module demonstrated to work on pre-generated simulation or experimental data sets.

D10.2 : Modular package for analysis of pertinent spectroscopic data and electrochemistry [24]

Modular package for analysis of pertinent spectroscopic data and electrochemistry developed.

D10.3 : Demonstration of linking active learning accelerated HTS and simulations [18]

Demonstration of linking active learning accelerated HTS and simulations.

D10.4 : Tiered theory and experiment screening pipeline as first test case for automatic reasoning calibration [36]

Report/paper on tiered theory and experiment screening pipeline as first test case for automatic reasoning calibration.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS15	M10.1: Successful delivery of active learning algorithm	3 - KIT	12	The working algorithm is working in synthetic (or simulated) data set. Associated risk R10.1.
MS16	M10.2: Demonstrate Figure Of Merit (FOM) extraction	3 - KIT	24	The FOM extraction are successful for selected

DRAFT

Schedule of relevant Milestones				
Milestone number[18]	**Milestone title**	**Lead beneficiary**	**Due Date (in months)**	**Means of verification**
				analyses from WP3/WP6 robots using modular analysis package. Associated risk R10.2.

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Work package number [9]	WP11	Lead beneficiary [10]	1 - DTU
Work package title	Battery Interface Genome		
Start month	1	End month	36

Objectives

WP11 seeks to unite the scientific results and approaches developed in the competence WPs: 2, 3, 5, 6 and the cross-cutting WPs: 7, 8, 9 and 10, to establish predictive deep learning based Battery Interface Genome models for (inverse) design and characterization of battery interfaces and interphases. The BIG-models will combine the spatio-temporal characterization of the interfaces with physics- and data-driven generative models to predict dynamic events at multiple time and length scales, e.g. from the atomic scale to the micron scale. WP11 will develop and utilize hierarchical latent variable generative models to integrate the fundamental "genomic" knowledge of battery interfaces and interphases through time, space and chemistries, e.g., in connection with WP3 (Task 3.2). When focusing on interfaces and interphases, one can ensure the transfer of useful information across different chemistries (Task 11.5) by developing a platform to measure, understand and rationalize the different processes occurring from the atomic/molecular to the materials/interface scale. Identification of the multitude of descriptors (or genes) coding for the spatio-temporal evolution of battery interfaces is a prerequisite for inverse design process, which simply cannot be established within existing methodologies. The BIG-models developed in WP11 will lay the groundwork for establish a fully predictive framework for linking the chemical composition of the battery interface and 3D-resolved morphologies, porosity, tortuosity, as a function of time, capturing the impact of their evolution on, e.g., electrochemical response, stability and capacity fading.

Description of work and role of partners

WP11 - Battery Interface Genome [Months: 1-36]
DTU, KIT, CNRS, NIC, CSIC, CNR, UCAM, UOXF, ESRF, CID, UMI, UNIBAS, 3DS
Task 11.1: Integration of multi-fidelity data from all domains
Task leader: ESRF; Partners involved: 3DS, CNR, CNRS, CSIC, DTU, KIT, Oxford; M1-M18
The successful development of the BIG models relies extensively on BIO (WP7) and standards (WP8), as well as the holistic data infrastructure developed in WP7 and WP9, respectively. Deep learning models are particularly well suited to optimize data collection and building bridges between the data sets, helping to solve the biggest challenges of battery interphases. Ideally, the ML algorithms should be fed large data sets from high-fidelity simulations and high-fidelity experiments. However, high-fidelity data is often very expensive and/or time-consuming to obtain and consequently scarce. Integrated multi-scaling approaches, e.g. through hierarchical latent space generative models (Task 11.3), requires curated interlinked data on the structure of the interphases over broad range of time- and length-scale. This task focuses the development on capabilities for multi-scale modelling, (WP2 and WP3), AI and systematic multi-modal characterization of battery interfaces, including operando characterization (WP5), to generate/collect comprehensive sets of high-fidelity data that will feed a common AI-orchestrated data-infrastructure in the MAP. A central element is to know which experimental or computational technique can provide the most relevant/pertinent data at the lowest cost (in terms of time and/or resources) for optimizing the model. At certain times, large, low-cost data set with moderate-to-low fidelity can be more useful in improving the predictive accuracy and lowering uncertainties than a limited, high-cost/high-fidelity data set, e.g., in highly sparse and unexplored regions of parameter space, and vice versa. The goal of this task is to demonstrate integration of multi-fidelity data from simulations, experimental characterization, testing to create a unified description of chemical and spatio-temporal evolution of the battery interface in a cost effective manner. ESRF will lead the experimental fidelity activities, with support from Oxford and CNRS, while CSIC will lead the computational efforts with support from 3DS, CNR, DTU and KIT.

Task 11.2: Dynamic interface/interphase descriptors
Task leader: DTU; Partners involved: UCAM, CNRS, KIT, Oxford; M6-M24
BIG is closely related to the concept of descriptors in catalyst design, where the binding energy of important reaction intermediate scale with that of other intermediates and thus becomes the descriptor for the catalyst activity. The identification and quantification of optimal binding energy enables an inverse search for better catalysts. Identifying the multitude of descriptors or genes that encode the spatio-temporal evolution of battery interfaces and interphases is a prerequisite for inverse design process. To make the descriptor discovery process semi-autonomous, semi-supervised deep learning will be used to cluster battery interphase into groups with similar performance defining physical processes. This is followed by identification of the physical descriptors, using existing data points within the group for which

reliable information exists. Infusion of domain knowledge through predefined chemical and physical variables is utilized to make the ML framework more data efficient. Furthermore, it helps to create and disseminate battery design principles at different scales at accelerated pace, by keeping the ML framework explainable. The goal of this task is to use the data from Task 11.1 and develop methods to autonomously identify dynamic interface/interphase descriptors. DTU will lead the method development for automated feature/descriptor identification with support from KIT, while UCAM, CNRS and Oxford will perform the experimental validation and testing needed. Transfer of pertinent descriptors to WP10 (Task 10.3) for accelerated discovery will also be performed.

Task 11.3: Hierarchical latent space multi-scale models
Task leader: DTU; Partners involved: 3DS, UBAS, CID, CSIC, KIT; M12-M30
The goal of this task is to develop a novel ML methodology for modelling time evolution of dynamic systems simultaneously at multiple time and length scales with a unified approach using hierarchical latent variable models (Figure 1.8). This task leads to generative deep learning models for the prediction of interface structures that utilizes computational and experimental data spanning multiple time- and length-scale for model training and aims to achieve parameterization-free bridging of scales.
A generative model is a probabilistic model for the data features we have access to. For example, as an atomic (interface) structure generator, the model should capture the probability distribution over all the possible atomic configurations and allow the generation of new structures from this distribution. Real space variables such as atomic coordinates are not completely independent of each other due to restrictions imposed by physical laws. It is therefore efficient to represent such data in the latent space. A successful deep generative latent variable model is the Variational Autoencoder (VAE). In this task, we will introduce the concept of hierarchical latent space models, which can represent features from different scales in multiple - but interconnected - latent spaces, which is needed for consolidated encoding of interphase evolution data that encompass wide range of time- and length-scale. Task 11.3 will use coupled encoders/decoders for the hierarchical latent space encoding of materials system information across scales (atomic to macro), enabling parameterization-free, multi-scale simulation and integrated design according to the target properties of the interface. Multi-scale characterization data obtained from the BIG-MAP databases will be utilized for hierarchical latent space model development. DTU will lead the hierarchical latent space model development with support from complementary internal activities, UBAS, 3DS and in particular KIT to ensure the direct link to Task 3.3 (AI enhanced models). These models will be validated experimentally by data gathered by CID and from the BIG-MAP databases.

Task 11.4: Uncertainty-guided spatio-temporal models
Task leader: DTU; Partners involved: UBAS, CNR, CSIC, KIT; M15-M36
In silico interface design requires tight bounds on the predictive uncertainty of the models and the underlying data sources. The ability to draw conclusions and make predictions while working with uncertain data is a vital aspect of the developed BIG-MAP framework, given the vast complexity of interface evolution across scales. Methods and workflows for autonomous uncertainty quantification and error correction therefore play a critical role in enabling prediction of the spatio-temporal evolution of battery interfaces and interphases. Such uncertainties stem from the generative deep learning model, but also from the training data gathered though characterization experiments and physical simulations (Task 11.1). Uncertainty propagation methods integrated within the probabilistic latent space generative models will be used to provide predictive uncertainties that take into account both data and model uncertainties. The goal of this task is to develop a unique framework comprising self-correcting unsupervised deep models for uncertainty-aware predictions. Clarity on sources of uncertainty within the models provide the basis for autonomous selection of additional training data generation effort through experiments and physical simulations such that high level of data efficiency is achieved. Additionally, within this task, we will build and validate the critical components of a system that autonomously predicts interfacial reactions and structure evolution, e.g., from a graph neural network model, and automatically identifies and corrects uncertainty and errors in the modelled and experimental data. The model should be able to track the propagation of uncertainty through all steps of the predictive modelling of the dynamic evolution of battery interfaces. DTU will lead the actual model development and ultilize synergy with the existing project SURE, while UBAS, CNR, CSIC and KIT will focus on methods for uncertainty quantification in the training data at different scales.

Task 11.5: Transferability of developed methodology to other materials
Task leader: CID; Partners involved: Oxford, NIC, CNRS, CSIC, DTU, UMI; M21-M36
This task is dedicated to the demonstration and testing of the versatility and transferability of the developed methodologies, e.g. Task 11.3, to a novel chemistry and/or structure of active materials or electrolyte (KD12). The transferability of the methodologies developed within BIG-MAP framework will be transferred from the investigated lithium-based batteries to other monovalent and multivalent system, more specifically to divalent batteries. The main objective of this task is to perform the initial testing of whether the developed methodologies can be utilized in combination with other (multivalent) metal anodes. This task will provide directions for upgrading the developed methodologies in future projects, towards a general scheme applicable for different types of interfaces/interphases in

all electrochemical storage systems. CID, CNRS and Oxford will lead the testing activities on Na-ion, NIC and CSIC will transfer developed solutions and test them in the combination with magnesium and calcium electrodes, while DTU and UMI will focus on the general transferability of the models.

Participation per Partner

Partner number and short name	WP11 effort
1 - DTU	51.00
3 - KIT	14.00
4 - CNRS	6.00
UPJV	2.00
7 - NIC	12.00
13 - CSIC	18.00
15 - CNR	5.00
17 - UCAM	6.00
18 - UOXF	22.00
21 - ESRF	12.00
24 - CID	24.00
26 - UMI	2.00
30 - UNIBAS	6.00
32 - 3DS	12.00
Total	192.00

List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
D11.1	Initial model for dynamic fidelity assignment	21 - ESRF	Report	Confidential, only for members of the consortium (including the Commission Services)	12
D11.2	Identification of interphase descriptor dynamics for test system	1 - DTU	Report	Public	18
D11.3	Multi-scale representation of interface with scale bridging descriptors from simulation and experimental data	1 - DTU	Other	Confidential, only for members of the consortium (including the Commission Services)	24
D11.4	1st generation uncertainty-guided	1 - DTU	Other	Confidential, only for members of the	32

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List of deliverables

Deliverable Number[14]	Deliverable Title	Lead beneficiary	Type[15]	Dissemination level[16]	Due Date (in months)[17]
	hybrid physics- and data-driven model of battery interfaces			consortium (including the Commission Services)	
D11.5	Demonstrate transfer of select model(s) to novel battery materials/ chemistry	24 - CID	Demonstrator	Public	36

Description of deliverables

D11.1: Initial model for dynamic fidelity assignment (ESRF, M12)
D11.2: Identification of interphase descriptor dynamics for test system (DTU, M20)
D11.3: Multi-scale representation of interface with scale-bridging descriptors from simulations & experiments (DTU, M24)
D11.4: Demonstration of an uncertainty-guided hybrid physics- and data-driven battery model (DTU, M32)
D11.5: Demonstrate transferability of select model(s) to novel battery materials/chemistry (CID, M36)

D11.1 : Initial model for dynamic fidelity assignment [12]

Report/paper submitted on the Initial model for dynamic fidelity assignment.

D11.2 : Identification of interphase descriptor dynamics for test system [18]

Report/paper on the identification of interphase descriptor dynamics for test system.

D11.3 : Multi-scale representation of interface with scale bridging descriptors from simulation and experimental data [24]

Multi-scale representation of interface with scale bridging descriptors from simulation and experimental data.

D11.4 : 1st generation uncertainty-guided hybrid physics- and data-driven model of battery interfaces [32]

1st generation uncertainty-guided hybrid physics- and data-driven model of battery interfaces developed.

D11.5 : Demonstrate transfer of select model(s) to novel battery materials/chemistry [36]

Demonstration of transfer of select model(s) to novel battery materials/chemistry completed.

Schedule of relevant Milestones

Milestone number[18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS17	M11.1: Successful completion of a latent space multi-scale model	1 - DTU	30	The multi-scale model enable hierarchical scale-bridging in latent space. Associated risk R11.1.
MS18	M11.2: Concept of uncertainty-guided hybrid data-driven and physical model demonstrated	1 - DTU	32	Delivery of the 1st generation of hybrid physics- and data-driven model of battery interfaces. Associated risk R11.2.

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1.3.4. WT4 List of milestones

Milestone number[18]	Milestone title	WP number[9]	Lead beneficiary	Due Date (in months)[17]	Means of verification
MS1	M2.1: Delivery of full protocol to achieve the exploration of chemical space for selected battery systems	WP2	2 - UU	12	The protocol is delivered from full QM data set and force field available. The delivery on time of D2.3 is the mean of verification. Associated risk R2.1.
MS2	M3.1: Incorporation of an AI-enhanced multi-scale model into the workflows of Task 3.1	WP3	3 - KIT	24	The correct incorporation of the AI-enhanced model is validated by the ability to run simulations in production mode. Associated risk R3.1.
MS3	M3.2: Integration of multi-scale workflow	WP3, WP9	3 - KIT	32	The workflow is integrated in BIG-MAP App-store into WP9. Associated risk R3.2.
MS4	M4.1: Specifications are defined	WP4	10 - Fraunhofer	6	Material classes and interfaces to AI materials discovery, decision-making authority and handling of data are all defined and available at M6. Associated risk R4.1.
MS5	M4.2: Hardware integrated and software architecture developed	WP4	10 - Fraunhofer	30	The integration of hardware and development of architecture is validated by the installation of robotic system for synthesis including sensors (D4.2). Associated risk R4.2.
MS6	M5.1: State-of-the-art experimental matrix completed	WP5	6 - CEA	6	Confirmation that the state-of-the-art is delivering all available parameters available in the literature for the matrix: scales, resolutions, operando mode, availability, etc. Associated risk R5.1.
MS7	M5.2: Technical implementation of the Demonstrator workflow (KD4)	WP5	6 - CEA	12	Framework for the running of coordinated multi-techniques experiments to acquire multi-scale data is operational. Associated risk R5.2.
MS8	M6.1: Establish and validate HTS assay and testing methodology for liquid electrolyte-based lithium batteries	WP6	33 - FZJ	12	The methodology enable optimization in electrolyte formulation, preparation of inorganic coatings, selected characterization and analysis. Associated risk R6.1.
MS9	M6.2: Establish interface between the	WP6	33 - FZJ	18	The HTS is deployed experimentally including AI orchestration to obtain raw

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Milestone number[18]	Milestone title	WP number[9]	Lead beneficiary	Due Date (in months)[17]	Means of verification
	HTS systems and AI orchestration				results to enable analyses for data lineage tracking. Associated risk R6.2.
MS10	M6.3: Critical review of the different methodologies and proposed evolution directions	WP6	33 - FZJ	24	The SEI/CEI investigations enable decisions on the optimum high throughput electrochemistry for neutral lithium-based chemistry. Associated risk R6.3.
MS11	M7.1: Consistent representative description of battery interface ontology	WP7	8 - SINTEF	6	A survey sent to relevant WP members to determine if the BIO is being adopted and provides value. Associated risk R7.1.
MS12	M7.2: Integration with BIG-MAP AI and database platforms	WP7	8 - SINTEF	21	Successful operation of a case study of the critical battery interfaces identified in the project. Associated risk R7.2.
MS13	M8.1: Creation of standards	WP8	4 - CNRS	6	The parameters for standards are battery cycling, characterization (large- and laboratory scale), and modelling at several scales made available online for the battery community. Associated risk R8.1.
MS14	M9.1: Successful delivery of automated integrated workflow	WP9	16 - EPFL	18	The workflow enable the creation of microscopic representative sample of battery materials. Associated risk R9.1.
MS15	M10.1: Successful delivery of active learning algorithm	WP10	3 - KIT	12	The working algorithm is working in synthetic (or simulated) data set. Associated risk R10.1.
MS16	M10.2: Demonstrate Figure Of Merit (FOM) extraction	WP10, WP3, WP6	3 - KIT	24	The FOM extraction are successful for selected analyses from WP3/WP6 robots using modular analysis package. Associated risk R10.2.
MS17	M11.1: Successful completion of a latent space multi-scale model	WP11	1 - DTU	30	The multi-scale model enable hierarchical scale-bridging in latent space. Associated risk R11.1.
MS18	M11.2: Concept of uncertainty-guided hybrid data-driven	WP11, WP3	1 - DTU	32	Delivery of the 1st generation of hybrid physics- and data-driven model of battery

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Milestone number[18]	Milestone title	WP number[9]	Lead beneficiary	Due Date (in months)[17]	Means of verification
	and physical model demonstrated				interfaces. Associated risk R11.2.

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1.3.5. WT5 Critical Implementation risks and mitigation actions

Risk number	Description of risk	WP Number	Proposed risk-mitigation measures
1	R1.1: A partner is leaving consortium during the project. Risk level = (S: severity and P: probability arising; 1 is low and 3 is high): (1*1) = 1	WP1	BIG-MAP is designed to cover the whole value chain of battery discovery in Europe, including several key partners per segment of value chain. The activities left by the leaving partner will be reassigned by the coordinator in agreement with WP leaders involved.
2	R2.1: Failure to deliver a full protocol. Risk level (3*1) = 1	WP2	The a priori check on QM data and FF will enable tracking of delays. Extra resources will be assigned if needed to deliver the full protocol on time.
3	R3.1: Failure to close a gap in the model spectrum because of lack of predictive power in the AI enhanced model. Risk level (2*2) = 4	WP3	The development period for AI enhanced model will be extended to reach predictive power.
4	R3.2: Lack of integration tools to execute heterogeneous workflows on the BIG-MAP computational infrastructure. Risk level (2*1) = 2	WP3	The heterogeneous workflows will be run with minimal integration tools.
5	R4.1 Specifications are insufficient for hardware and software integration. Risk level: (3*1) = 3	WP4	Follow standard operating procedures to ensure well formulated and usable spec sheets
6	R4.2 Software integration not successful. Robot system not functional. Risk level (2*2) = 4	WP4	Prolong scientific/engineer visits at location of integration (FISC, ULIV) for joint, rapid development and problem solving.
7	R5.1 Complexity in scientific issues and challenges resulting in delayed assemble of the effective matrix. Risk level (2*1) = 2	WP5	The number of parameters to be taken into account will be reduced.
8	R5.2 Unavailability of a universal sample environment for an integrated characterization workflow between lab- and large-scale facilities. Risk level (2*2) = 4	WP5	The “reduced-perimeter” sample environment will be defined and agreed among the WP partners.
9	R6.1 No validation of HTS assay and testing methodology. Risk level (2*2) = 4	WP6	The iterative work upstream will enable tracking of delays. If needed, extra-resources will be assigned.
10	R6.2 AI orchestration of HTS systems is not operational. Risk level (3*2) = 6	WP6	Extra-resources will be allocated at mid-term check to obtain the critical AI orchestration.

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Risk number	Description of risk	WP Number	Proposed risk-mitigation measures
11	R6.3 No roadmap for evolution directions. Risk level (3*1) = 3	WP6	A minimum roadmap of evolution for demonstration and available samples will be proposed instead.
12	R7.1 The complexity of the battery interface might delay the development of the ontology. Risk level (3*2) = 6	WP7	In agreement with other WPs, rather than a more complete description, a reduced ontology will be developed based on the immediate needs of BIG-MAP.
13	R7.2 The erosion of common standards and/or different platforms could hinder the integration of the ontology. Risk level (2*2) = 4	WP7	A preferred platform will be selected.
14	R8.1 Issues in implementing the different standards due to the consortium size. Risk level (2*1) = 2	WP8	Working groups will defined more precisely the optimum standards.
15	R9.1 Delay or not delivery of automated workflow. Risk level (2*3) = 6	WP9	Extra-resources will be assigned if needed after a check of status at M12.
16	R10.1 Failure for the algorithm to run in synthetic (or simulated) data set. Risk level (2*2) = 4	WP10	Extra resources will be allocated to run the algorithm either in synthetic or simulated mode.
17	R10.2 No delivery of the demonstration of Figure of Merit (FOM) extractions. Risk level (1*3) = 3	WP10	Extra-resources will be assigned if needed after a status check at M18.
18	R11.1 Coupling of multiple scales in latent space is too complex. Risk level (2*2) = 4	WP11	The multiple scales will be reduces to optimum parameter for completion of the model.
19	R11.2 Available training data is insufficient. Risk level (2*3) = 6	WP11	Extra resources will be assigned to obtain training data for the demonstration.

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1.3.6. WT6 Summary of project effort in person-months

	WP1	WP2	WP3	WP4	WP5	WP6	WP7	WP8	WP9	WP10	WP11	Total Person/Months per Participant
1 - DTU	36	24	12	0	24	0	12	0	12	24	51	195
2 - UU	1	35	24	0	24	0	0	12	12	0	0	108
3 - KIT	1	0	53	0	0	14	0	0	14	57	14	153
4 - CNRS	1	0	0	0	39	0	0	93	0	0	6	139
· UPJV	0	0	14	0	0	0	0	0	0	0	2	16
5 - WWU	1	12	23	0	0	0	0	0	0	0	0	36
6 - CEA	3	1	8	11	48	11	0	0	1	0	0	83
7 - NIC	1	0	27	12	3	0	5	0	0	0	12	60
8 - SINTEF	1	11	0	0	0	0	23	0	0	0	0	35
9 - PDT	1	0	35	0	0	0	0	0	0	0	0	36
10 - Fraunhofer	1	0	0	40.70	0	9.30	0	0	0	3	0	54
11 - CTH	1	23	0	0	27	0	0	0	9	0	0	60
12 - WUT	1	0	0	47	0	24	12	0	0	0	0	84
13 - CSIC	12	0	12	0	6	0	6	0	0	0	18	54
14 - TUD	1	0	0	0	31	0	0	0	6	0	0	38
15 - CNR	1	12	24	0	0	0	0	0	12	0	5	54
16 - EPFL	6	6	0	0	0	0	18	0	42	0	0	72
17 - UCAM	1	49.90	0	0	19.30	0	0	12	0	0	6	88.20
18 - UOXF	1	0	0	0	15	0	0	15	0	0	22	53
19 - UT	1	0	0	24	0	0	0	0	0	0	0	25
20 - ULIV	1	0	0	42.20	0	0	0	0	0	38	0	81.20
21 - ESRF	1	0	0	0	12	0	0	11	6	0	12	42
22 - ILL	1	0	0	0	23	0	0	12	6	0	0	42

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	WP1	WP2	WP3	WP4	WP5	WP6	WP7	WP8	WP9	WP10	WP11	Total Person/Months per Participant
23 - SOLEIL	1	0	0	0	15	0	0	12	14	0	0	42
24 - CID	1	0	8	0	0	36	0	0	0	12	24	81
25 - EMIRI	12	0	0	0	0	0	0	0	0	0	0	12
26 - UMI	1	5	0	0	2	6	0	0	0	4	2	20
27 - SOLB	1	0	0	5	0	4	0	0	3	5	0	18
28 - BASF	2.50	0	3	0	0	11	0	1.50	0	3	0	21
29 - NVOLT	1	0	0	0	0	12	0	0	0	8	0	21
30 - UNIBAS	1	36	0	0	0	0	0	0	0	0	6	43
31 - ITU	1	0	0	41	0	0	0	0	0	4	0	46
32 - 3DS	1	12	0	0	0	0	0	0	23	0	12	48
33 - FZJ	1	0	12	12	0	89	0	0	0	12	0	126
34 - SAFT	1	0.50	0.50	0	5.50	12	0	0	0	0	0	19.50
Total Person/Months	99.50	227.40	255.50	234.90	293.80	228.30	76	168.50	160	170	192	2105.90

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1.3.7. WT7 Tentative schedule of project reviews

Review number [19]	Tentative timing	Planned venue of review	Comments, if any
RV1	18	to be decided in due time	
RV2	36	to be decided in due time	

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1. Project number

The project number has been assigned by the Commission as the unique identifier for your project. It cannot be changed. The project number **should appear on each page of the grant agreement preparation documents (part A and part B)** to prevent errors during its handling.

2. Project acronym

Use the project acronym as given in the submitted proposal. It can generally not be changed. The same acronym **should appear on each page of the grant agreement preparation documents (part A and part B)** to prevent errors during its handling.

3. Project title

Use the title (preferably no longer than 200 characters) as indicated in the submitted proposal. Minor corrections are possible if agreed during the preparation of the grant agreement.

4. Starting date

Unless a specific (fixed) starting date is duly justified and agreed upon during the preparation of the Grant Agreement, the project will start on the first day of the month following the entry into force of the Grant Agreement (NB : entry into force = signature by the Commission). Please note that if a fixed starting date is used, you will be required to provide a written justification.

5. Duration

Insert the duration of the project in full months.

6. Call (part) identifier

The Call (part) identifier is the reference number given in the call or part of the call you were addressing, as indicated in the publication of the call in the Official Journal of the European Union. You have to use the identifier given by the Commission in the letter inviting to prepare the grant agreement.

7. Abstract

8. Project Entry Month

The month at which the participant joined the consortium, month 1 marking the start date of the project, and all other start dates being relative to this start date.

9. Work Package number

Work package number: WP1, WP2, WP3, ..., WPn

10. Lead beneficiary

This must be one of the beneficiaries in the grant (not a third party) - Number of the beneficiary leading the work in this work package

11. Person-months per work package

The total number of person-months allocated to each work package.

12. Start month

Relative start date for the work in the specific work packages, month 1 marking the start date of the project, and all other start dates being relative to this start date.

13. End month

Relative end date, month 1 marking the start date of the project, and all end dates being relative to this start date.

14. Deliverable number

Deliverable numbers: D1 - Dn

15. Type

Please indicate the type of the deliverable using one of the following codes:

R	Document, report
DEM	Demonstrator, pilot, prototype
DEC	Websites, patent fillings, videos, etc.
OTHER	
ETHICS	Ethics requirement
ORDP	Open Research Data Pilot
DATA	data sets, microdata, etc.

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16. Dissemination level

Please indicate the dissemination level using one of the following codes:

PU	Public
CO	Confidential, only for members of the consortium (including the Commission Services)
EU-RES	Classified Information: RESTREINT UE (Commission Decision 2005/444/EC)
EU-CON	Classified Information: CONFIDENTIEL UE (Commission Decision 2005/444/EC)
EU-SEC	Classified Information: SECRET UE (Commission Decision 2005/444/EC)

17. Delivery date for Deliverable

Month in which the deliverables will be available, month 1 marking the start date of the project, and all delivery dates being relative to this start date.

18. Milestone number

Milestone number:MS1, MS2, ..., MSn

19. Review number

Review number: RV1, RV2, ..., RVn

20. Installation Number

Number progressively the installations of a same infrastructure. An installation is a part of an infrastructure that could be used independently from the rest.

21. Installation country

Code of the country where the installation is located or IO if the access provider (the beneficiary or linked third party) is an international organization, an ERIC or a similar legal entity.

22. Type of access

VA	if virtual access,
TA-uc	if trans-national access with access costs declared on the basis of unit cost,
TA-ac	if trans-national access with access costs declared as actual costs, and
TA-cb	if trans-national access with access costs declared as a combination of actual costs and costs on the basis of unit cost.

23. Access costs

Cost of the access provided under the project. For virtual access fill only the second column. For trans-national access fill one of the two columns or both according to the way access costs are declared. Trans-national access costs on the basis of unit cost will result from the unit cost by the quantity of access to be provided.

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Battery Interface Genome – Materials Acceleration Platform BIG-MAP

H2020-LC-BAT-12-2020 - Novel methodologies for autonomous discovery of advanced battery chemistries.
Type of action: RIA; Duration: 36 months
Name of the coordinating person: Tejs Vegge (DTU), teve@dtu.dk, +45 51641787

Table 0.1 – History of changes

	Changes to Part A
1	The timeline for the following four deliverables has been updated in Table 3.1c: **D1.3**: Minutes of kick-off meeting (M2), **D1.8**: Minutes of 5. bi-annual project meeting (M31); **D1.12**: Interim Exploitation plan (M12); **D1.14**: Final Exploitation plan (M36).
2	Three additional deliverables have been included in Table 3.1c: **D4.7**: Design of robotic system for organic synthesis completed (M18); **D4.8**: Design of robotic system for inorganic synthesis completed (M18); **D5.5**: Design of workflow for a European experimental multimodal platform completed (M18).
3	The following types of deliverables have been updated in Table 3.1c: **D1.2**: Data Management Plan: Type changed from "R" to "ORDP"; **D2.1**: Initial QM data sets for ML-training and analysis: Type changed from "R" to "DATA"; **D2.2**: 1st demonstrator QML interface potential for experimentally relevant electrode-electrolyte system. Type changed from "R" to "DEM"; **D9.1**: Prototype of the BIG-MAP App-store. Type changed from "R" to "DEC"; **D9.5**: Updated BIG-MAP App-store. Type changed from "DEC" to "ORDP"
4	The following deliverables have been changed from "CO" to "PU": **D1.13**, **D4.1**, **D4.5**, **D4.7**, **D4.8**, **D5.1**, **D5.2**, **D7.1**, **D7.3**, **D7.4**, **D10.4**, **D11.2.**
5	Small adjustments in the budgets for Partner 18 (UOXF) and 29 (NVOLT) have been made to increase the budget for Other Direct Cost (ODC) to include materials cost for the proposed testing. Corresponding reductions of 3 PMs has been made in WP5, WP8 and WP11 for UOXF and in WP10 for NVOLT. Partner 1 (DTU) has made a small reduction in ODC and a corresponding increase in PM.
	Changes to Part B
6	Page 32 and Table 3.4b: A more detailed description has been provided for the €350.000 that has been allocated (specified as subcontracting in the budget for Partner 1: DTU) to secure funding for **Stakeholder Initiated Initiatives (SII)**, as well as for the matching €350.000 for **BIG-MAP** partners (under "Other direct costs" in the DTU budget) agreeing to undertake additional tasks to meet the request specified in the SII proposal, e.g., for development of specific **apps and interfaces** between the **BIG-MAP** infrastructure and LC-BAT-1x-2020 projects or software widely used in the community.
7	Page 32: A clarification of the open call process and assessment procedures for the application for funding of **stakeholder initiated initiatives** has been provided, specifying that the decision on the allocation of funds is made by the Executive Board (EB) following a set of predefined criteria.
8	Page 32: It is now specified that all grantees from the **stakeholder initiated initiatives** will automatically obtain membership in the **Priority Stakeholder** group, while other requests for membership in the Priority Stakeholder group are assessed by the Project Coordinator.
9	Page 38: Additional virtual meetings of the Executive Board every 3 months have been included.
10	Page 40 and Table 3.4b: A more detailed description has been provided for the allocation of €100.000 (in the DTU budget) to ensure and strengthen the close collaboration between the partners for support of longer stays of key researchers with a partner organization. Allocation of extra mobility funds is based on a short application to the PC, who then recommends to the EB for final approval of funding.
11	More detailed descriptions of the other direct costs have been provided in Table 3.4b, including descriptions for Partner 18 (UOXF) and 29 (NVOLT).
12	A clarification of the use of a linked third party (LTP) for CNRS, i.e. UPJV, has been included in Section 4.1 and 4.2, while the incorrect mentioning of LTP has been removed for WWU (Section 4.2).
13	Two additional Letters of Intent for Priority Stakeholder status have been included in Section 6.

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MAIN ABBREVIATIONS

AI	ARTIFICIAL INTELLIGENCE
BIO	BATTERY INTERFACE ONTOLOGY
BIG	BATTERY INTERFACE GENOME
CEI	CATHODE ELECTROLYTE INTERFACE
DL	DEEP LEARNING
DFT	DENSITY FUNCTIONAL THEORY
DMP	DATA MANAGEMENT PLAN
EB	EXECUTIVE BOARD
EMMC	EUROPEAN MATERIALS MODELLING COUNCIL
EMMO	EUROPEAN MATERIALS MODELLING ONTOLOGY
FF	FORCE FIELD
GA	GENERAL ASSEMBLY
GrA	GRANT AGREEMENT
HPC	HIGH PERFORMANCE COMPUTING
HTS	HIGH THROUGHPUT SCREENING
IP	INTELLECTUAL PROPERTY
KPI	KEY PERFORMANCE INDICATOR
KD	KEY DEMONSTRATOR
LSF	LARGE-SCALE FACILITY
MAP	MATERIALS ACCELERATION PLATFORM
MD	MOLECULAR DYNAMICS
ML	MACHINE LEARNING
MST	MANAGEMENT SUPPORT TEAM
PC	PROJECT COORDINATOR
QM	QUANTUM MECHANICAL
QML	QUANTUM MACHINE LEARNING
SEI	SOLID ELECTROLYTE INTERPHASE
TRL	TECHNOLOGY READINESS LEVEL
WP	WORK PACKAGE

1 Excellence

1.1 Objectives

Large scale deployment of intermittent renewable energy and the electrification of the transportation sector critically depend on the availability of low cost, high-performance, environmentally friendly and scalable energy storage. Unlocking technological access and optimization of green energy storage solutions is essential for ensuring and accelerating the transition towards a net-zero CO_2 emission European Union by 2050. Further development of sustainable, high-performance battery technologies and materials plays a central role in ensuring and accelerating this transition. However, the existing paradigm for battery innovation and development is too slow and too costly to address the urgency of the societal challenges resulting from global warming. These challenges call for radical and accelerated technological innovation to reduce the global CO_2 emission to meet the goals of the Paris Agreement.

The 2019 Nobel prize in chemistry was awarded to Profs. John Goodenough, M. Stanley Whittingham and Akira Yoshino for their ground-breaking discovery and development of the lithium-ion battery technology. In doing so, The Royal Swedish Academy of Sciences recognized the disruptive influence the Li-ion battery has had on Society, but they also celebrated a largely Edisonian (trial-and-error based) discovery process with a 20-year timespan from Stanley Whittingham's initial idea about intercalation in 1972 to the commercial Li-ion battery (Sony, 1991). A battery concept and architecture which has remained unchanged ever since and still relies on scarce materials like cobalt, nickel and lithium. In a traditional sequential battery development process (Figure 1.1), each step of the discovery value chain is dependent upon the successful completion (green arrows) of the previous step(s). In contrast, failure (red arrows) sets the process back by one or more steps.

Figure 1.1: Traditional sequential and trial-and-error based battery discovery & development.

With the development of the **Battery Interface Genome – Materials Acceleration Platform** (**BIG-MAP**), we are proposing a **radical paradigm shift** in battery innovation, which will lead to a dramatic speed-up in the battery discovery and innovation time; reaching a 5-10 fold increase relative to the current rate of discovery within the next 5-10 years. **BIG-MAP** relies on the development of a unique R&D infrastructure and accelerated methodology that unites and integrates insights from leading experts, competences and data across the entire battery (discovery) value chain with Artificial Intelligence (AI), High Performance Computing (HPC) and autonomous synthesis robotics.

The large-scale European Research Initiative **BATTERY 2030+**[1] stands united behind the **BIG-MAP** consortium for the LC-BAT-12-2020 call. The **BIG-MAP** consortium comprises an unprecedented gathering of world-leading scientific experts and industry leaders, spanning the full battery discovery value chain, from fundamental discovery to advanced battery materials and cell production. In addition to 13 core partners from BATTERY 2030+, the **BIG-MAP** consortium includes a number of leading European experts from complementary research areas such as Quantum Machine Learning (QML) (UCAM, UBAS), deep learning (DTU), autonomous synthesis robotics (ULIV, ITU, UT), European large-scale synchrotron/neutron facilities (ESRF, ILL, SOLEIL), HPC & data infrastructure (CNR, EPFL, 3DS), as well as battery materials producers (BASF, SOLB, UMI) and battery cell producers (SAFT, NVOLT).

The **BIG-MAP** proposal represents the **ramp-up implementation and demonstration phase** of the collective long-term vision and strategy of BATTERY 2030+ for the development of a novel "chemistry neutral" methodology and data/research infrastructure, "*to invent the batteries of the future, bringing together the smartest brains in Europe to join forces in speeding up scientific discoveries, creating synergies and avoiding over-redundant research*". In short,

[1] https://www.battery2030.eu

BIG-MAP aims to *reinvent the way we invent batteries* and to develop core modules and **Key Demonstrators** of a Materials Acceleration Platform[2] specifically designed for accelerated discovery of battery materials and interfaces.

Over the last year, we have outlined, presented and discussed the **BIG-MAP** vision in the **BATTERY 2030+ Roadmap**[3] and collected valuable input and insights from the European battery community through the written consultation and stakeholder workshops. Many of these contributors will also be directly connected to the project through our **BIG-MAP** stakeholder initiatives discussed below. Only by a united effort of the entire **European battery community** can we achieve the breakthrough development in battery innovation presented here, which will place Europe (back) in a leading position for battery discovery, development and production.

1.1.1 Context and positioning of BIG-MAP

Today, advanced materials account for nearly half of the manufacturing costs[4] of clean energy technologies such as high-performance Li-ion batteries, and this figure is expected to reach eighty percent in the future[5]. Relying on existing trial-and-error based development processes, the discovery of novel high-performance battery materials and cell designs entails considerable effort, expense, and time – traditionally over 10 years from initial discovery to commercialization. Historically, these innovation cycles rely on cost reduction by accelerated manufacturing and engineering rather than deployment of new "Quantum leap" technologies.

Experience has shown that when developing new battery chemistries or introducing new functionalities into an existing battery technology, interfaces hold the key to exploit the full potential of the electrode materials and to develop **ultra-high performance, sustainable and smart batteries**. The European battery R&D landscape consists of a multitude of research institutions, laboratories and companies, many of which pursue complementary approaches to tackle this challenge at a local scale. Here, we will bring together this expertise with cross-sectoral competences, industrial partners and end-users to establish the **Battery Interface Genome (BIG)** and accelerate the development of radically new battery technologies.

One of the key challenges in establishing **BIG** is to automate the acquisition, curation and analysis of enormous data sets that will be generated as part of a community-wide European battery "**Materials Acceleration Platform**" or (**MAP**), which will be applied to key challenges in battery research. In line with the Mission Innovation Clean Energy Materials Innovation Challenge IC6 Roadmap[2], a MAP utilizes a number of complementary approaches, including AI, to integrate and orchestrate data acquisition and utilization from a number of complementary and cross-sectoral approaches and technologies. The MAP concept can be applied to diverse classes of materials, and here it will be developed specifically with battery applications in mind. This innovation pipeline will feed **physics-aware data-driven hybrid models** (section 1.4.5.3) that aid in better understanding and predicting properties of battery interfaces. While the MAP will provide the platform to accelerate our findings, BIG will develop the necessary understanding to control the formation and dynamics of the crucial interfaces and interphases (section 1.4.2.1), which are limiting battery performance.

The proposed **BIG-MAP** **infrastructure is modular and versatile**, in order to be able to accommodate and handle all emerging battery chemistries, materials compositions, structures, formulations and interfaces. **BIG-MAP** should integrate relevant cross-sectoral technologies, including emerging research strategies, to accelerate materials design. In the long-term, we envision the development of a "**chemistry neutral**" **BIG-MAP**, which will enable the community as a whole to take up and pursue discoveries with greater agility.

BIG-MAP will provide an accelerated path to disruptive battery technologies with ultra-high performance, full sustainability and smart operation

Next-generation batteries necessitate advancements in computational and experimental techniques across **multiple time- and length-scales** with a linkage between *in-* and *ex operando* conditions. Such advancements pose a challenge to the scientific community as a new level of collaboration between theory- and experiment-driven research groups is necessary – **BIG-MAP** seeks to overcome this hurdle through a **unique domain-bridging data infrastructure** and embedding of materials and data from simulations and experiments. Experimental results are needed to identify realistic input parameters for the development of new computational models, and modelling results need to be validated against experimental results. Likewise, the extraction of insights from experiments can be done with greater certainty when cross-referenced with theoretical models and simulations.

In addition to the continuous improvement and development of new experimental techniques and methodologies, a radical new way of combining experimental, computational and data driven techniques will be necessary. Advanced physics-based hybrid models and simulation techniques have to be developed for the interpretation of cutting-edge

[2] Mission Innovation; Clean Energy Materials Innovation Challenge (IC6), "Materials Acceleration Platform—Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence" (2018)
[3] Battery 2030+ Roadmap: "Inventing the Batteries of the Future – Research Needs and Future Actions" 2020. (battery2030.eu/roadmap)
[4] Schmuch R. et al Nat Energy 3, 267–278 (2018)
[5] Fabrice Stassin, Director of EMIRI (2018)

operando experiments. More efficient methods for utilizing large data sets to determine **descriptors**[6] for multi-scale processes and multi-structure theories have to be developed. With these technical advancements, new insights will follow, which will allow us to control the access to a fine-tuning of battery interfaces and thus develop the next generation of ultra-performance batteries. Rather than empirical development of battery chemistry and assembly, we aim at developing a framework for **inverse design of batteries** driven by application specifications, i.e. inverting the design process and letting the materials targets determine the optimal composition/structure.

BIG-MAP will develop a modular, closed-loop infrastructure and methodology to bridge physical insights and data driven approaches to accelerate inverse design of future battery chemistries and technologies

1.1.2 BIG-MAP specific objectives

The ultimate +10 year vision and ambition of BATTERY 2030+ are to develop a **fully autonomous battery Materials Acceleration Platform** capable of performing accelerated closed-loop materials discovery, cell design and manufacturing of sustainable, ultra-high performance batteries in Europe, utilizing data from all elements in the battery value chain from raw materials to end-users, e.g. on-the-fly data from EV users across Europe (Figure 1.2).

Figure 1.2: Overview of the long-term BIG-MAP objectives and benefits in Europe

This will **not be achievable in three years**, but the **BIG-MAP** consortium has identified a set of **Specific Objectives** and **12 Key Demonstrators** (Table 1.2) for the 3-year ramp-up phase addressed in this proposal that will develop and demonstrate the infrastructural backbone needed to achieve a 5-10 fold acceleration in the discovery process. In summary, the Specific Objectives are:

O1 **Develop the scientific and technological building blocks and models for accelerated battery discovery**

Sub-objectives	Key Performance Indicator (KPI)
AI-accelerated atomic-scale simulation techniques for battery materials and interfaces	Acceleration through potentials from Quantum Machine Learning (QML) for battery electrode-electrolyte system (>10^4 longer simulation times)
Multi-scale modelling by coupling AI with multi-fidelity data from simulations and experimentation	Scales successfully bridged with AI-assisted identification of interface descriptors/features in multi-scale models for interface evolution (from TRL 1 to 3)
Demonstration of an open-source framework for seamless integration of software, hardware and robotics modules to enable autonomous synthesis processes for advanced battery materials and cells	Increase 'levels of autonomy' reached in core steps of the synthesis and characterization process for direct (coatings: manual to semi-automated) and indirect (formulations: automated to semi-autonomous) alteration of interface properties due to **BIG-MAP**

[6] Nørskov J.K. & Bligaard T. Angew. Chemie Int. Ed. 52, 776–777 (2013).

Development of a European multi-modal characterization platform for battery interfaces and interphases bridging lab- and large-scale facilities (LSF) and techniques	Number of lab-scale and LSF instruments and/or chemistries successfully bridged (>4 instruments successfully bridged)
Optimized discovery process for advanced electrolyte and electrode materials using High-Throughput Screening (HTS) guided by advanced hybrid AI-models	Reduction in the time/resources needed to identify and demonstrate new materials and/or additives through HTS of electrolyte formulations, and documenting improved interface performance (factor of 2 or more)

O2 Deliver cross-cutting initiatives to ensure implementation and use of project data and results across the battery discovery value chain

Sub-objectives	KPI
Develop a Battery Interface Ontology (BIO) to ensure interoperability between multiple scales, techniques, and domains in the battery discovery process. Facilitate battery experts in different fields to convert real-life observations to a common digital representation	Inclusion of the BIO in community accepted ontology platforms like the European Materials Modelling Ontology (inclusion in EMMO GitHub repository completed)
Creation of a common European web-platform for materials and battery testing with community-wide accepted standards and protocols	European organizations and institutions adopting and/or co-developing the standards and protocols for battery interfaces (>20 organizations outside Battery 2030+)
Development of a shared software infrastructure platform with simulation and experimental control, and data handshaking, enabling automated simulations and experiments	Number of registered users at the project website www.BIG-MAP.eu at the end of the project period (>500 registered users)
Implement a cross-cutting framework to accelerate materials discovery and optimization in experiments and *in silico* using AI, active learning, automated analysis and reasoning to accelerate materials experiments, synthesis routes, and simulations	Number of successful demonstrator projects by the consortium or external users, where automated analysis and/or optimization has been achieved using **BIG-MAP** modules/apps (>10 examples)
Development of an uncertainty-guided hybrid physic- and data-driven generative BIG-model to predict the spatio-temporal evolution of battery interfaces, and enable inverse materials design	Development of predictive generative models which can successfully predict performed simulations and experiments (from TRL 1 to 3)

O3 Disseminate and reach the battery community all along the battery value chain, to boost EU advanced battery development and manufacturing

Sub-objectives	KPI
Develop a **BIG-MAP** App-store, where the software modules, automated analysis tools and workflows, as well as remote data access protocols developed in **BIG-MAP** can be made available for community download	>1000 downloads of data sets and/or software through the website, and >500 uploads of data sets from external users
Arrange stakeholder engagement, ESR training events, workshops and webinars to disseminate **BIG-MAP** to key stakeholders in the European battery community. Present and discuss the **BIG-MAP** vision and blueprint.	>150 participants at workshop co-hosted by the LC-BAT-12/13/14/15-2020 projects, and >30 registered participants for ESR training events
Initiate activities to strengthen the education of students and training of the workforce (life-long learning) through the web interface, e.g. (e-learning) courses and virtual laboratories	To increase the educational aspect of **BIG-MAP**, a section of the App-store is developed to share online (e-learning) courses and virtual laboratories
Use of Social media channels like LinkedIn and Twitter to actively publish information about breakthroughs, scientific publications and project events and updates to reach a broader audience	>1000 unique followers of **BIG-MAP** through social media platforms, i.e. Twitter and LinkedIn

1.2 Relation to the work programme

BIG-MAP addresses the topic *LC-BAT-12-2020: "Novel methodologies for autonomous discovery of advanced battery chemistries" (RIA)*. The solutions **BIG-MAP** brings to the specific challenges and scope of the topic are briefly summarized in Table 1.1 below, while the impact is addressed in Table 2.1.

Table 1.1 – Relation between BIG-MAP and LC-BAT-12-2020

Challenge	BIG-MAP relevance to challenge
The performance and durability of existing batteries are limited due to insufficient knowledge in managing the complex and dynamic processes taking place in the materials and in particular at the interfaces/interphases within the battery cell. *The long term challenge is to integrate advanced multi-scale computational modelling, materials synthesis, characterization and testing to perform closed-loop autonomous materials findings and interphase engineering that would accelerate by at least a factor of 5 the discovery of new battery chemistries with ultra-high performances.*	The **BIG-MAP** infrastructure is designed to produce and utilize large curated data sets to fill in gaps in the understanding of the complex phenomena happening at battery interfaces/interphases and utilize machine learning (ML) methods to enhance the obtainable understanding of dynamic process from both experiments and multi-scale simulations. **BIG-MAP** aims at developing an infrastructure to accelerate the discovery of battery materials and interfaces by combining computational models at various length and time scale and AI models with synthesis robotics and autonomous characterization. The expected acceleration will be well beyond a factor of 5-10.
Scope	**BIG-MAP relevance to scope**
The target is to develop a pilot materials platform for computational and experimental material characterization that would pave the way towards the development of a full-scale autonomous battery Material Acceleration Platform (MAP) enabling closed-loop materials discovery, automated characterization, device-level testing and addressing aspects related to manufacturability and recyclability. The pilot MAP should deliver a complete blueprint of the targeted autonomous material discovery platform and demonstrate key features such as: the ability to use modelling, simulation and machine learning techniques to determine optimal materials composition, the ability to autonomously direct an automated material synthesis robot in optimizing selected battery materials and the ability to perform autonomous analysis and interpretation of experimental data and of deriving previously unknown structures and compositions. *The pilot MAP should demonstrate the potential of this novel approach on a specific test case targeting the optimization of specific advanced or emerging battery chemistries. It should be sufficiently flexible to be adaptable for future disruptive battery chemistries, concepts and technologies and for integrating aspects like manufacturability, ageing, degradation and recycling of importance to the entire battery lifecycle.* *Proposals should be specifically targeting battery interfaces such as the Solid Electrolyte Interphase and the Cathode Electrolyte Interphase that are critical for the battery functionality, as well as controlling their formation, composition and morphology.*	**BIG-MAP** will develop a pilot battery MAP capable of demonstrating the acceleration achievable by closed-loop materials discovery. 12 Key Demonstrators (Table 1.2) will be developed during the 3-year ramp-up to show-case this. The initial **BIG-MAP** infrastructure will be developed and trained on a specific set of advanced battery materials and chemistries, but be general enough also to serve as a base for future chemistries and concepts. We will apply the techniques and infrastructure for a specific combination of state-of-the-art (SoA) Li-ion electrode materials and electrolyte materials (see section 1.4.1). These have been selected because they display an optimal balance between theoretical performance, interfacial challenges for commercialization and develop the possibility to utilize existing literature and industrial data for the training of the models, and, finally, they are produced and delivered by leading European producers of battery materials. The developed models and modules will be targeted towards the formation and initial evolution of the SEI and CEI on the identified advanced Li-ion electrode materials, and used to discover and optimize electrolyte formulations, as well as to guide automated synthesis of protective coatings for enhanced performance. The developed approaches will be sufficiently modular and versatile to warrant use outside the original development cases, e.g. use the developed deep learning techniques to understand and predict materials/interface degradation[7]. **BIG-MAP** will disrupt the state-of-the-art of infrastructures and methodologies for discovery of battery materials by integrating all relevant data streams for battery materials and interfaces. The ultimate scope is to develop an unprecedented AI-orchestrated infrastructure capable of closed-loop linking of modelling, synthesis, characterization and testing at multiple length and time scales, such that AI and machine learning can be used across all areas to synergistic effect.

[7] Nash W. et al npj Mater Degrad 2, 37 (2018)

1.3 Concept and methodology

1.3.1 Concept and approach

BIG-MAP's strategy is to cohesively integrate ML accelerated simulations and AI-orchestrated experiments to expedite battery materials discovery and optimization by a factor of 5-10

The identified necessity for rapid advancement in the fundamental way battery research is conducted today requires the joint forces of accelerated computational and accelerated experimental methods, which is at the heart of the **BIG-MAP** concept. This novel approach to research thrusts from the **top research groups for battery research in Europe** and will transform partners in industry and academia into a homogenous world leading research and development community, as the proposed platform would be worldwide unique in terms of fidelity (i.e. the ability to represent real world properties), throughput, scale and accelerated integrative concept. We believe that machine learning (ML) can be used to merge these disjunct perspectives onto the underlying physics to provide a more detailed understanding. Here, ML act as the translating layer and with a versatile data management ensure rapid and frictionless exchange of data and insights. Recent advances in AI-orchestrated experimentation and ML accelerated computational methods, like the Chemputer, ChemOS and the Electrolyte Genome[8], provides the foundation for the integrated **BIG-MAP** platform. Figure 1.3 illustrates the conceptual flow of data in **BIG-MAP** between the 8 core modules and the central AI (i.e., the central AI-orchestrator and optimizer/explorer), supplying the structured layers needed to operate the autonomous laboratory and plan the optimization, synthesis and evaluation feedback-loop (discussed in sections 1.4.4 and 1.4.5). Below, we also discuss why we focus on specifically on interfaces, and why we believe AI and a common data infrastructure are the conceptual keys to making **BIG-MAP** a success.

Figure 1.3: BIG-MAP concept for advancing autonomous discovery of battery materials

Why study interfaces and interphases?

It is widely accepted that interfaces and interphases are of the utmost importance for the operation of batteries, and understanding, controlling and designing their functions is key for the development of ultra-performing, smart and sustainable batteries. Any globally leading approach trying to master and (inverse) design battery interfaces must therefore combine the characterization of these interfaces in time as well as in space (**spatio-temporal characterization**) with physical and data-driven models integrating dynamic events across multiple scales, e.g. from the atomic scale to the micron scale. **BIG-MAP** therefore aims at establishing a fundamental "**genomic**" knowledge of battery interfaces and interphases through time, space and chemistries.

Interfaces and interphases have always been both a blessing and a major limitation to the development of batteries. The interfaces are the places where the energy storage in batteries is facilitated, but also where many degradation phenomena are initiated. In Li-ion batteries, it was realized that one major aging mechanism, the growth of the so-called **Solid Electrolyte Interphase (SEI)** on graphitic anodes (and the related **Cathode Electrolyte Interphase (CEI)**) is also one of the most crucial properties to ensure the cycling stability of the battery. In this example, interfacial reactivity, when mastered, helps to extend the thermodynamic stability of organic electrolytes used in

[8] Gromski P.S. et al, Trends in Chemistry, 2, 1, 4-12 (2020); Dave A. et al. ChemRxiv. Preprint.10.26434/chemrxiv.10282112.v1 (2019); Whitacre J.F. et al, J. Electrochem. Soc. 166, 16 (2019)

batteries, owing to the formation of this passivating interphase that allows ions but not electrons to diffuse through (Figure 1.4). When these interfacial reactions and surface modifications are not controlled, continuous parasitic reactions may occur, thus limiting the life cycle of the battery.

Indeed, a slight modification of electrode structure and/or electrolyte formulation, as well as the presence of impurities or defects, can lead to a drastic change in the chemical composition as well as the morphology of the SEI or CEI. This may induce a complete reversal from the ideal scenario to an uncontrolled one, hence driving significant research efforts in studying such interfacial processes.

Figure 1.4: Schematic representation of interfacial processes (LTGM: long-term growth mechanisms).[9]

The **Battery Interface Genome** is related to the concept of descriptors in catalyst design[6], where the binding energy of other important reaction intermediates scales with that of the descriptor, and the identification and quantification of the descriptor value enables an accelerated and accurate prediction of the rate of the total reaction. Identifying the multitude of descriptors (or genes) coding for the spatio-temporal evolution of battery interfaces and interphases is a prerequisite for the proposed inverse design process, and simply cannot be established within existing methodologies. This requires improvements of the capabilities of multi-scale modelling and systematic multi-technique characterization of battery interfaces, including *operando* characterization, to generate/collect comprehensive sets of high-fidelity data that will feed a common AI-orchestrated data-infrastructure in **BIG-MAP** (Figure 1.3).

Despite decades of research, the details of interfacial reactions in the complex electrochemical environments in batteries remain a conundrum, e.g. the composition and function of the SEI and CEI. The structural properties depend in a highly complex and elusive manner on the specific characteristics of the composition of the electrolyte and structures of the electrode materials, as well as the external conditions. The complexity of such interphases arises from a multitude of reactions and processes spanning a wide range of time- and length scales that define their formation, structure and, ultimately, their functionality in the battery.

Key challenges include the development of new multi-scale modelling concepts including physics-aware data-driven hybrid models to identify **dynamic interphase descriptors**, the development of new characterization techniques and **standardization of experimental data** and observables as inputs to physical models to make the link between observables and descriptors.

Understanding and tracking different types of uncertainties in the experimental and simulation methods, as well as the ML framework for, e.g., generative deep learning models[10] (section 1.4.5.3) is crucial for controlling and improving the fidelity in the predictive design of interfaces. Predictive modelling and design of interfaces holds the key improved battery performance and durability. Simultaneous utilization of data from multiple domains, including data from apparently failed experiments[11], can accelerate the development of generative models that enable accelerated discovery and inverse design of durable high-performance interfaces and interphases in future batteries.

Why use AI and machine learning?

We have identified a pressing need to deploy a MAP capable of revolutionarily accelerating the way we conduct materials research on batteries by an order of magnitude or more. This necessity originates in the combinatorial explosion of possibilities in the **multi-dimensionality of chemical space**. Chemical space is comprised of a multitude of parameters that cross influence each other. Examples for batteries are: composition of electrodes, combination of electrodes, formulation of electrolytes, processing, packaging, and cell aging. The combinatorics of this space with well **above 10^9 possibilities** surpass even exhaustive search capabilities of state-of-the-art HTS equipment, motivating a primary focus on experiments that aid in both improving battery performance and in unravelling the underlying physics and chemistry. Within **BIG-MAP**, we aim to *reinvent the way we invent batteries* through integrating the core research tasks[15] in the MAP, while also **accelerating the individual research task**

[9] H Horstmann B et al. Current Opinion in Electrochemistry 13, 61-69 (2019)
[10] Maaløe, L. et al. arXiv Prepr. arXiv1704.00637 (2017)
[11] Raccuglia, P. et al. Nature 533, 73 (2016)

through the efficient use of ML, e.g. active/sequential learning[12]. **Active learning** holds the promise to achieve the combined goal of improving material and model performance through efficient exploration and exploitation. Recent results suggest **acceleration factors above 30x**[13] compared to exhaustive search strategies. Combined with the accelerations possible through HTS compared to manual experimentation, as well as proper integration between research tasks, we believe that the **BIG-MAP** will be able to **demonstrate a breakthrough acceleration** of research pace in battery discovery. A precursor for the efficient orchestration of experiments by means of active learning and for building BIG is using a **ML-amendable representation** of materials and experiments. Such representations are ideally continuous and aid in conveying complex information in highly compressed form, but also aid in the translation between domains and scales. Several examples exist where features of materials are represented as SMILES, SELFIES, or **latent space vectors** using, e.g., autoencoders [14]. In **BIG-MAP**, we aim to use these embedding methods to represent battery materials, interfaces and experiments to accelerate the optimization of batteries, while unravelling the underlying physics and chemistry. This entails the translation across scales and fidelity (bridging), to, e.g., predict optical absorption spectra from simple materials images[15]. Other examples include the automated unravelling of fundamental insights from multi-fidelity experiments such as print composition, Raman spectroscopy and electrochemistry[16], or predicting materials functionalities in unexplored processing spaces using generative models[17].

Atomic-scale simulations can provide chemical and physical understanding of battery systems and can also be guided by AI in the search for novel battery materials[18]. Simulations with Quantum Mechanical (QM) approximations such as density functional theory (DFT) can be orders of magnitude more cost efficient than physical experiments. However, the complexity of battery systems forces an unavoidable trade-off between cost and accuracy of simulations, often rendering them impractical battery interface studies with currently used methodologies. Various ML approaches can be combined with QM approximations to form **QML models** capable of changing the trade-off towards significantly faster and/or accurate simulations. As both QM and ML models by virtue are *in silico*, they complement each other well in terms of data generation and utilization. A ML model can be trained on QM data and work independently[19], act as a surrogate to increase the speed of QM simulations[20], or be used for fidelity bridging and enable the use of less demanding QM methods[21]. These approaches in various ways enable simulations of model systems closer to real physical systems and exploration of a large chemical space than otherwise feasible.

A prerequisite for any ML/AI study in materials science is **data access** and management beyond lab books and standard reporting. For **BIG-MAP** we need to achieve data management and **data lineage tracking** beyond FAIR guidelines,[22] such that **data is automatically pushed for analysis and reported back**. Additionally, data needs to be accessible and ingestible with little to no human supervision, while protecting Intellectual Property (IP) of, e.g., industrial partners (see section 2). An integral part of the MAP is therefore **autonomously orchestrateable robotics**, that are used as the experiment initiator, worker and checker in an autonomous feedback loop. Robots are automated pieces of instrumentation, often part of a HTS setup, that are externally interfaced. In classical HTS, such instruments scan a materials library over a fixed e.g. spatial grid and log the data. In **BIG-MAP**, robots are externally interfaced and analyse and deposit the measurement data on the fly. All prior experimental and simulation data will be accessible from a **central BIG-MAP database** to facilitate dynamic planning of subsequent experiments and simulations. Early examples in experimental materials science include the optimization of organic hole transport materials[23] and multinary organic photovoltaic cells[24]. Through vigilant data management and analysis tightly integrated into these **robot workflows**, a new era of closed-loop experiments comes into reach. Within **BIG-MAP**, we seek to adopt proven methods from in-depth characterization in, e.g., photo-electrochemistry[25] and large scale manufacturing. From the latter **BIG-MAP** will **adapt an existing automated electrolyte formulation and coin cell production line for AI-orchestration**. This setup[26] will deliver pertinent information on system/stack level effects and long-term battery life. For early and intermediate battery lifetime with a focus on interfacial properties, **BIG-MAP** will employ

[12] Cohn D.A. et al Journal of artificial intelligence research, 4, 129–145 (1996)
[13] Rohr B. et al. ChemRxiv. Preprint. 10.26434/chemrxiv.11303606.v1
[14] Gómez-Bombarell R. et al. ACS Cent. Sci. , 4, 2, 268-276 (2018); Krenn et al., arXiv:1905.13741v1 (2019)
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[16] Umehara M. et al. npj Computational Materials 5, 34 (2019)
[17] Banko L. et al. arXiv Prepr. arXiv 1910.09468 (2019)
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[19] Chang J. et al J. Phys.: Condens. Matter, 31, 325901 (2019); Sivaraman G. at al. arXiv:1910.10254 (2019); Deringer V. et al. Adv. Mater. 31, 1902765 (2019); v Lilienfeld A. et al. arXiv:1911.10084 (2019)
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[21] Zaspel P. et al. J. Chem. Theory Comput. 15, 3, 1546-1559 (2019)
[22] Wilkinson M.D. et al. Sci Data. 3: 160018. (2016)
[23] MacLeod B.P et al. arXiv Prepr. arXiv:1906.05398
[24] Langner S et al. arXiv Prepr. arXiv:1909.03511
[25] Sliozberg K et al. ChemSusChem, 8, 7, 1270-1278 (2015)
[26] www.uni-muenster.de/news/view.php?cmdid=10123

a series of, e.g., scanning droplet cells, which will allow the characterization of **thousands of millimetre sized batteries** in three electrode cell configuration and subsequent SEI and CEI characterization using a plethora of spectroscopic techniques.

Many of these spectroscopic techniques yield complex data that requires post-processing and in-depth analysis. One of the most prominent examples of large and hard to interpret data sets are X-ray diffraction phase maps, that required expert crystallographers up until recently to analyse hundreds of diffractograms. Through the efficient use of AI and data management background subtraction and noise rejection,[27] these can now be fully automated and phase maps are automatically generated[28] using physical constraints. Adapted, these methods would enable ML for accelerated in line characterization and deep learning for prediction of the spatio-temporal evolution of battery materials.

Why develop a shared data infrastructure and automated workflows?

A key aspect of the novelty of **BIG-MAP** is in the full integration of battery modelling, synthesis, characterization and AI in a way that enables not only the fluid exchange of data, but also enables each domain to directly query the others to fill in gaps in (training) data and/or understanding, suggest new materials/interfaces and to verify/disprove results (Figure 1.5). As illustrated in the figure, the uninterrupted flow of data and queries between the different domains is crucial, e.g., in the continuous optimization of parameters and analysis of new target materials and cells. This requires three crucial components: **Interoperability**, i.e., both standards and tools to exchange data fluidly and faithfully; **shared data infrastructure**, i.e., hardware and hosted databases to store and quickly access data in a uniform way; **automated workflows**, i.e., procedures for encoding of knowledge from one domain (e.g. experiments) in a workflow capable of automatically launching procedures in another domain (e.g. simulations) in fully reproducible way.

Figure 1.5 AI-orchestrated BIG-MAP workflow

1.3.2 The key results of the project and the future with BIG-MAP

Currently, **no such integrated platform exists in the World** that enables characterization, either by experiment or theory, or optimization of battery materials and their critical interphases/interfaces. Building such a platform is a **community effort** that reflects community requirements and as such will incorporate new ways, of, e.g., ensuring **protection of IP**, as well as **provenance tracking** of data from different sources. The **BIG-MAP** project will deliver the key components and a **blueprint of the infrastructural backbone** of such a platform, and the novel methodologies needed to integrate them into a community tool that enables a paradigm shift in the development of battery materials and cells.

No large-scale database of battery-oriented interface properties that compares to existing structure databases for organic and inorganic materials[29] is currently available publicly. The implementation of such an European database

[27] Ament S.E. et al. npj Computational Materials 5, 77 (2019)
[28] Gomes C.P. et al. MRS Commun. 9, 2, 600-608 (2019)
[29] Zakutayev, A. et al. Sci. Data 5, 180053 (2018); ICSD - Inorganic Crystal Structure Database.

requires the further development and utilization of characterization techniques capable of providing a high-fidelity description of the interfaces and their dynamics, and track the provenance of the data. This needs the definition of generic, **community-wide keywords** and labels to include, e.g., **suitable metadata**[30]. Both lab-scale and LSFs are needed to achieve this goal, depending of the level of data resolution or quality needed in the workflow. This would allow a general classification of phenomena and categorization of interfaces, which is currently missing. This would help to establish the "shared features" and any potential deviations from these into **BIG-MAP**, regarding, e.g., the chemical, structural evolution of solid/liquid and solid/solid interfaces, as well as the dynamic restructuring of complex electrodes. It is important to stress that the proposal only covers the ramp-up phase and blueprinting of a **+10 year vision** for a ground breaking autonomous infrastructure, but we have identified **12 Key Demonstrators** to visualize and quantify the impact achievable in the ramp-up phase (Table 1.2).

Table 1.2 – 12 Key Demonstrators from the BIG-MAP ramp-up phase

	Key Demonstrators
KD1	**QML Demonstrator** of an interface potential for an experimental electrode-electrolyte system (**D2.2**)
KD2	**AI-enhanced Multi-scale Demonstrator** for accelerated scale-bridging (**D3.4)**
KD3	**Demonstration of Autonomous Synthesis Robotics** of protective electrode coatings (**D4.6)**
KD4	**Multi-modal Characterization Demonstrator** capable of running coordinated multi-technique experiments to acquire multi-scale/multi-fidelity data (**D5.3)**
KD5	**HTS SEI Demonstrator** using integrated high-throughput electrochemistry and *ex situ* high-throughput spectroscopy to optimized electrolyte formulations and materials (**D6.4**)
KD6	Development of a community-wide European **Battery Interface Ontology** (BIO) (**D7.5**)
KD7	An **Open European Platform** with **BIG-MAP** standards & testing protocols for battery materials (**D8.8**)
KD8	**Automated Workflow Demonstrator** for integrated simulations and experiments (**D9.2**)
KD9	Development of a **BIG-MAP App-store** for automated analysis modules and workflows (**D9.5**)
KD10	Modular packages for **Autonomous Analysis** of spectroscopic and electrochemical data (**D10.2**)
KD11	Demonstration of **uncertainty-guided hybrid physics and deep-learning battery model** (**D11.4**)
KD12	**Transferability demonstrated** for Li-ion hybrid models to novel battery chemistries (**D11.5**)

1.3.3 The BIG-MAP consortium and partner activities linked to the project

The **BIG-MAP** consortium members are extremely active and participate in a multitude of European and (inter)national initiatives connected with the development of sustainable high-performance batteries and advanced methodologies to enable their research and development. A select list of recent projects is reported in Table 1.3.

Table 1.3 – Selected, recent national and European projects for the BIG-MAP partners

Research activities that feed into BIG-MAP	**Funding**	**Acronym or webpage of the project**	**Start /End**	**BIG-MAP Partners**
Next generation of ultra-high-performance, sustainable and safe batteries	H2020	www.battery2030.eu	2019 2020	13 Partners
Modelling, synthesis and characterization of electrodes, electrolytes and electrolyte additives in Al-S batteries	H2020	www.salbageproject.eu	2017 2020	CSIC, DTU
Modelling, synthesis and characterization of electrodes, electrolytes and electrolyte additives in Mg-batteries	H2020	www.e-magic.eu	2019 2022	CID, DTU, KIT, CSIC, CEA,
Development of a multi-scale simulation tool for battery systems	Euro-Stars	SimBa	2017 2020	DTU, UMI
Development of first-principles codes and materials informatics platform HPC of battery components	H2020	www.max-centre.eu	2018 2021	CNR, EPFL, CSIC

[30] The European Materials Modeling Council. The EMMC RoadMap 2018 for Materials Modelling and Informatics (2018)

Calcium rechargeable battery technology	H2020	CARBAT	2017 2020	CSIC, CTH
Calcium and magnesium metal anode based batteries	H2020	CAMBAT	2017 2021	CSIC
Post-lithium electrochemical energy storage	CoE	POLiS	2019 2025	KIT
Development of Na-ion batteries	H2020	NAIMA	2019 2022	CNRS
Open innovation test bed for electrochemical energy storage materials	H2020	www.teesmat.eu	2019 2022	CEA, ESRF, UMI
Safe and pre-lithiated high energy density batteries based on sulphur and silicon chemistries	H2020	www.project-spider.eu	2019 2022	CEA, FZJ CIDETEC, SOLVAY,CIDS OLB
Optimization of scalable real-time models and functional testing for e-drive concepts	H2020	www.obelics.eu	2017 2020	NIC
Digital Ontology-based Modelling Environment for Simulation of materials with focus on cathode materials for Li-ion batteries	H2020	www.simdome.eu	2019 2023	PDT, UMI
All solid-state reliable battery for 2025	H2020	ASTRABAT	2020 2023	CEA, UMI, FRAUNHOFER
Addressing the challenges in all solid-state batteries	Faraday Inst.	www.solbat-faraday.org	2018	OXFORD
Next generation cathode materials	Faraday Inst.	CATMAT	2018	OXFORD, UCAM
Interface characterization and modelling (multi-scale multi-physics) of advanced hybrid ceramic-electrolyte in lithium- Ni rich cells	H2020	SAFELIMOVE	2020 2023	CID, CEA, SAFT, UMI
Battery design and manufacturing optimization through multi-physics modelling	H2020	DEFACTO	2020 2023	CID, CEA

1.3.4 Methodology

1.3.4.1 Overall methodology for BIG-MAP

With **BIG-MAP**, we are proposing a paradigm shift in the battery discovery process. This transformative shift requires a combination of transitioning from the sequential thinking in the traditional battery discovery process, and a number of **scientific breakthroughs** in key research and development areas for batteries, as well as complementary research areas like AI and autonomous robotics. This cannot be achieved using traditional methodologies and project organization structures, so we propose a fully connected matrix organization (section 3.1.1) bridging a set of **five Competence Pillars** with **five Cross-cutting Initiatives**, establishing a **new methodological framework** for bridging the traditionally separated competence domains.

1.3.4.2 BIG-MAP competence pillars

We have identified the following core competence pillars, where scientific/methodological breakthroughs must – and can – be achieved within the 3-year ramp-up phase:

- **Accelerated Atomic-scale Simulations** (WP2; led by UU). Connecting the accuracy of Quantum Mechanical calculations with machine learning (i.e. QML) provides a pathway to massively accelerate the exploration of the vastness of chemical compound space. Specifically, exploring the complexity of electrode-electrolyte interfaces without drastically compromising the accuracy/fidelity.
- **Multi-scale Modelling** (WP3; led by KIT). Developing predictive scale-bridging models for battery interfaces/interphases on the basis of the atomic constituents of the materials involved. Using AI to enhance the scale-bridging and validating the models against first-principles calculations and experimental data. Physics based models that lack predictive power, will be augmented with data to generated predictive AI-enhanced models that can be integrated into the multi-scale modelling chain.
- **Modular Synthesis Robotics** (WP4; led by FRAUNHOFER). Accelerating the materials synthesis procedures by extending automatic robotics from formulation to synthesis. Development of an open-source framework of hardware and software modules to be seamlessly integrated to automate specific synthesis processes. The developed framework will implement optimized molecules and novel materials for, e.g., protective coatings.

- **Characterization** (WP5; led by CEA). Construct a European experimental platform organized for multi-modal characterization using standardized cells/protocols/data collection, treatment and analysis. Organize the access to beamtime at the European level for the investigation of model/real battery interfaces. Define effective feed-back loops with multi-scale modelling, and evaluate AI modules for optimization of data acquisition and analysis.
- **HTS and Testing** (WP6; led by FZJ). Through strong interaction and complementarity, a new degree of integration in the high-throughput formulation-characterization-performance evaluation chain across time and length scales will be achieved. This will enable establishment of a chemistry neutral and versatile materials characterization, as well as a HTS performance evaluation module within the **BIG-MAP**.

1.3.4.3 BIG-MAP cross-cutting initiatives

To complement and connect the scientific and methodological breakthroughs, a set of cross-cutting initiatives can – and will – provide new ways of connecting the breakthroughs in their respective fields to yield synergy.

- **Battery Interface Ontology** (WP7; led by SINTEF). The development of a Battery Interface Ontology will ensure interoperability between multiple scales, techniques, and domains in the discovery process. The BIO will facilitate the work of battery experts in different fields to convert real-life observations to a common digital representation.
- **Standardization and Protocols** (WP8; led by CNRS). Working closely together with BATTERY 2030+ (LC-BAT-15-2020) and Batteries Europe, we will establish community-wide standards for battery data and metadata formats, as well as experimental procedures and testing protocols. These are essential for ensuring the transferability, interoperability and usability of the generated results.
- **Infrastructure and Interoperability** (WP9; led by EPFL). Developing a web-based shared infrastructure and the capabilities (software infrastructure, simulation/experimental control and data handshaking) leading to automated simulations and experiments to access these capabilities and data; and to have simulations and experiments communicate with each other.
- **AI-accelerated Materials Discovery** (WP10; led by KIT). Accelerating materials discovery and optimization in both experiments and *in silico* through close collaboration with multiple WPs. This cross-cutting initiative will provide the technology and implementation of sequential (active) learning methods, automated analysis and reasoning to accelerate materials experiments and synthesis routes.
- **Battery Interface Genome** (WP11; led by DTU). Developing BIG models for characterization and (inverse) design of battery materials and interfaces that combine the spatio-temporal characterization of the interfaces with physics and data-driven generative models to predict dynamic events across time and length scales, e.g. hierarchical latent space multi-scale models.

1.3.4.4 Project Management and Coordination, Exploitation and Outreach

A dedicated work package (WP1) will be needed to ensure Project Management and Coordination, Education, Exploitation and Outreach. WP1 will also work together with the Project Coordinator (PC) and the Executive Board (EB) to ensure the progress of the project (see section 3).

1.3.4.5 Gender aspects

BIG-MAP aims for a representative gender balance in the consortium, based on equal opportunity principles during the recruitment phase. The consortium fully subscribes to the **policy of the European Union on gender equality in general and in science** (e.g. article 2 and 3 in the Treaty of Amsterdam, COM (99)76 final, working document "Women and Science: Excellence and Innovation – Gender Equality in Science" in 2005) and the initiative Helsinki Group on Women in Science.

The consortium will ensure that gender bias and gender discrimination is avoided. Each partner will promote gender awareness and equality within the project at organizational level. This is guaranteed since all partners are already providing equal job opportunities to men and women, facilitating flexible working arrangements and care services in view to allow men and women to reconcile their private and professional lives.

BIG-MAP ensures the sex and gender requirements set by the European Commission are followed. **BIG-MAP** has three female work package leaders and three female WP co-leads, plus a significant percentage of female key personnel (see details in Part B Section 4-5). In addition, numerous tasks will be coordinated by female scientists.

1.4 Ambition

The ambition of **BIG-MAP** is to develop core modules and to deploy the infrastructural backbone of the BATTERY 2030+ vision for a battery MAP that demonstrates the capability of highly accelerated exploration, discovery and optimization of new active battery materials, electrolytes and interfaces/interphases. The battery MAP will enable autonomous closed-loop materials discovery and development through the use of **AI as an accelerator** for efficient orchestration of data acquisition, handling and analysis. The MAP will feed off multi-scale computer simulations,

high-throughput and high-fidelity experiments and testing. Utilizing both existing and generated data from the large community in academia, industry, and (ultimately) end-users. **BIG-MAP** pushes for advancements in autonomous high-throughput synthesis robotics and experiments with targeted utilization of European large-scale synchrotron/neutron facilities.

Central to **BIG-MAP** is the development of a **BIO** (WP7), **standardized testing and characterization protocols** (WP8) and the **shared data infrastructure** (WP9). This data infrastructure will be capable of performing autonomous acquisition, analysis, management and **data lineage tracking** from all sectors and domains of battery innovation and development. Once fully implemented, the European value chain for battery development and manufacturing will supersede any existing innovation network due to its **interoperable data infrastructure**.

Battery interfaces are arguably the least understood part of advanced batteries, notwithstanding that most of the critical reactions responsible for the battery performance occur here. **BIG-MAP** therefore focusses scientifically on the interfaces and specifically on the SEI and CEI. Accelerated design of battery materials requires a detailed fundamental understanding of the Battery Interface Genome, but to date interfaces and interphases have mainly been studied "post mortem" and with *ex situ* experimental techniques. The unique combination of multi-scale modelling, *in* and *ex situ* experiments with methods such as machine/deep learning will unravel **translational descriptors** that enable deeper insights and ultimately design capabilities. Experimentally, this means studying and **controlling interfaces and interphases *in operando***, i.e. while the battery cell is in operation. Computationally, it requires frontier developments of methods and codes capable of taking advantage of recent advancements in pre-exascale HPC facilities. This will enable fast and large steps towards better and more reliable batteries of the future (WP10). Through integration, the aim is to establish predictive and interpretable BIG models depicting the spatio-temporal evolution of interfaces/interphases, which will be integrated into the MAP.

We will develop novel AI-based tools and hybrid physics and data-driven models (WP11) to utilize the vast amounts of existing and generated data, with a strong emphasis on battery materials, interfaces and interphases. The data will be generated across different length and time scales, using a wide range of complementary approaches discussed above.

The **Key Demonstrators** (Table 1.2**)** will be developed during the first 3 years of the **BIG-MAP** ramp-up phase to *"demonstrate the potential to achieve a 5-10 fold acceleration in the materials discovery process"* and to exemplify the level of acceleration achievable with the **BIG-MAP** approach, within central parts of the battery discovery cycle.

1.4.1 Availability and fidelity of training data and materials

The achievable acceleration with the **BIG-MAP** approach is largely dependent upon the **availability, fidelity, curation and interoperability of the (training) data**, which is accessible on the specific battery materials and interfaces under investigation. Substantial amounts of data on advanced battery materials already exist, e.g., in the scientific literature, crystallographic and computational databases, as well as in presently inaccessible results, either **raw, bad, unpublished or proprietary industry data**, but the searchability and exploitability of the data is very low, even when using unsupervised natural language processing.[31] This is largely due to heterogeneity of the data and the **lack of data standards and provenance.**

Depending on the characteristics of the phenomenon or process under investigation, different experimental and computational techniques have **different levels of fidelity**, but also the quality and quantity of the accessible **metadata** is important. High-fidelity indicates an experiment or simulation that reproduces reality with a high degree of accuracy. Both high- and low-fidelity data are important for the proposed AI-based materials design and discovery, depending on the specific need for training data at any given time. Transferability and interoperability between high throughput laboratory and costly large-scale synchrotron and neutron scattering experiments, e.g., in terms of sample environments and characterization protocols, will play a critical role in ensuring the acquisition of multi-fidelity data describing battery materials and interfaces. Similar needs exist for expensive **first-principles calculations** and analytical simulation models. This calls for the ability to perform **autonomous, on-the-fly analysis** of the vast amounts of data generated at laboratories, synchrotron/neutron and HPC facilities across Europe.

Demonstrator electrode and electrode materials: To enhance the data and materials fidelity, **BIG-MAP** will focus on a limited and predefined of set of high-performance Li-ion electrode materials, which will be produced and delivered by a single partner and distributed to all other partners. We have selected **graphite/silicon for the negative electrode** (produced by CID), and **NMC-811** (produced by UMI) and **LNO** (Lithium Nickel Oxide) (produced by BASF) for the positive electrodes, while the formulation of new organic electrolytes will be developed and optimized in the project (SOLV). This will allows us to demonstrate the potential of the **BIG-MAP** approach to optimize the particular electrode/electrolyte compositions/formulations to a specific interface/interphase challenge, using

[31] Tshitoyan, V. et al. Nature 571, 95–98 (2019)

(pre-)commercial high-performance materials combinations, while simultaneously demonstrating its ability to utilize existing (lower-fidelity) training data from multiple source and databases.

Figure 1.6 Relevant time and length-scales for multi-scale approaches for batteries.

1.4.2 Bridging multi-scale models and experiments

1.4.2.1 State-of-the-art

Interfaces and interphases: The interfaces between the electrodes and the electrolytes are where the energy conversion redox reactions occur, i.e., where ions and electrons are exchanged. Although an ideal interface generally consists of one atomic and one molecular layer, the interface between the electrode and the electrolyte is instead characterized by a larger region stretching up to several tens of atomic and molecular layers to either side[32]. If the chemical composition of the electrolyte is also changed close to the interface, this comprises the **interphase**. Both interfaces and interphases are several orders of magnitude smaller than the electrodes (nm vs. µm) and **interfacial reactions are therefore easily masked by their surroundings**. Furthermore, battery performance and lifetime are determined by multiple processes that occur not only on a vastly different length scale, but also on different time scales[33]. The time-scale for interfacial reactions spans from the picosecond (charge transfer) to the seconds/minutes (nucleation/growth phenomena), as well as hours/days/years for stability and lifetime issues (Figure 1.6). Experimental and computational techniques which are highly surface sensitive and display exceptionally high resolution and fidelity are therefore specifically targeted when studying interfaces/interphases in **BIG-MAP**.

Within computational (virtual) materials design, a single computational model that encompasses all these phenomena is beyond the limits of current computing power and methods. To address this challenge, individual models that describe a given time and length scale must be coupled together, e.g. by **passing key physical parameters from one scale to another,** in a chain to create a complete picture of battery performance, a technique known as **multi-scale modelling**. Today, multi-scale simulations utilize a number of different models and conceptual approaches. Properties of materials and interfaces are commonly studied with first-principle methods on the electronic and atomic scales, e.g. DFT and molecular dynamics (MD). Such atomic-scale models (among others) can be combined to screen the suitability of new materials[34] and predict important parameters describing thermodynamic[35], kinetic[36] and structural properties[35], as well as transport phenomena[37] in batteries. Multi-scale modelling techniques are currently being developed, for example, to optimize real and virtual electrode microstructures, study the effects of the fabrication process on cell performance, and electrode surface film growth[38].

1.4.2.2 Challenges and bottlenecks in state-of-the-art

[32] Philippe, B. et al. J. Electrochem. Soc. 163, A178–A191 (2016); Tripathi, A. M. et al. J. Chem. Soc. Rev. 47, 736–851 (2018).
[33] Franco, A. A. et al. Chem. Rev. 119, 4569–4627 (2019).
[34] Husch T. & Korth M. Phys. Chem. Chem. Phys. 17, 22596–22603 (2015).
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[38] Feinauer, J. et al. J. Comput. Sci. 31, 172–184 (2019); Ngandjong, A. C. et al. J. Phys. Chem. Lett. 8, 5966–5972 (2017); Röder, F et al. J. Electrochem. Soc. 164, E3335--E3344 (2017).

The experimental characterization of batteries interface has been a **long-standing challenge**. While techniques are available for independently studying the micro-structural or the chemical properties of the interphases separately, very few are currently capable of breaking that partitioning and provide a full description of the evolution of an interface or interphase. Thus, sorting characterization techniques depending on their sensitivity in space and time is crucial to design an **integrated experimental and computational strategy to fully characterize and control the interphase formation and evolution**, where the most efficient techniques can be identified and used at any given stage of the interphase evolution (as indicated by the shading in Figure 1.7). It remains highly challenging to directly probe the interfaces and efforts were thus focused in the past to provide 2D or 3D visualization and quantification of gradients and/or heterogeneities at the relevant scales, e.g., from atomic (local chemical environment, coordination numbers, modified surface layers, strain and stresses), to nano-meso-microscales (morphology, porosity etc.) up to macroscale (dendrites, cracks, delamination (Figure 1.7). Real-time observations of electrochemical reactions/events at the interfaces have thus been pursued. For that, available characterization tools for battery investigations form an extremely rich experimental suite consisting of electrochemical (charge transfer/performance), spectroscopic (chemical information), direct-space (amicroscopy) and indirect-space (X-rays/neutron) techniques are needed.

Figure 1.7 Dynamic fidelity assessment of experimental and computational techniques (adapted from Vegge et al. [43]).

The root of the multi-scale challenge is that it is **not known how best to couple and link models at different scales** in an efficient and robust way. For example, in linking electronic and atomistic models "upwards" for a certain material, it is usually not known which of the **physical and chemical features** of the electronic model need to be carried over to the atomistic model to preserve the crucial elements of the description (**feature extraction**), nor what model expression is needed to capture these features. Going in the opposite direction ("downwards") is often even more challenging and plays a key role in the **inverse materials design** process. The large gain in time and accessible size in models on larger scales generally entails a sacrifice in detail and resolution. In order to provide both morphological and chemical information about the interphases to the data-driven models, there is a growing **need for coupling several computational and experimental techniques** to cover multiple length scales of interest and to correlate processes occurring at the atomic level with those at the scale of the electrode[39]. The development of such coupled techniques is still in its infancy but represents the next frontier to conquer in order to achieve a complete understanding of the battery interface in operation.

ML techniques would prove to be critical in providing the glue between the experimental characterization methods that provide high accuracy structural information at specific scales and physics simulations methods. This is especially useful for gathering data on the time evolution of the system as *in situ* characterization of buried interfaces are often very difficult or outright impossible. Appropriate physics simulation needs to be combined with intermittent characterization experiments to reconstruct the system (interphase) evolution. The challenge is also to conceive predictive machine/deep learning models that can generate lower level structural details (e.g., atomic structure) based on observations done at a higher level (e.g., grain orientation or microstructure). **Ingenious ML/DL techniques** need to be invented for performing such scale bridging across many orders of magnitude of time and length scales.

1.4.2.3 Addressing challenges and ambition

X-ray and neutron-based techniques are illustrative examples of techniques that can be combined to gain complementary information about battery interfaces. Common for these techniques is that they are used to their full potential at large-scale facilities (LSF), where the resolution (spatial, energy, time) and the energy range are superior to lab-scale instrumentation. This allows researchers to perform more advanced materials characterizations in which they can better differentiate the details of the battery interfaces. The characterization methodology as well as the materials understanding is therefore also highly driven by the research performed at these large-scale laboratories. Access to LSFs being limited, it is then important to also develop improved understanding of battery interfaces using

[39] Müller, S. et al. Nat. Commun. 9, 2340 (2018); Tardif, S. et al. ACS Nano 11, 11306–11316 (2017); Chattopadhyay, S. et al. Chem. Mater. 24, 3038–3043 (2012); Pietsch, P. et al. Sci. Rep. 6, 27994 (2016)

in house techniques, which can be used as a first characterization level or to provide specific data sets quickly. Finally, for achieving high-throughput levels, characterisation techniques should be organised in a way that they manage automated investigations of a large number of samples. This requires the development of workflow processes for characterisation to generate large quantities of data automatically. Either, the instrumentation and protocols are designed in a way to accelerate the acquisition of data, or the acquisition time itself could be reduced. Thus, it is a key challenge to maximize the efficiency of data acquisition, by combining information from characterization experiments in cheaper and faster setups and that in LSFs. While such workflows are conceivable at a specific scale, radical approaches are required to do so across multiple scales.

Recently developed generative deep learning methods in related fields[10,17] would be helpful for optimal exploration of the chemical and structural space for improved battery interfaces. State-of-the-art ML/DL techniques can be extended to automate the parameter/data sharing between from two adjoining scales of experimental or simulation methods. Traditional data representation differs significantly between multiple length scales as well as between experimental and simulation methods. A critical bottleneck in developing ML/DL-based integrated multi-scale characterization and simulation approaches is **scale/method agnostic structural data representation**, as well as a modelling strategy that can encompass all scales while maintaining acceptable fidelity in data and predictive models.

Such robust and predictive models for the key battery processes spanning multiple scale are thus needed to perform closed-loop discovery of battery materials. This pertains both to physics/simulation-based and data-driven materials discovery strategies. It is unrealistic that individual institutions and groups can develop the holistic approach required to enable breakthroughs in the discovery of materials for future ultra-high-performance batteries. For this reason, mechanisms must be instituted to **enable the curation of models and data sets of the highest quality** for the outstanding materials challenges (depth challenge), while at the same time **ensuring the availability of such models and data for the community at large**, i.e. beyond the groups/consortia that curate models and data for specific scales (width challenge). Only the full integration of physics/simulation-based and data-driven multi-scale models generated under the exploitation of AI technology with automated synthesis and characterization technologies will enable the envisioned breakthroughs required for the implementation of fully autonomous materials discovery. Key bottlenecks towards the realization of closed-loop discovery are the concurrent availability of data and models outside the groups that generate them essentially in real-time. There is thus a need for a paradigm shift and to generate **automated workflows** that not only assures for a complete reproducibility of the results but also allow for **AI-orchestrated launching of the required experiments, simulations and tests at appropriate scales**, without the direct input from the researcher. **BIG-MAP** will be a cornerstone in the development of tools that enable such integration of research tools by providing platforms for decentralized data access with qualified access protocols that enable the exploitation not only of FAIR[40]/open source but also existing proprietary data.

Releasing the full potential of inverse multi-scale modelling and characterization to support new materials, interface and device design requires radically new approaches to bridge scales beyond the state-of-the-art that cannot be achieved by research communities in individual countries. The ML techniques and physics-guided data-driven models can be used to identify the most important parameters, features or fingerprints[41]. Coupling and linking the efforts among disparate research communities working across time and length scales will be a key effort for a battery MAP to create a stronger, more competitive European battery community and contribute to the efforts of, e.g. The European Materials Modelling Council (EMMC) on ensuring interoperability. **BIG-MAP** will exploit European LSFs and computational infrastructures, such as PRACE and the EuroHPC supercomputers, e.g. LUMI (Large Unified Modern Infrastructure) when it becomes operational[42], as well as the results of prior and ongoing EU and national funding efforts, such as former and ongoing centres of excellence in HPC applications like NOMAD, MaX and EoCoE.

The inability to limit and control interfacial processes like dendrite and SEI/CEI formation, which span numerous time- and length scales, is currently preventing us from exploiting the full potential of new electrolytes and electrode materials. Inverse design and engineering of high-performance interfaces/interphases has remained an **elusive dream**, but hybrid physics- and data-driven models trained on large multi-fidelity data sets from multi-scale simulations, experiments and databases may hold the key to unlocking the dream[43]. This would not only allow for **leapfrogging the performances of existing Li-ion batteries** but also unlock the development of new chemistries with great promises for applications such as grid storage and electric vehicles. **BIG-MAP** provides a key step in the ambitions to go beyond the current limitations by mapping the chemistry of the battery and all its components/interfaces.

[40] Wilkinson, M. D. et al. Sci. Data 3, 1–9 (2016)
[41] Reichstein, M. et al. Nature 566, 195 (2019)
[42] datacenter.csc.fi/wp/about-lumi/
[43] Bhowmik, A. et al. Energy Storage Mater., 21, 446-456 (2019)

Attempts to find **dynamic interface descriptors** capable of capturing the kinetics for the interphase formation[44] have had little success so far owing to the difficulty of capturing a single physical property defining the dynamic nature of the interface[45]. Rather than a single physical property, a **multi-scale/multi-feature** approach combining multiple tools will certainly be necessary to grasp the dynamics of the interface at different scales[46]. One of the most important issues is to link physical observables such as thermodynamic potential, diffusion coefficient, activation energies, pair correlation functions and low energy phases to descriptors. Identifying the multitude of **interface descriptors or genes** that encode the spatio-temporal evolution of battery interfaces and interphases is a prerequisite for the inverse design process, and simply cannot be achieved with existing methodologies.

The reliability of the physical and ML/DL models needed for **BIG-MAP** will be assessed continuously through **uncertainty quantification**. Predictions with unknown uncertainty are potentially useless results, since the discovery process is dealing explicitly with the identification of "**unknown unknowns**"[47]. Errors and uncertainties in predictive models arise from both the accuracy of the model but also from the uncertainties in the data used to build those models. Uncertainty quantification and (dynamic) fidelity assessment of individual experimental and computational techniques (data sources), as well as in generative deep learning poses a key challenge. Uncertainty estimation is often used in the characterization of batteries, e.g. in estimations of state of charge (SoC), state of health (SoH), etc., with ML, and has recently also been applied in computational techniques[48]. However, the concept is less established in DL techniques[43]. Generative and predictive neural network models are generally not reliable when they encounter conditions that have not been sampled during model training[49].

Figure 1.8 Coupled hierarchical latent space model for bridging of multiple scales in simulations and experiments.

We propose to develop an integrated multi-scale approach through a **generative hierarchical latent space model** (Figure 1.8). This requires curated and interlinked data on the structure of the interphases over multiple time and length scales. Indeed, no such unified interface descriptor currently exists, and empirical reasoning still prevails in attempts to harness the dynamics of the interfaces. However, by linking BIG and MAP together using AI, physics-guided AI-orchestrated materials discovery can go beyond the current limitations. To provide sufficient data to the models, high throughput will be required, asking for organizing characterization techniques in a way that they manage the investigation of a large number of samples. This new type of organization requires the use of automated experimentation and workflow processes, as discussed above. In a second step of the workflow, higher quality/fidelity data have to be acquired requiring more complex and advanced techniques able to provide high resolution data and precise operando measurements.

Furthermore, the development of multi-modal characterization techniques that can be performed on the functioning system, i.e., operando measurements, must be privileged since they enable probing the interaction and functions of the battery components in real-time, going from measurement of the static battery system to the dynamic battery system, and set-ups capable of performing operando measurements of applied systems for LSFs must be developed. To accelerate our findings, specific cell setups must be constructed in **BIG-MAP** to allow carrying out measurements in a systematic fashion with transferable sample environments; these cells would ideally allow one to obtain multi-techniques information/data about the same materials/interfaces.

[44] Giordano, L. et al. J. Phys. Chem. Lett. 8, 3881–3887 (2017); Boyer, M. J. & Hwang, G. S. Curr. Opin. Chem. Eng. 13, 75–81 (2016).
[45] Kristoffersen, H. H. et al. Chem. Sci. 9, 6912–6921 (2018)
[46] Franco, A. A. et al. Chem. Rev. 119, 4569–4627 (2019)
[47] Jia et al. Nature, 573, 251–255, (2019)
[48] Christensen, R. et al. J. Phys. Chem. C 120, 24910–24916 (2016)
[49] Kendall A. & Gal Y. arXiv Prepr. arXiv: 1703.04977 (2017)

1.4.3 Data management, infrastructure and interoperability

1.4.3.1 State-of-the-art

A central requirement for the accelerated, rational design of battery materials and interfaces is easy access to and the interoperable data from multiple sources and domains. Unfortunately, no such large database currently exists for battery-oriented interface properties (such as existing crystal structure database for materials). The implementation of such an European database would first require the development of characterization and modelling techniques/methods capable of providing a high-fidelity description of the interfaces (and their dynamics), and allowing a **general classification of phenomena and categorization** of model interfaces.

There are substantial ongoing efforts to establish standardized infrastructures that allow users to store, preserve, track, and share data in a curated, well defined format that can be **accessed from different platforms** and for various purposes. Over the last decade, the development of several theoretical databases[50] like The Materials Project, AFLOWLIB, Open Quantum Materials Database (OQMD), the Computational Materials Repository (CMR) and **The Materials Cloud[50]** have emerged to complement experimental ones[51] like The Inorganic Crystal Structure Database (ICSD), Springer Materials, the ICDD database, the High Throughput Experimental Materials (HTEM) Database, and the Materials Experiment and Analysis database (MEAD). Although these databases contain several million of datapoints, there is a **need for infrastructure tools that enable bridging between databases**, between experimental and theoretical data, between different length and time scales[52]. A number of large-scale European projects in this area are MaX[53], MARVEL[54], which develop repositories as well as a Materials Encyclopedia and Big Data Analytics tools for materials science and engineering, but with a strong focus on electronic structure codes.

The development of more comprehensive databases is closely connected with the implementation of workflows to automate materials discovery. FireWorks[55] and AiiDA[56] are two examples of infrastructures that have been implemented for managing workflows and data. Currently, each workflow, as it happens for databases, cover at most few concatenate experiments or simulations, which in most cases only describe the (ground state) properties of the materials at a single scale.

1.4.3.2 Challenges and bottlenecks in state-of-the-art

The development of predictive models to design future batteries requires thorough validation using **curated data sets**. In particular, the validation of the complex models to be used for the inverse design of battery materials and interfaces requires the integration of high/multi-fidelity data covering complementary aspects of the materials and device characteristics. Presently, such data sets are too sparse and cover only a fraction of the required phase space.[57]

Data generated by academic and industrial R&D groups across Europe today is generally not available to other stakeholders. Further, there is no well-established procedure to share curated data, which means that existing high-fidelity data may be difficult to find and complement. **Access to suitable training data is essential**, and establishing cross-disciplinary strategies for efficient (re)use of existing experimental, computational and resource databases is a key challenge. Other important challenges include **access to 'bad' data**, e.g., from failed experiments, and strategies to enable users to retain IPR of their data.

The data set size required by a fully implemented **BIG-MAP** is difficult to assess, but we can use geosciences as an example with comparable complexity. Here, many petabytes of data is available, but **generative models for predicting long-time scale events are limited by the model uncertainty**[41], i.e., tomorrows weather forecast is easy, while drought prediction remains out of reach. Comparable or possibly larger data sets can be required for the inverse design of dynamic battery interphases, which stresses the need for **community-wide standardization and curation of data** across research disciplines and domains, including the industrial sector (BASF alone generates >70 million electrochemical data points per day[58]).

Intensive efforts have been devoted in the last years to uncover the complexity of the battery interface dynamics and to control its reactivity and functionality, generating large data sets by individual group that remain largely under-exploited. Hence, a paradigm shift is needed in order to address this fundamental challenge. For that, data must be

[50] Jain, A. et al. APL Mater. 1, 011002 (2013); Taylor, R. H. et al. Comput. Mater. Sci. 93, 178–192 (2014) ; Kirklin, S. et al. npj Comput. Mater. 1, 15010 (2015); Materials Cloud (www.materialscloud.org); Landis, D.D. et al. Comput. Sci. Eng. 14, 51–57 (2012)
[51] Bergerhoff, G. & Brown, I. D. in Crystallographic Databases (ed. F.H. Allen et al.(Hrsg.)) (International Union of Crystallography, 1987); ICSD - Inorganic Crystal Structure Database and ICDD (2019). PDF-4+ 2019 (Database (International Centre for Diffraction Data, 2019) and Zakutayev, A. et al. Sci. Data 5, 180053 (2018); Soedarmadji E. et al., npj Comput. Mater., 5, 79 (2019)
[52] Zheng, C. et al. npj Comput. Mater. 4, 12 (2018)
[53] MaX - Materials design at the Exascale. European Centre of Excellence for HPC (www.max-centre.eu)
[54] NCCR MARVEL (nccr-marvel.ch)
[55] Jain, A. et al. Concurr. Comput. Pract. Exp. 27, 5037–5059 (2015)
[56] Pizzi, G. et al. Comput. Mater. Sci. 111, 218–230 (2016)
[57] Strmcnik D. et al., Nature Catalysis 1, 255 (2018) Cao C. et al. Joule, 3, 762-781 (2019)
[58] Hartmann Leube, Senior Vice President BASF, AABC Europe, Wiesbaden, January 2019

collected, handled and analysed in a more systematic and automated manner, e.g., to be accessible to the central AI orchestrating the accelerated discovery process. To ensure a meaningful synergy between experiments, simulations and AI-based models, the simulations and models should become more realistic and closer to experimental conditions. Similarly, the experimental conditions should be made as ideal and reproduceable as possible to decouple the different effects and reactions, especially for the initial training of hybrid physics-aware data-driven models, i.e. data-driven models where the parameter space is bound by physical laws and insights (section 1.4.5.3).

1.4.3.3 Addressing challenges and ambition

In order to facilitate community-wide access to the **BIG-MAP** data, we plan to develop a **Battery Interface Ontology** (BIO), i.e., a common knowledge-based representation system to ensure interoperability between different scales, techniques and domains in the battery discovery process. The BIO will facilitate the work of battery experts in different fields to **convert real-life observations to a common digital representation**. As a basis of this effort, we will **lead a community-wide effort to standardize experimental protocol and data formats** to orchestrate the level of complexity that AI, multi-scale models and different experimental techniques bring to the picture.

A **common data-infrastructure and web-interface** will be developed to help ensure interoperability and integration of experimental data and modelling in a closed-loop materials discovery process across institutions in real time. Realization of such an infrastructure will make the data generated by individual consortia (instantly) available to the community at large and drastically shorten the R&D cycles. **BIG-MAP** will pioneer such an infrastructure based on a decentralized access model, where data, simulation protocols and AI-based discovery components from different sources can be used via **qualified access protocols**. The infrastructure will be based upon the structure of **The Materials Cloud** and exploit existing EU results regarding computational protocols, data-organization and resources at an unprecedented scale, while at the same time ensure more **secure protection of the data and IP** (e.g., through self-generated DOIs for data sets). Such a comprehensive model will facilitate identification of missing parts of the required data space. The European Materials Modelling Ontology (EMMO)[59] and ontology initiatives in closely related area like materials synthesis[60] will be actively used to ensure maximum efficiency and complementarity.

In collaboration with other EU activities, such as the MarketPlace projects, we will develop a **BIG-MAP App-store**, where data access, simulation/experimental protocols and automated analysis modules will be made available to the community at large and thus be accessible outside the groups who originally developed the protocols. This approach will generate a large set of **freely available apps and automated analysis modules** that address key development challenges of **BIG-MAP**, but also ensures the correct data formats are used when uploads are made to the **BIG-MAP databases**. Linking the modules into codified workflows, which will also be made available in the App-store, will enable the participants of the project and the community at large to address ever more complex challenges related to battery development. Through a Priority Stakeholder initiative (section 2.3.1.2), we will co-develop modules and **BIG-MAP** interfaces to external codes and techniques used in the community. Ultimately, even modules that remotely control robotic synthesis and characterization will be added to enable community wide autonomous discovery campaigns, albeit this goes beyond the ramp-up phase.

BIG-MAP will offer a unique opportunity to leverage the size of this effort towards the standardization of data from the entire battery value chain, by exploiting **semantic access protocols** enabled by EMMC and EMMO, as well as private groups with the goals of connecting academia and industry, materials modelling and engineering[61]. Here, there is a common need for the development of an **Open Innovation Platform**, which will facilitate the sharing of infrastructures and data between partners and the integration of modelling into industrial processes to close the gap between *in silico* design of materials, battery cell manufacturing and their end-use in electric vehicles and other everyday life devices. This requires an international standardisation of infrastructures, data formats and repositories, metadata, etc. The scope is to define **uniform European protocols** to cover all aspects of the battery materials and interfaces, from the material itself, to the physical law and models, over data acquisition and storage, to post-processing of data. Realization of such standards will make data interpretable, interoperable and reusable beyond the groups and communities that generate it, towards data and **meta-data formats** that can be easily used in an AI context. This will also allow for a more consistent and accurate verification and validation of the models, which is needed for an accelerated materials discovery. The "materials Modelling Data" (MODA) protocol has been developed to provide a systematic description of simulations at different levels (user case, model, solver and post-processor)[62], and a comparable strategy will be applied here.

1.4.4 Autonomous material synthesis

1.4.4.1 State-of-the-art

[59] Ghedini E. et al., EMMC Workshop on Interoperability in Materials Modelling (2017)
[60] Kim, E. et al. Chem. Mater. 29, 9436–9444 (2017); Kim E. et al. Matter 1, 8-12 (2019); Ashino, T., Data Sci. J., 9, 54–61 (2010)
[61] Goldbeck Consulting. Materials Modelling - Connecting communities: science to engineering, academia to industry. (2017)
[62] MODA – The European Materials Modelling Council. (https://emmc.info/moda/)

Another central element in the closed-loop materials discovery process[63] is the development of **autonomous and modular synthesis robotics**, which can be controlled and directed by a central BIG-MAP AI. Highly automated high-throughput synthesis is gradually becoming state-of-the-art for organic and pharmaceutical research[64], and examples are also emerging in the development of solids and thin-film materials[65], as well as for complex wet chemical processes[66]. Also, in the field of energy storage materials, robot-assisted synthesis and automation have opened the field to HTS of functional electrolytes and active materials comprising anode and cathode[8]. Correlation of structure-property relations and performance of active battery materials has, in combination with computational approaches such as data-mining, had a significant impact on the discovery of novel and promising materials.[64]

HTS is an experimental and computational paradigm, comprising the (virtual) evaluation of large materials libraries for functional properties. That is, the HTS achieves a rapid assessment of large formulation spaces, e.g. for electrolytes and compositions of electrode materials of selected battery chemistries, via the use of automation, miniaturization, and large-scale data analysis. The HTS paradigm in itself allows for the rapid identification of active and inactive battery components suitable for the targeted application domain beyond the identification of top performers and trends. A few examples of fully automated HTS systems for electrolyte formulation, cell assembly and selected relevant electrochemical measurements are now available (within the consortium)[67]. For systems comprising the assembly of two- and three-electrode cells as an additional HTS module, a systematic and effective measurement of the key electrochemical properties is possible through, e.g., scanning droplet electrochemistry[68]. Its efficiency gain of **two orders of magnitude is comparable to industry-based HTS systems**[69]. HTS systems represent a highly valuable, proven to be reliable[70], tool that enables the European community to accelerate the search towards identifying optimized electrolyte candidate formulations, as well as electrolyte/electrode interphases. Furthermore, based on the technical know-how built up during the years of construction and optimization, research domain specific improvements for accelerated battery research are ready to be implemented by the consortium.

In the field of organic synthesis, symbolic AI and Monte Carlo tree search procedures have recently been used to establish **computer-aided retrosynthesis**, which is a cornerstone for the inverse materials design [71]. In the field of inorganic crystal synthesis, new classes of phosphates and carbonophosphate have been obtained by developing a new model derived from ICSD data. By substituting ions in long known inorganic compounds/structures, new potential electrochemically active materials could be synthesized[72]. For AI accelerated experiments in large chemical spaces, a recent benchmarking study[13] suggests an acceleration of experiments by >10x. Combined with the already accelerated pace of HTS, a realistic acceleration of experiments of up to three orders of magnitude compared to conventional experimentation is potentially obtainable.

An emergent observation in literature [73] is that the deployment of an isolated, automated HTS workflow or development of an optimization scheme is not a grand challenge, but the integration of subsequent research tasks and the interoperation of instrumentation and algorithms is. The integration of knowledge and insights from theory and experiment welded together by AI to achieve targeted research has not been demonstrated to date.

1.4.4.2 Challenges and bottlenecks in state-of-the-art

Even though ML and AI will further expedite computational and automated development of molecular battery components (e.g., electrolyte systems) in the short term, radically new developments and innovation are needed to achieve autonomous closed-loop materials discovery. Until today, comprehensive electrochemical characterization of battery materials and the testing on the cell level is one of the major bottlenecks for the development of new electrolyte formulations, active electrode materials and combinations thereof. Despite a large number of approaches for high-throughput testing of battery materials in literature[74], **virtually none focus on short time scales processes or mechanisms**; in particular, cycling experiments may last days to weeks. Thus, it is essential to integrate the HTS with a **tiered screening pipeline** to identify lead candidates. For this purpose, a systematic initial characterization, including a large number of relevant electrochemical and transport properties, has to be performed on the materials'

[63] Coley C.W. et al. Angew. Chem, (2019), Accepted Manuscript (10.1002/anie.201909987)
[64] Gromski P.S. et al. Trends Chem., 2, 1, 4-12 (2020); Gromski P.S. et al. Nat. Rev. Chem., 3, 119–128 (2019); Tabor D.P. et al. Nat. Rev. Mater. 3, 5–20 (2018); Greenaway, R.L. et al. Nat. Commun. 9, 1–11 (2018)
[65] Huo, H. et al. npj Comput. Mater. 1–7 (2019); MacLeod B.P et al. arXiv Prepr. arXiv:1906.05398
[66] Steiner S. et al. Science, 363, 6423 (2019)
[67] www.uni-muenster.de/news/view.php?cmdid=10123&lang=en
[68] Sliozberg K et al. ChemSusChem, 8, 7, 1270-1278 (2015); Gregoire, J. M. et al. Rev. Sci. Inst. 84, 024102 (2013)
[69] chemspeed.com
[70] Alberi, K. et al. J. Phys. D, 52, 1 (2019)
[71] Segler M.H.S. et al. Nature 555, 604–610 (2018); Coley C.W. et al. Chem. Sci. 10, 370-377 (2019); Schwaller P. et al. ACS Cent. Sci., 5, 9, 1572-1583 (2019)
[72] Hautier G. et al. Inorg. Chem. 50, 656–663 (2011)
[73] Stein H. & Gregoire J.M. Chem. Sci.,10, 9640-9649 (2019)
[74] Hahn R. et al. Microsyst. Technol. 25, 1137–1149 (2019); Spong A. et al. J. Power Sources 119–121, 778–783 (2003); Lyu Y. et al. J. Mater. 3, 221–229 (2017)

level in an efficient and automated manner. In addition, the integration of new sensor systems, e.g., developed in LC-BAT-13-2020, will give a better-resolved state of the cells, including electrodes, interphases and gas evolution.

Further, demonstrating the capability of direct integration of (multiple) advanced on-the-fly autonomous analysis modules in HTS setups is needed. Combined with a fidelity-aware central AI (see section 1.4.5), this will enable accelerated determination of whether the most valuable information is obtained by performing additional characterization tests under different conditions, and/or modify the electrolyte formulation to obtain valuable new training data.

1.4.4.3 Addressing challenges and ambition

Whereas a complete software and hardware robotics infrastructure capable of performing fully autonomous synthesis of electrode materials and electrolytes is beyond the scope of the 3-year ramp-up phase and should be further addressed in subsequent projects, **we will develop a set of demonstrator modules to illustrate the value of the process automation.** This includes the key demonstrator **KD3**: "Demonstration of Autonomous Synthesis Robotics of protective electrode coatings", where protective organic and inorganic coatings will be developed using automated synthesis robotics guide by fundamental insights (see details in WP4). Further examples will include modular and process variable battery assembly, high-throughput electrochemistry based on scanning droplet cells and the development of protective electrode coatings (**KD5**).

A weakness in many HTS protocols utilizing automated synthesis, formulation and characterization robots is a large degree of customization for a specific task. Both hardware and software are often tailor-made for a specific purpose and for each other. As a result, they are inherently difficult to be used by the researchers outside the development team. The transferability of tangible assets between research institutions can be cumbersome and slow the development. **BIG-MAP** will facilitate the generation and maintenance of a universal and modular system for autonomous synthesis with widespread use.

For these activities, we will rely extensively on existing infrastructure within the consortium, e.g., hardware at the Materials Innovation Factory (ULIV) and FRAUNHOFER, while focusing on developing a flexible adaptation to the specific modules for advanced battery materials. Autonomous robotics for chemical synthesis of organic[64] and inorganic[65] materials should be further investigated and prioritized in dedicated subsequent projects.

1.4.5 AI and ML applied to battery development

1.4.5.1 State-of-the-art

Rapid advancements in ML and computational capabilities in the past decade have revived the field churning out breakthroughs towards universal AI in record time. Lighthouse examples include AlphaGo and AlphaZero, capable of surpassing human capabilities in two of the world's most complicated board games, Go and chess.[75] The promise of AI and deep learning in materials science offers tremendous opportunity[76] but the complexity and challenges faced in **AI-orchestrated, closed-loop discovery** of novel battery materials and interfaces are much greater than any isolated research project. To unravel the BIG for inorganic battery materials and organic/inorganic interfaces requires pertinent descriptors to "teach a computer chemistry". One of the major challenges is the acceleration of and integration between research tasks. Here, the availability of sufficiently large[77], curated data sets[78] for the training of the models is a prerequisite for the successful deployment of AI/ML techniques. While it is critical to achieve a full understanding of the SEI/CEI and similar interphases/interfaces when aiming to design smart interfaces for all types of batteries, it is experimentally challenging to probe a buried interface. Suitable surrogate descriptors that can aid in obtaining a full understanding of SEI/CEI formation and ageing processes must be established.

The central idea is accelerating the related research through ML/AI and a key tool in this endeavour is the description of a material in such a way that is amendable to an algorithm. These descriptions are typically referred to as embeddings or **latent space representations**. Famed examples are continuous representations of molecules like SMILES and SELFIES that allow rapid inverse chemical design for drug manufacturing[14]. A major challenge is the application of the same method for solid state materials due to the almost infinitely larger latent space that is only sparsely sampled by known crystal structures. However, limited generative models for solid-state materials exist that are capable to inversely designing new crystal structures[79]. There is a growing number of representations for compositions and elemental descriptors that often perform only mediocre in predicting out of limit materials[80]. Towards the deployment of an AI-accelerated MAP, **experiments need to be well-represented and automatically**

[75] Silver D. et al. Nature 529, 484 (2016); Silver D. et al. arXiv Prepr. arXiv:1712.01815 (2017); Silver D. et al. Science 362, 1140–1144 (2018)
[76] Coley C.W. et al. Angew. Chem, (2019), Accepted manu. (10.1002/anie.201909987); Umehara M. et al. npj Comput. Mater. 5, 34 (2019)
[77] Soedarmadji E. et al., npj Comput. Mater., 5, 79 (2019)
[78] Stein et al. Scientific Data volume 6, Article number: 9 (2019); Bölle F.T. et al. Batteries & Supercaps Accepted manu. (10.1002/anie.201909987)
[79] Noh J. et al. Matter, 1, 5, 1370-1384 (2019)
[80] Xiong Z. et al., Comp. Mat. Sci., 171, 1, 109202 (2020)

analysed. The combinatorial materials science community has demonstrated great progress in the field of automated materials experiment analysis in the past two decades surmounting fully automated analysis tools onto a proven foundation of accelerated research[70]. However, there are very few examples of ML directly applied to experimental data for battery research, in part due to the lack of well-curated data sets. A notable exception is the recent battery lifetime prediction from early battery cycling[81] that has the largest public experimental database to date of 124 batteries. There are, however, several methodologies in AI-enhanced materials research that directly pertain to **BIG-MAP** efforts. For the efficient acceleration of experiments, there are emergent demonstrations of autonomous orchestration[82] and benchmarking results suggesting high acceleration factors. Automated data analysis is largely performed in combinatorial materials science with exemplary demonstrations of AI-assisted signal extraction with superhuman capabilities[27] and fully automated phase mapping with crystal structure matching.

1.4.5.2 Challenges and bottlenecks in state-of-the-art

AI-orchestrated data acquisition is a central aspect in the development of a holistic infrastructure for materials data to facilitate agile communication between all branches of the materials discovery cycle. Developing **versatile and robust software packages** to control, orchestrate and synchronize automated instrumentations, handle multiple databases, and interact with various learning modules and AI algorithms is therefore essential.

While ML can potentially yield massive acceleration in the screening/identification of, e.g. structure-property relations of inorganic energy materials by combining ML, Genetic Algorithms and surrogate ML-models to increase the speed of discovery by many orders of magnitude[83], a key challenge within utilization of AI in the discovery of battery materials and interfaces is the development of **autonomous workflows for extraction of fundamental relations and knowledge from sparse data sets**[76] spanning a multitude of experimental and computational time- and length scales.

Key challenges in the current state-of-the-art: Translating across time and length scales in computational modelling, efficient interfacing instrumentation using AI orchestration, integrating computational and experimental workflows, fully automating data analysis using AI

Computational modelling at different scales can be used to, e.g., propose new electrode coatings[84] and provide valuable insights into the spatio-temporal evolution of interfaces and interphases. Coupling back experimental insights to these models has not yet been demonstrated (a key demonstrator (**KD8**) in **BIG-MAP**). Feedback loops typically hinge upon communication protocols and data management which, for the most part, is not properly performed. An emergent realization[85] is therefore to establish standardized measurement protocols and reporting schemes beyond FAIR. For the dynamic description of interfaces, the massive challenge of ensuring interoperability and the coupling of scales is critical since interphase structures often extend to the nanometre scale and have influence on both adjacent bulk phases (electrode and electrolyte). To capture the complete influence of the interphase on the full cell behaviour is therefore not possible without further upscaling to the continuum scale, nor without integration of the mathematical theories used on each scale[30]. A coupling with AI-based physics-aware data-driven methods (**KD11**) would strongly enhance the quality of the determination of interface descriptors, features and parameters, by enriching the physical simulation with validated correlations between idealized physics/chemistry-based simulations and data from real materials.

Coupling theories with completely different mathematical structures is particularly critical at interfaces. Hence, for interfaces between electrodes and electrolytes, predictive modelling of the electrochemical properties and reaction kinetics between complex solid surfaces with defects and chemically different liquid electrolytes containing ions, neutral solvents molecules and additives is highly challenging, but insights and approaches in the consortium can be transferred from other electrochemical interfaces, e.g. electrocatalysis.[45,86] To understand and predict, e.g., the accessible power density but also the safety of batteries, a deep understanding of the kinetics of interfacial reactions, ion transfer reactions and side reactions is essential. A complete and closed mathematical description of the whole reaction mechanism is enormously challenging, since coupled ionic and electronic transfer reactions in electrochemical relevant environment include usually coupled multistep reactions[87].

For the acceleration of instrumentation there is a critical need for **fully automated data analysis**. While the analysis of most pertinent electrochemical data for batteries is largely automated, there is limited progress in automated analysis of, e.g., current voltage curves for redox phenomena and electrochemical impedance spectroscopy (EIS).

[81] Severson K.A. et al., Nature Energy, 4, 383–391 (2019)
[82] Roch L.M. et al., Science Robotics, 3, 19 (2018)
[83] Jennings, P.C. et al. npj Comput. Mater. 5, 46 (2019)
[84] Tian Y. et al. Joule 3, 1037–1050 (2019); Xiao Y. et al. Joule 3, 1252–1275 (2019); Chen, T. et al. Frontiers in chemistry 7, 1–10 (2019)
[85] Aykol M. et al. Matter, 1, 6, 4, 1433-1438 (2019)
[86] Kristoffersen H. et al. Chem. Commun., 56, 427-430 (2020)
[87] Bruce P.G. & Saidi M.Y. J. Electroanal. Chem. 322, 93–105 (1992); Lück, J. & Latz, A. PCCP. 20, 27804–27821 (2018)

Such analysis currently require expert mediation and existing AI amended data analysis and extraction techniques will need to be adapted.

Besides the data analysis challenge, there is a practical need for orchestration platforms. Commonly employed frameworks such as the Robot Operating System (ROS)[88] from ULIV and ChemOS[82], e.g., combined with advanced Bayesian optimizers like Phoenics and Dragonfly or exploration algorithms like Curiosity [89], have been deployed for autonomous materials science but have a steep learning curve. There is a need for rapid deployment of more versatile and robust autonomous orchestration capabilities to reach community acceptance and adaptation. These demand an agnostic instrumentation/computation framework and efficient scheduling of autonomously orchestrated experiments. Developing more agile and versatile orchestrators and optimizers will be a challenge that stretches beyond the ramp-up phase, so a first objective here is ensuring the standardization and interoperability of the data streams.

1.4.5.3 Addressing challenges and ambition

A flexible plug-in architecture ultimately needs to have the capability of dynamically ingesting new kinds of information from external sources, be it databases, computational models for materials and retrosynthesis or manufacturability data. Continuing development and deployment of HTS and autonomous robotics for synthesis and testing will evidently grow a valuable knowledge foundation that **BIG-MAP** needs to utilize to further expand and enhance autonomous synthesis planning and evaluation in real time.

Generative models, i.e. probabilistic models for the observed data for the spatio-temporal evolution of battery materials and interfaces, are at the centre of **BIG-MAP**. **Generative deep learning** is a class of models that combine generative modelling approach with deep neural networks[90]. One of the main reasons for employing deep generative models is that it **enables the prediction of new data points**, e.g. in regions of phase space where limited data is available. Recent examples include the generation of materials images from optical absorption spectra[91] or thin film morphology from deposition parameters[92]. Developing hybrid physics and data-driven models will be an essential part of **BIG-MAP**. Emblematic are models incorporating physical constrains similar to phase mapping algorithms obeying the Gibbs phase rule, the extraction of fundamental knowledge from materials databases and literature[31], or operando characterization data from synthesis and materials/cell level testing.

Figure 1.9 Uncertainty-guided generative deep learning model for interface evolution (adapted from [43]).

Inverse design enables the generation of candidate materials and interfaces/interphases that are specifically **designed to meet specific performance targets**, cost and compatibility requirements of a given battery technology, in principle without imposing *a priori* constraints on the composition and/or structure of the material/interface. Interfaces specific performance metrics can be achieved, while retaining a (reasonable) degree of control over how the interface evolves over the battery lifetime. Inverse design of battery materials and interfaces, i.e., optimizing and engineering materials and interfaces from the starting point of a particular desired functionality without defining a specific starting composition, structure, etc., has until now been unfeasible for most battery challenges due to the massive complexity. However, the complexity of the design space makes inverse design based on generative deep learning models particularly enticing in the development of ultra-high-performance, sustainable batteries. A first demonstration will be provided (**KD11**), but further developments will be needed in subsequent projects.

AI-assisted multi-scale models for modelling, e.g. transport phenomena self consistently coupled with local reaction kinetics within the battery electrodes will require the development of adequate mathematical frameworks, which will have to deal with the massive amount of experimental data that will be made available, and with the separation of length- and time-scale between homogeneous nucleation (a rare molecular event) and molecular growth and

[88] Quigely et al. ICRA Workshop on Open Source Software (2009) (www.ros.org)
[89] Hase et al, ACS Cent. Sci 4, 1134-1145; Kandasamy et al. arXiv:1903.06694 (2019); Grizou et al, chemrxiv.6958334.v1 (2019)
[90] Yeh R. A. et al. in Proceedings of the IEEE Conf. on Comp. Vision and Patt. Recog. 5485–5493 (2017)
[91] Stein et al. Chem. Sci.,10, 47-55 (2019)
[92] Banko et al. arXiv Prepr. arXiv:1910.09468 (2019)

aggregation. Current approaches[93] will have to be unified with new simulation paradigms, based on innovative coarse-graining techniques[94].

1.4.6 BIG-MAP ambition all over the battery value chain

The **European battery value chain critically depends on generating new IP and concepts**, and **BIG-MAP** aims to deliver this through the accelerated research strategy. Emerging markets and governmental financing of large-scale battery production facilities have leveraged the economics of scale in battery production prices. Production capabilities have grown exponentially in the past decade such that the learning curve of price-vs-production plummeted the prices for modern Li-ion batteries. Scarcity of CRMs and virtually no additional capital gains through cost reduction, there is a pressing need to develop economically viable alternatives for battery production in Europe. **BIG-MAP aims to be the precursor for a battery manufacturing revolution** in Europe, by targeting virtually all (low TRL) steps of the value chain[95]. By providing a blueprint (D1.15) of a **modular and chemistry-neutral research platform**, emergent battery technologies such as Na-, Ca-, or Al-ion batteries can potentially achieve similar or superior performance as Li-ion batteries. During the **BIG-MAP** ramp-up phase, the **12 Key Demonstrators** will be developed on the basis of SoA advanced materials for Li-ion to ensure availability and fidelity of materials, techniques and data, and to open up collaborations with industry. We will also build the foundation for future adoption of next-generation battery chemistries and materials (**KD12**). A hybrid approach of demonstrating the capabilities and offering novel battery chemistries promises to leverage the full thrust and trust of the industry whilst securing future-readiness.

The experimental capabilities of **BIG-MAP** targets the entire battery value chain, i.e. raw processed materials, over battery components to cell manufacturing and ecologic considerations. **BIG-MAP** will employ autonomous synthesis robots to target new organic electrolytes and coatings in an agile manner, offering the possibility for controlled composition and processing variation through a combinatorial synthesis of electrode materials, fully automated electrolyte formulation with interface and cell level analysis and complete battery manufacturing and testing with unprecedented throughput (**KD5**). These developments feed on the expertise of partners/Pis form their involvement in related initiatives, e.g., Mission Innovation (IC6), JCAP, TRI-AMDD, Power2X, and many more that all advanced capabilities of high-throughput screening instrumentation and data analysis. Our contributions aim to offer open community tools with possible technology transfer to benefit various other clean energy projects globally. When fully developed and deployed, **BIG-MAP** will offer the possibility to screen and manufacture several hundred of battery materials a day. Industrial interactions are therefore possible for electrode and electrolyte materials, cell- and stack-level optimization and deliver an edge over competitors for the European battery value chain.

2 Impact

2.1 Expected Impact

The electrification of the energy and transportation sectors in Europe remains a key roadblock in reducing CO_2 emissions and in EU's implementation of the Sustainable Development Goals.[96] A commercially viable and environmentally sustainable domestic production of battery cells in Europe is of critical importance for the ongoing **transition of the European automotive industry towards e-mobility**. Therefore, the European Commission placed the highest priority on accelerating the establishment of a competitive and sustainable European battery industry. A globally competitive battery value chain in Europe can only be achieved through a world-leading research and innovation ecosystem bridging scientific excellence and industrial leadership. BATTERY 2030+ and **BIG-MAP** specifically strive to establish the **fundamental and long-term framework** (**TRL 1-3**) that directly benefits both the short-to-medium term implementation (e.g., Strategic Energy Technology Plan and Batteries Europe) and the commercialization (e.g., the **European Battery Alliance**).

2.1.1 BIG-MAP impact overview

BIG-MAP will create the infrastructural backbone of a versatile and chemistry neutral framework capable of reaching a 10-fold increase in the rate of discovery of novel battery materials and interfaces in Europe

Key impacts for the European battery value chain may be summarized as follows:

- Data standards and testing protocols: Together with Battery 2030+ and Batteries Europe, **BIG-MAP** will be the driving force in the creation of European battery research community standards for data management and testing protocols (WP8). This requires defining a BIO to bridge battery data from all sources and all fidelity

[93] Todorović M. et al. npj Comput. Mater. 5, 35 (2019)
[94] Salvalaglio M. et al. Proc. Natl. Acad. Sci. U. S. A. 112, E6-14 (2015)
[95] European Battery Alliance (EBA)
[96] Europe Sustainable Development Report (2019)

levels (WP7). This is of fundamental importance for an accelerated discovery of novel battery materials and interfaces, where computational models, AI, and experimental evidence is needed.

- Web-platform and database: A www.BIG-MAP.eu website will be created with links to the **BIG-MAP App-store** and **databases** to collect, analyse and share implementations and battery data created within **BIG-MAP**, as well as **community contributions** (WP9). This infrastructure assures the protection of data and IPR when required. New standards for preservation and dissemination of software and data are thus created.
- Multi-scale and multi-fidelity models and techniques: **BIG-MAP** will deliver a number of novel **predictive models** (WP11) and multi-modal experimental setups (WP5) that will address key challenges in the description, understanding and design of battery interfaces/-phases by incorporating information across all fidelity levels. True predictive power beyond simple model systems necessitates data from several length and time scales (WP3).
- Demonstrators: **12 Key Demonstrators** will showcase **BIG-MAP**'s ability to accelerate materials research by a factor of 5-10 during the ramp-up phase, e.g. ML-accelerated atomic-scale interface simulations (WP2), ML-accelerated synthesis robotics (WP4) and experimentation (WP6), ML translation of results from experiments to computation and back (WP10). Automated workflows integrating experiments and computational efforts and an associated **BIG-MAP** App-store will be also be demonstrated (WP9).
- Hybrid physics and data-driven interface models: **BIG-MAP** proposes that **integration of physical and data-driven models** can achieve predictive accuracy and enable inverse materials design for systems and materials governed by multi-scale phenomena (WP11). Achieving the **highest level of data/cost efficiency** will reduce innovation barriers for new battery materials and interfaces. The demonstration of such hybrid modelling approaches can pave the path for a similar 10x acceleration in other engineering systems design.

The specific impact of **BIG-MAP** relative to LC-BAT-12-2020 call is summarized in Table 2.1.

Table 2.1 – Contributions towards the specified impacts in the LC-BAT-12-2020 call

Expected Impact of LC-BAT-12-2020	How will this be addressed in BIG-MAP
Demonstrate a fundamental paradigm shift in the materials discovery process for clean energy materials that can significantly accelerate the development cycle for future battery materials and technologies, which cannot be achieved using conventional Edisonian type trial-and-error approaches.	The developed **interoperable data infrastructure** in **BIG-MAP** will provide and demonstrate a true paradigm shift in the battery discovery and development process by enabling direct orchestration of experiments and computation whilst allowing **real-time access to data from all domains.** **BIG-MAP** will develop a new class **of integrated workflow**s that builds upon the shared data standards and ontology (BIO) to automate the **seamless integration of simulations and experiments**, e.g., subsequent to a HTS experiment, a high-fidelity benchmarking LSF experiment is launched, and/or a complimentary computer simulation at the relevant scale(s) to simulate the reaction/structure/evolution matching the specific materials/interface and experiment performed. This will be made possible by utilizing the **full data lineage/provenance of the discovery cycle** (i.e. providing unique materials, experimental and simulation identifiers) and facilitate a fast identification of feature vectors and interface descriptors bridging different time- and length-scales. **Uncertainty-based hybrid physics- and data-driven and models** for the predictions of the spatio-temporal evolution of the battery materials and interfaces will additionally rely on the tools for dynamic fidelity assessment to acquisition to optimal cost-to-value data for (unsupervised) training.
Demonstrate the potential to achieve a 5-10 fold acceleration in the materials discovery process, e.g., through a reduction in the number of required experimental trials.	Through the development of the **12 Key Demonstrators** (Table 1.2), we will show-case the ability to accelerate critical/rate-limiting steps in the discovery process. One example is the ~10^5 speed-up in the atomic-scale modelling of SEI evolution using novel ML potentials to describe the interface reactions between silicon/graphite electrodes and the organic electrolyte (**KD1**). Providing ML-based analysis modules for **autonomous on-the-fly analysis** of characterization and testing data (**KD8**) will facilitate significantly accelerated analysis and utilization of (all) the acquired/accessible data. This will also enable "intelligent" use of otherwise unpublished and discarded data. The enhanced data access and the utilization of active learning will provide an unprecedented agility in terms of adaptation and adjustments, e.g., in **reducing the number of (unnecessary) experiments**. The autonomous synthesis robotics (**KD3**) will be guided by the model predictions, e.g., synthesizability of new materials/interface suggested before launching a new synthesis

	process; thereby **limiting the number of redundant synthesis attempts** to develop improved interfaces (**KD5**).
Demonstrate the ability to improve the performance of the selected battery interfaces with the developed methodologies.	The core focus of the 3-year ramp-up phase of the **BIG-MAP** project (covered in this application) will be on the development and demonstration of the **fundamental methodologies and infrastructure**. We have identified a set of specific battery interfaces to demonstrate how the performance can be optimized. In **BIG-MAP**, the developed hybrid models (**KD11**) will be used to optimize the electrolyte formulation for the electrode materials and intended operating conditions of the battery. By direct interrelation of e.g. electrolyte formulation to model predictions (**KD5**) of the SEI/CEI formation and, e.g., on-the-fly Electrochemical Impedance Spectroscopy (EIS) measurements, we will be able to improve the performance by **optimizing the electrolyte formulation** (**KD10**) and/or create **new protective electrode coatings** (**KD3,KD5**).

2.1.2 BIG-MAP impacts and the short, medium and long terms

The long-term vision of BATTERY 2030+ is to develop a versatile and chemistry neutral framework capable of reaching a 5-10 fold increase in the rate of discovery of novel battery materials and interfaces. The infrastructural backbone of this vision, the **BIG-MAP** in its final form will enable the inverse design of ultra-high-performance battery materials and interfaces/interphases. Through a modular approach and the integration of cross-cutting constraints like **manufacturability** and **recyclability** can directly influence the discovery process by introducing a bias towards materials compositions and structures, which favour, e.g., *in situ* recycling[97]. When fully implemented, **BIG-MAP** will also rely heavily on the direct integration of the insights, **smart sensors** and **self-healing approaches** developed in the **LC-BAT-13-2020 and LC-BAT-14-2020 projects** and other advances in the area of sustainable, ultra-high-performance batteries (D1.15).

To illustrate the full concept, we envisage having embedded sensors monitoring the stability and evolution of the electrode-electrolyte interface. Input from these sensors can then be sent to **BIG-MAP**, where a generative deep learning model provides a spatio-temporal prediction of the interface evolution. If the model suggests, e.g., increased gas evolution, information can be sent directly to the Battery Management System (BMS), which can then initiate the release of a self-healing agent by application of external stimuli. Such **pre-emptive self-healing** would facilitate **enhanced battery life** and **extended battery warranty**, and the resulting competitive advantages, e.g. to the automotive sector.

In order to achieve these ambitious goals, a number of short-, medium and long-term objectives have been identified:

2.1.2.1 Immediate impact (within the LC-BAT-12-2020 project)

- Develop a **shared and interoperable data infrastructure** for battery materials and interfaces, spanning data from multiple domains of the battery discovery and development cycle
- Establish community wide characterization/testing **protocols and data standards** for battery interfaces
- **Demonstrate acceleration capabilities** for select key demonstrators
- Autonomous modules for **on-the-fly analysis** of characterization and testing data using AI and simulations
- Integrated **experimental and computational workflows** to identify and pass features/parameters between different time and length scales
- Develop multi-modal high-throughput/high-fidelity interface characterization approaches
- Demonstrate uncertainty-based hybrid physics- and data-driven models of select battery materials

2.1.2.2 Medium-term impact

- **Fully autonomous platform** capable of integrating computational modelling, materials synthesis and characterization (**BIG-MAP**)
- Develop predictive hybrid models for the spatio-temporal evolution of battery interfaces
- Demonstrate successful **inverse design of battery materials and interphases**
- **Direct integration of data from embedded sensors** in the discovery and prediction process, e.g. to orchestrate proactive self-healing.

2.1.2.3 Long-term impact

- Full autonomy and **chemistry neutrality** in the **BIG-MAP** platform established and demonstrated
- Integration of battery **cell assembly** and **device-level testing**
- Inclusion of **manufacturability and recyclability** in the materials discovery process

[97] Zhang, X. et al. Chem. Soc. Rev. 47, 7239–7302 (2018)

- Demonstrate **5-10 fold acceleration in the full materials discovery cycle**
- Demonstrate **full transferability** of the **BIG-MAP** approach to novel battery chemistries and interfaces
- **Digital twin** for ultra-high throughput testing on cell level implemented and validated

2.2 Other impacts

2.2.1 New market opportunities, competitiveness and growth

The **BIG-MAP** consortium consists of a substantial number of global industrial leaders in core areas of the developed methodologies and infrastructure, i.e. **Dassault Systemes** in 3D computational design and engineering software, for battery materials and systems, etc. **BASF**, **Solvay** and **Umicore** as material producers for advanced lithium-ion batteries and other clean energy technologies, as well as **Northvolt** and **SAFT** in the production of advanced and sustainable battery cells. All of these companies will benefit directly from enhanced competitiveness and new market opportunities with the developed **BIG-MAP** models and infrastructure, as discussed in the detailed description in the Exploitation Strategy (Section 2.2.1.4).

2.2.2 Environmental benefits

The current production of Li-ion batteries relies extensively on the availability and access to **critical raw materials** (CRM), in particular lithium, nickel and cobalt. In addition to the high cost and scarcity of the CRMs, the materials are extracted in countries with geopolitical instability and/or under significant ecological damage. Critical concerns also remain regarding the **security of supply** and the scalability of, e.g., the cobalt production to the expect cell production demands in 2030 and beyond.[98] The "cost function" in the materials optimization in the **BIG-MAP** infrastructure will be designed to be able to include **availability, scalability and recyclability** of the battery materials and concepts directly into the discovery process. Similarly, the **manufacturability and CO_2 footprint** of the materials processing can also be integrated to optimize the ratio of performance-to-environmental impact. The development of a versatile and chemistry neutral battery discovery infrastructure is a critical step towards alternative battery technologies based on **abundant raw materials**, which are crucial to meet **future demand for sustainable battery capacity.**

In contrast to the active materials in current Li-ion batteries, many of the abundant elements in the earth's crust are produced in Europe. There is a possibility to reduce or avoid cobalt and other CRMs completely by targeting alternatives that can be optimized, characterized and synthesised using **BIG-MAP**.

The accelerated discovery process will also have direct implications on **minimizing the energy consumption during the discovery and development process** of the battery materials and interfaces. For example, the environmental impact of the materials supply is dominated by the material itself (exploitation, extraction from ores, etc.), and a main environmental impact of **BIG-MAP** is thus a reduced need of material in each cell, due to increased energy density.

Beside the focus on optimization of environmentally benign materials, production processes and related upstream chains, **BIG-MAP** will optimize the **ecological impact of downstream chains**. On the one hand, production related waste streams will be evaluated regarding their potential of recycling and/or reuse. On the other hand, products will be designed in a best possible "closed-loop" thinking, i.e., choosing materials and production methods enabling a feasible and efficient end of life, second life or re-life. The strong focus on both **environmental and techno-economic assessments** together with the optimization of production, use and end-of-life handling from environmental and economic perspectives make it possible to develop a product that is as environmentally friendly as possible and, at the same time, to maintain or even **enhance profitability** from producer and end-user perspectives.

2.2.3 Societal benefits

The automotive sector is one of the largest single employers in the European Union, with 13.8 million employees and a generated turnover representing over 7 % of the EU GDP, which is larger than e.g. the pharmaceutical and machinery equipment manufacturing sectors. With the current paradigm shift from fossil based transportation to electric vehicles, the **BIG-MAP** infrastructure can play a critical role in ensuring and **strengthening the European automotive industry**. Industry leading innovation helped European automotive manufacturers capture and retain significant portion of the profitable high value car market over the years. The battery pack is the single most expensive and performance limiting component of an electric vehicle. As the industry transitions, to remain the innovation leader, EU car industry must work with the battery industry and battery researchers towards **leapfrogging American and Asian companies** who already have an advantageous head start.

[98] Olivetti et al, Joule, Vol. 1, 229-243 (2017)

Shortening the laboratory-to-production time-lag is necessary. Maintaining a technological lead, i.e., owning the IP of ground-breaking methodologies and battery technologies, which are both safe, sustainable and with high energy/power density, and control over the overall production value chain is critical for the economic wellbeing of this industrial bedrock. Self-sufficiency from battery-pack production to finished cars, will maintain and expand the coveted manufacturing job numbers in EU countries. **BIG-MAP** aims at a 10x expedited innovation track for battery technologies, which will pave the path for industrial competitiveness and help achieve this target.

Finally, energy storage through large stationary batteries are becoming key to energy grid security as share of fluctuating renewable are increasing fast in the grid. The modularity of the **BIG-MAP** infrastructure would also make it adaptable other battery concepts like flow batteries, with the addition of future modules.

2.2.4 Main barriers for achieving the expected impacts

The main barriers and obstacles related to **BIG-MAP** are analysed through a **PEST** (Political, Economic, Social and Technological) analysis and is listed in Table 2.2.

Table 2.2: Barriers affecting Expected Impact

BARRIER CLASSIFICATION	BARRIER DESCRIPTION	IMPACT	MEASURES TO OVERCOME BARRIERS
Political	Hard Brexit and the potential ramifications regarding participation and funding of UK partners.	MEDIUM	In the case of Hard Brexit that blocks the UK groups (Oxford, UCAM, ULIV) from participating, other partners within the consortium will take over responsibility for these activities, e.g. EPFL for UCAM.
Political	Regulatory barriers and political uncertainties regarding data standards and intra-European data sharing.	MEDIUM	**BIG-MAP** will play a key role in solving the issues related to uncertainties in data standards and sharing. This is one of the key deliverables of the project (KD7).
Economic	IPR and data safety issues related to sharing and utilization of existing/generated data and/or new materials/interfaces.	HIGH	**BIG-MAP** will work together with industrial and academic partners to ensure the highest level of security for the data and IPR protection. The **BIG-MAP** infrastructure will take advantage of national and European initiatives already working with protected data.
Economic	The implementation costs are too high for the industry to adopt the **BIG-MAP** infrastructure.	MEDIUM	The modularity of the **BIG-MAP** approach will ensure value/return on investment for the industrial/academic users, even for individual modules.
Social	The lack of consumer/end-user confidence and acceptance of the materials, interfaces and cells identified with the closed-loop **BIG-MAP** approach.	LOW	The use of AI in (materials) science is well-accepted by the community. Deeper integration between AI and aspects of the battery materials discovery will increase the confidence in the methodology; dissemination activities planned.
Social	The sustainability and scalability of the materials and interfaces are insufficient to meet social and ecological demands.	LOW	**BIG-MAP** has identified specific challenges to address during the three years of the project. In the long-term perspective, the methodology is targeted to address sustainability challenges.
Technological	The availability and/or fidelity of the training data is insufficient to train generative deep learning models for the spatio-temporal evolution of interfaces.	MEDIUM	**BIG-MAP** will focus on the research area, where a significant amount of data is available. Should the generated and available data sets be insufficient during the ramp-up, a demonstrator with reduced complexity will be developed.
Technological	The infrastructure development is too slow compared to traditional and/or alternative approaches, e.g., developed in the US or Asia.	HIGH	The key demonstrators developed within **BIG-MAP** will ensure a head start in the three-year period. The implementations will be generic and agile to ensure the longer-term goals, but follow-up projects are needed to remain ahead.

Technological	The EuroHPC/LUMI and PRACE resources and/or beamtime at large-scale facilities (LSF) are not made available in time or insufficient quantity for the HPC/LSF applications and demonstrators.	MEDIUM	Direct interaction with the relevant boards in EuroHPC/LUMI and PRACE to ensure dedicated channels beyond the standard proposals mechanisms. Reduced-scale calculations on available machines. Block Allocation Group (BAG) access agreement to be arranged with LSF partners.

2.3 Measures to maximise impact

2.3.1 Dissemination and exploitation of results

The **dissemination and exploitation** of results will be carried out in WP1 Project Management, Exploitation & Outreach, to ensure a coherent strategy and planning for taking the innovation developed in the project to the market. An Interim Dissemination and Communication plan (D1.9) and an Interim Exploitation Plan (D1.12) presenting strategies and related actions will be delivered in month 18 and month 36, respectively. The Dissemination and Communication plan will present actions to maximize the visibility and impact of the project results. The Exploitation Plan will describe the exploitation strategy and how the results from **BIG-MAP** will be used in commercialization by relevant stakeholders. The Dissemination and Communication Plan and Exploitation Plan will then be updated to obtain the Final dissemination report (D1.13) and Final Exploitation Plan (D1.14).

2.3.1.1 Stakeholder-oriented dissemination and exploitation

The plans for exploitation and dissemination, included in the **developed web-interface (KD9)**, will also include a potential stakeholder/user set (target groups and organizations for **BIG-MAP** dissemination measures) to be updated continuously during the project's lifetime. These target groups include:

Table 2.3: Target groups for BIG-MAP

Type of target group	Target group	Planned Action
The broader scientific community	University researchers, research organizations, large-scale research facilities (experimental and computational) and R&D centers	- Presentation at partner PhD schools, e-learning courses, etc. - The **BIG-MAP** App store - Conferences and workshop - Publications in scientific journals
Industry and investors	European Battery Alliance (EBA250)	- Webinars - Stakeholder training events - Continuing education programmes
European and international platforms with activity related to batteries, energy storage, HPC, robotics and accelerated materials discovery	BATTERY 2030+; ETIP Batteries Europe; MaX; EoCoE; EuroHPC; Alistore ERI; RS2E; CELEST, Polis; EIP on Raw Materials; EuMaT; euRobotics; 31nravell MaterialDigital	- Awareness of the **BIG-MAP** technology and its impact on European Society. - Alistore, MaX, RS2E and CELEST, Polis, etc. are already represented in the **BIG-MAP** consortium
Sector relevant associations and organizations	EMIRI; EASEM; RECHARGE; Mission Innovation (IC6)	- Joint workshops and events under BATTERY 2030+ - Participation in MAP/IC6 activities
Standardization bodies	Standardization committees such as CENELEC, IEC or ISO	- Will be kept up-to-date on the progress within standardization
Students and citizens	University and high-school students as well community organizations	- The **BIG-MAP** App-store - e-learning courses and virtual reality tools for education - knowledge sharing with non-experts
Professional/ business organizations/third parties	Automotive industry, technology developers in clean energy, engineering/manufacturing services	- Invitations to stakeholder events. - Commercialization of the **BIG-MAP** technology and/or single modules
Government and policy makers	European Commission and Member State representatives	- National policy advocacy in innovation and green energy transition - Batteries Europe and Future Battery Technologies

Financial authorities	Innoenergy, The European Investment Bank	- Key stakeholders will approached for potential co-funding

2.3.1.2 Stakeholder activities

BIG-MAP has established an initial **Priority Stakeholder** group to ensure the implementation of the developed concepts, standards and infrastructure tools will be adopted by – and adapted to – the needs of the main stakeholder groups across the European battery value chain. A substantial number of Priority Stakeholders spanning industry SMEs and large enterprises, e.g. within the automotive industry (Volvo Cars), software developers (SCM, ChemOS inc.) and materials producers (Haldor Topsøe A/S), HPC CoE, research organizations and academic institutions have already been identified and signed **Letters of Intent** to interact closely with **BIG-MAP** (see full list in Section 6).

A total of €350.000 has been allocated (specified as subcontracting in the budget for partner 1: DTU) to secure funding for **Stakeholder Initiated Initiatives (SII)**. This funding is matched by an additional €350.000 for **BIG-MAP** partners (under "Other direct costs" in the DTU budget,) agreeing to undertake additional tasks to meet the request specified in the SII proposal, e.g., for development of specific **apps and interfaces** between the **BIG-MAP** infrastructure and LC-BAT-13/14/15-2020 projects or software products/techniques widely used in the community. The specific guidelines for the application for these funds will be announced in an open call at or prior to the first stakeholder event, and the decision on the allocation of funds is made by the Executive Board (EB) following a set of predefined criteria. All grantees will automatically obtain membership in the Priority Stakeholder group, while other requests for membership in the Priority Stakeholder group are assessed by the PC. Priority Stakeholders:

- Will receive invitations to **BIG-MAP** training events and workshops.
- Are offered early access to select software packages and models developed in **BIG-MAP**.
- Have the opportunity to **utilize BIG-MAP resources** to help develop interfaces between the **BIG-MAP** data infrastructure and our experimental/computational software.
- Have the opportunity to apply for **BIG-MAP** resources to assist in developing apps for the **BIG-MAP App store**, e.g. specialized automated data analysis modules.
- Agree to participate by consultation to the development of joint binding **BIG-MAP** data standards and protocols for acquisition and reporting of data to the **BIG-MAP** database(s).

As outlined in the Resource Allocation (Section 3.4), substantial funding has been allocated to the stakeholder activities, including training events, webinars and the development of apps and interfaces.

2.3.1.3 Education of future scientists

Most current day teaching is performed in a sequential and compartmented way, where competences are thought individually. **BIG-MAP** is also going to enforce a **paradigm shift in the training and education** of the next generation of scientists and researchers. To gain the competences required to (inverse) design materials and interfaces, even beyond batteries, the education of students needs to cover all the aspects of the new discovery process, from modelling and AI to synthesis, characterization and testing, in a more cohesive and interconnected way than what is done today.

BIG-MAP tackles this challenge by initiating the development of an infrastructure for e-learning courses and webinars, powered by **virtual laboratories**, virtual reality tools and remote access, for a realistic experience in a research setting, even when the facilities are not physically available. By making it available from the App-Store, it allows all the partners of **BIG-MAP** to share their expertise and disseminate the results. **BIG-MAP** targets different levels of education, from BSc and MSc basic courses to advanced courses for PhD students. This infrastructure have an impact also for continued education for researchers in the industrial sector. The online training and virtual design allows, in fact, to attend the classes remotely in the stakeholders locations.

2.3.1.4 Exploitation of the results

The **BIG-MAP** exploitation strategy will be carried out in WP1 and address how to **maximize the visibility and impact** of the project results. An **internal IP Manager** (IPM) will be appointed by the Project Coordinator to oversee IP right related issues. An exploitation strategy will be prepared to assess the dissemination strategy and how the **BIG-MAP** project results will be used in commercialization by relevant stakeholders, beyond the end of the project, and by using EC Horizon Results Platform. A list of exploitable result already identified are listed in Table 2.4, together with their exploitation strategy and the **BIG-MAP** partner that has the property of the results.

Table 2.4: Exploitation strategy of BIG-MAP partners

Partner	Type	Exploitation strategy
BASF, Umicore, Solvay	Materials	Patents and proprietary know-how on cathode active materials and surface coatings or modifications. Patents and proprietary know-how on new additives combination. Knowhow on designing specific additives adapted to electrode chemistries.
SAFT, Northvolt	Materials and Processes	Patenting and licensing
3DS	Multiscale simulation platform	Patenting and/or copyright; Industrialization and commercialization
Research organizations	R&D services	Patenting and licensing; Enhanced business competitiveness and capacity for innovation through accelerated discovery and development of new materials and processes for the industrial collaborators and customers
Large-scale facilities	R&D services	Increased value to academic and commercial customers
Research organizations , academia	Materials, processes, methods and tools, etc.	Enhanced innovation capability through accelerated discovery and development of new materials and processes; Patents; Licensing and/or start-up creation

2.3.1.5 Data management

BIG-MAP will generate data at multiple levels. Data will come from computational models (atomistic, mesoscopic and continuum levels), as well as ML models and from experiments and synthesis. The infrastructure needs to be able to adapt to collect the data from these different sources. Within the **BIG-MAP** consortium, we have already have demonstrated the capability to do so, e.g. EPFL and CNR (MaX) and the Materials Cloud platform, which will be used in **BIG-MAP**. We will use the most recent standards as indicated by the EMMC and work together with them to adapt and improve these standards. In addition, the continuation of the BATTERY 2030+ CSA (LC-BAT-15-2020) will contribute to generate new standards for the data ontology that will be used here. Project data, which is connected to a DOI by default, will be made available to all the partners of **BIG-MAP** (mostly) without restrictions using a **dedicated BIG-MAP section** of the **Materials Cloud platform**. When required, restricted access will also be possible at this level to ensure industrial participation. Materials Cloud already allows to store, share, re-use of data. Local hubs will be utilized for the data storage in **BIG-MAP**, e.g. at CNRS for the interface characterization and at EPFL/Materials Cloud for the computational data. Data protected by IPR will not be made available to the general public at this stage. Dedicated personnel will be responsible to curate and preserve the data and the functionalities developed within **BIG-MAP** (the cost will be covered by the project).

2.3.1.6 Knowledge management and protection

BIG-MAP will comply with the most recent standards for management and protection of the scientific knowledge and expertise produced within the project. A Consortium Agreement (CA) will be negotiated and signed, upon agreement of all Parties, in order to specify the terms and conditions pertaining to ownership, access rights, exploitation, dissemination of results and background. The consortium agreement will be based on the DESCA Horizon 2020 Model Consortium Agreement (www.desca-2020.eu) with the necessary adaptations considering the specific context and the Parties involved in the project. Particular attention will be paid to **ensure IP protection and sharing for co-developed BIG-MAP methodologies**, as well as for **novel materials and interfaces identified or developed by BIG-MAP or individual modules**.

While we will emphasize the openness of the project to the European citizens via peer-reviewed publications in Open Access or via institutional repositories and the www.BIG-MAP.eu web site, any sensitive IP will be protected prior to any disclosures, including participation in scientific conferences, workshops and other events related to materials and battery research (IBA, IMLB, etc.), PhD or master defences, etc. **BIG-MAP** will provide **free on-line access to selected (non IPR sensitive) data and information through the web-interface**. In addition, peer-reviewed scientific publications will be used to disseminate the **BIG-MAP** project results. Any partner wishing to disseminate project results must first inform the IPM with due time beforehand (according to the procedure defined and agreed upon in the CA). The IPM will archive related documents on the dedicated collaborative tool and inform all partners so that each can ensure that their interests are protected. The consortium will ensure that open access is provided to all publications resulting from the project, e.g., via a 'gold' or a 'green' model (depending on the journal policy and the potential impact of the publication on the scientific community).

2.3.2 Communication activities

Within **BIG-MAP**, we have identified 7 main channels to ensure a broad communication of the research activities and results. These are targeted an audience of experts and students (e.g., project website, conferences and workshops, peer-reviewed publications), as well as a broader scientific and non-scientific community (e.g., through popular journals, mass and social media). Outreach activities directed to society at different levels will serve to raise **general awareness of the nature of the research undertaken** and the benefits likely to accrue. Different types of actions are considered such as national popular science events like "Week of Science" or News and FAQ sections on the project website **explaining the basics of the battery MAP technology** and the project goals in an easily understandable non-scientific language. These activities are described below.

Table 2.5: Dissemination strategy of BIG-MAP partners

Communication channel	Description
Project website	The www.BIG-MAP.eu website will provide an overview of the project's objectives, activities, partners, dissemination activities and publications as well as direct access to the **BIG-MAP** database and App Store. The goal is to reach **>1000 unique stakeholder registrations and >500 downloads** (of data sets and/or software) through the website. This infrastructure aims to become a recommended repository to store and share battery data from major publishers and funding agencies. FAQ sections in the website explaining the basics of battery technology and the project goals in an easily understandable non-scientific language.
Project events	The **BIG-MAP** consortium plans yearly stakeholder meetings and training events, as well as online tutorials and webinars. We will co-host at least one international workshop/conference together with the other LC-BAT-13/14/15-2020 consortia, where stakeholders from industry and European associations will be invited as key note speakers and asked to provide feedback to the project progress and outcome. Further, 1-2 training seminars specifically targeting ESR (Early Stage Researchers) and industrial researchers in the field. **The goal for participants for the international conference/workshop is >150, while it is 30-50 participants for the seminars.**
Networking events	**BIG-MAP** partners are active in different European platforms, and will use these to promote the outcome of the project, specifically the data standard and testing protocols and well as the online tools and databases provided by the consortium to relevant industry and end users. **The consortium will participate and present the project in at least 25 networking events.**
Scientific conferences and workshops	The academic partners of the project will individually and in collaboration publish and present scientific advances at leading conferences and workshops in addition to the co-organized LC-BAT workshop/conference. A non-exclusive list of selected conferences and workshops: Meetings of ECS, IBA, MRS, e-MRS, ACS, CECAM, IEEE, ICRA, etc. **In total 100-150 conference/workshop presentations/posters are planned.**
Scientific journals	Expected scientific results range from new materials discovery accelerators, autonomous characterization modules, integrated experimental and computational workflows, breakthroughs in the **BIG-MAP** technology and new advanced materials and interfaces. These findings will be published in relevant high-impact journals like Chem. Sci., J. Mat Chem A, J of Power Sources, Energy & Env. Sci., Adv. Materials, Nature Comm., Nature Materials, J Am Chem Soc, ACS App. Energy Lett., Batteries & Supercaps, Energy Storage Materials, Adv. Energy Materials, Adv. Functional Materials, ACS App. Mater. & Interfaces. **In total 60-80 peer-reviewed publication planned by the end of the project.**
Mass media	**BIG-MAP** will communicate with the media about key results through press releases and interviews and communicate popular science articles targeting the general audience. Outreach activities directed to Society at different levels will serve to raise general awareness of the nature of the research undertaken and the benefits likely to accrue. Different types of actions are considered such as national popular science events. **The goal is to publish at least 2-3 popular science publications per year.**
Social media	Social media channels like LinkedIn and Twitter will be used actively to publish information about breakthroughs, scientific publications and project events and updates, e.g. quarterly live streaming interviews to reach a broader audience. Specific **BIG-MAP** accounts will be created and **the goal is to exceed 1000 unique followers through social media.**

3 Implementation

3.1 Work plan — Work packages, deliverables

In order to achieve the **Specific Objectives** established in Section 1.1, the **BIG-MAP** project will be developed in **11 Work Packages** (WPs) over a timeframe of 36 months. The **BIG-MAP** work plan is schematically represented in Figure 3.1, the timeline is shown in **Gantt chart** in Figure 3.2.

3.1.1 Overall structure of the workplan

To organize the work in **BIG-MAP** and to facilitate the envisaged paradigm shift in the battery discovery process, a transition from a traditional "siloed" approach to the discovery of battery materials (and other clean energy materials for that matter) is needed. As discussed in section 1.3.4, we have identified five scientific **Competence Pillars**, where specific focus and effort is needed to deliver the **scientific breakthroughs** in key research and development areas for batteries and complementary fields: WP2: **Accelerated atomic-scale Simulations**, WP3: **Multi-scale Modelling**, WP4: **Modular Synthesis Robotics**, WP5: **Characterization**, and WP6: **HTS and Testing** (details about the WP-activities are found in the following sections).

These WP activities will be linked through conventional exchanges of data, samples and models, but in addition to this, we have identified the five **Cross-Cutting Initiatives**, that provides **new ways to cross-fertilize the discoveries** in the diverse fields in the competence pillars and provide the framework for establishing the common "language", infrastructure and integrated workflow needed to achieve the scientific objectives in **BIG-MAP**. The cross-cutting initiatives are WP7: **Battery Interface Ontology**, WP8: **Standards & Protocols**, WP9: **Infrastructure & Interoperability**, WP10: **AI-accelerated Materials Discovery**, and WP11: **Battery Interface Genome**.

WP1: **Project Management, Exploitation & Outreach** will manage the successful coordination, interlinking and execution of the complex tasks in the project. WP1 will also ensure a high level and quality of the dissemination and outreach activities, e.g. to the priority stakeholders, and a dynamic analysis of the exploitation of the discoveries and breakthroughs. In addition to the **Executive Board** (section 3.2.1.4) and **General Assembly** (section 3.2.1.3), an **Advisory Board** (section 3.2.1.5) has also been established to assist the project management (figure 3.3).

Figure 3.1: the interconnected matrix structure of the Work Packages in BIG-MAP

		Month		Year 1				Year 2				Year 3			
	Workpackages/Tasks	Start	End	1-3	4-6	7-9	10-12	13-15	16-18	19-21	22-24	25-27	28-30	31-33	34-36
1	**Project management and education, exploitation and outreach**	**1**	**36**												
1.1	Administrative and financial management and reporting	1	36												
1.2	Participation in the Future Battery Technologies initiative and collaboration with LC-BAT projects	1	36												
1.3	Research Data Management	1	36												
1.4	Intellectual Property management and utilization	1	36												
1.5	Development and implementation of an Exploitation Plan	1	36												
1.6	Stakeholder activities and management	1	36												
1.7	Dissemination, outreach and communication	1	36												
2	**Accelerated atomic-scales simulations**	**1**	**36**				M2.1								
2.1	Data from QM calculations	1	36												
2.2	Train ML potentials	1	36												
2.3	ML in battery compound space	1	36												
2.4	Battery simulations at the atomistic level	1	36												
2.5	Modelling operando spectroscopies and atomistic-level characterization	6	36												
3	**Multiscale Modelling**	**1**	**36**								M3.1			M3.2	
3.1	Development and validation of multiscale modelling frameworks	1	18												
3.2	Verification and Validation of Scale-Bridging Protocols for SEI/CEI formation	1	36												
3.3	AI enhanced models	1	36												
3.4	Verification and Validation of Models for HTS experiments	12	32												
3.5	Workflow demonstrators	12	36												
4	**Modular Robotics and Syntheses**	**1**	**36**	M4.1									M4.2		
4.1	Specifications	1	6												
4.2	Hardware and software design, integration	6	30												
4.3	Integration and validation	12	36												
4.4	Synthesis of components for organic protective coatings	6	30												
4.5	Combinatorial synthesis and application of inorganic coatings	6	30												
5	**Characterization**	**1**	**36**	M5.1			M5.2								
5.1	Benchmark	1	30												
5.2	Workflow	1	36												
5.3	Data acquisition & visualization	6	36												
5.4	Data Analysis	8	36												
6	**HTS and Testing**	**1**	**36**				M6.1		M6.2		M6.3				
6.1	Preparation and characterization of "feeding" units for the HTS assays	1	36												
6.2	Formulation and characterization of advanced electrolyte components for HTS assays	1	36												
6.3	HTS analysis via selected methods	1	36												
6.4	HTS in electrolyte formulation, cell assembly and "filtration" measurements	1	36												
6.5	HTS of inorganic protective coatings	1	36												
7	**Battery Interface Ontology**	**1**	**36**	M7.1						M7.2					
7.1	Establish ontology standards to support interoperability and dissemination	1	36												
7.2	Design a general battery ontology	1	18												
7.3	Design the battery interface ontology (BIO)	3	36												
7.4	Implement the ontology to describe specific case studies	9	36												
8	**Standards and Protocols**	**1**	**36**	M8.1											
8.1	Selection and refinement of pre-existing initiatives regarding standards and protocols	1	6												
8.2	Creation of working groups and workflow	6	36												
8.3	Implementation of these standards and protocols	6	36												
8.4	Organization of European platforms for battery testing	24	36												
9	**Infrastructure and Interoperability**	**1**	**36**						M9.1						
9.1	Robust and reliable workflows for automated simulations	1	36												
9.2	Integration of the computational platforms	1	36												
9.3	Development of a software framework for data management, linkage and protection	1	18												
9.4	Deployment of a cloud platform for automated simulations and data access	1	36												
9.5	Integration of automated experiments and automated simulations	1	18												
10	**AI Accelerated Materials Discovery**	**1**	**36**				M10.1				M10.2				
10.1	Accelerating experiments with active learning	1	18												
10.2	An automated data analysis framework	1	24												
10.3	Transfer learning and new fundamental insights	1	24												
10.4	Automatic reasoning and materials funnel	1	36												
11	**Battery Interface Genome**	**1**	**36**										M11.1	M11.2	
11.1	Integration of multi-fidelity data from all domains	1	18												
11.2	Dynamic interface/interphase descriptors	6	24												
11.3	Hierarchical latent space multi-scale models	12	30												
11.4	Uncertainty-guided spatio-temporal models	15	36												
11.5	Transferability of developed methodology to other materials	21	36												

Figure 3.2: BIG-MAP GANTT chart

3.2 Management structure, milestones and procedures

3.2.1 Organisational structure and decision making

An organizational structure (figure 3.3) has been established with management procedures and decision-making mechanisms that are suitable for the scale of the project. This structure will be implemented to ensure the smooth implementation of **BIG-MAP**. The GA shall handle strategic and impact related decision-making, the EB including the WP leaders, topical managers and key representatives (Table 3.2.1) will be in charge of implementing the decisions. The AB provides guidance and the MST provides day-to-day support to the PC and the EB.

Figure 3.3: BIG-MAP organisational structure

3.2.1.1 Project coordinator (PC)

The Coordinator of **BIG-MAP** is Prof. Tejs Vegge (DTU) who has substantial experience in managing large international projects and groups, see short CV in the partner description (Part B Section 4-5). Prof. Vegge has the overall responsibility for the project management and shall perform all tasks assigned as described in the Grant Agreement (GrA) and the CA. As chairman of the GA, responsibilities of the PC will include:

- Monitor partner compliance regarding obligations and proper project implementation
- Act as the intermediary for all communications between the partners and the EC including financial compensation of partners by EC and track and distribute partner contact information
- Request and review any documents or information required by the EC and verify their completeness and correctness before passing them on to the EC, this includes submission of deliverables and reports
- Transmit documents and information connected with the project to any other partners concerned

As chairman of the Executive Board, the PC will take over the day-to-day management of the project consisting of both strategic (technical & innovation management, risks, external opportunities...) and operational EU project (animation, communication, reporting…) management tasks with support from MST. The PC will be in charge of:

- Organizing (methodologies, tools, knowledge management) and piloting at project level the S&T management carried out by the WP leaders
- Follow-up the project level indicators (balanced scorecard) included in the dashboard
- Timely organization of deliverable reports and contributions for the progress and financial reports
- Ensuring that the internal quality processes, common templates and communication tools decided by the GA are properly used by the consortium members
- Implementing the global risk management linked to Milestones as detailed below and identifying project specific needs (funding, people, management related)
- Ensuring on a daily basis the communication between the different partners

DTU has a long and successful track record both as participant and as coordinator in European projects with more than 400 projects in H2020, where DTU has coordinated multiple of these, and hence there is additional qualified staff to provide support to the PC. The involved department, DTU Energy, has detailed knowledge of management and administrative support of EC contracts, as well as the experience to help handle any conflicts and other challenges that may occur in the consortium.

3.2.1.2 Management support team

A The MST will assist and facilitate the work of the PC. It will be an adviser for partners on administrative matters related to reporting and day-to-day management. The MST is also responsible for setting up and facilitate an electronic infrastructure to ease communication within the Consortium, for controlled and shared access to project documents. The MST team consist of the Project Coordinator Assistant and a Legal Adviser from DTU.

3.2.1.3 General Assembly (GA)

The General Assembly is the ultimate decision making and conflict resolution body of the project. It will be **chaired by the PC** and attended by one representative of each partner. The GA will be responsible for the overall strategic orientation and policy of the project. It will make sure that the adopted strategy is respected in order to reach excellence. Its tasks include:

- Assessment / agreement on project progress and resources status and allocations
- Changes of GrA & technical annex to be submitted for EC approval

- Changes to the work programme and its timing
- Modifications to CA notably to validate background IPR to be included
- Evolution of the consortium: conditions of entry & withdrawal of parties, identification of breach by a party or defaulting party
- Ensuring the leverage effect of the project and achievement of expected impacts and external opportunities

The GA will meet physically **every 6 months**. Exceptional sessions (telephone or web conference) may be called upon and organized when needed or requested.

3.2.1.4 Executive Board (EB)

Chaired by the PC, the EB will be responsible for the proper execution and implementation of the decisions of the GA. It will monitor the effective and efficient implementation of the Project. In particular the EB will:

- Every 6 months report progress, IPR, dissemination, communication etc. and resources status of the project
- Assess the compliance of the partners, if necessary, propose modifications and manage stakeholder requests
- Resolve conflicts on technical, financial and strategic issues and consult GA if needed
- Support EC meeting preparation with data and deliverables
- Approve and time press releases and joint publications by the consortium or proposed by the EC
- Propose and set up internal quality processes, common templates and communication tools

The EB members' appointment will be validated by the members of the GA (first proposal in Table 3.2.1a). The EB will meet virtually every 3 months and physically every 6 months. Additional meetings by teleconference may be organized when needed/requested by a partner by 1 month notice.

Table 3.2.1a: BIG-MAP Executive Board members

EB members		Names	
Project Coordinator		Tejs Vegge (DTU)	
Dissemination and Exploitation Manager		Rosa Palacin (CSIC)	
IP Manager		Simon Perraud (CEA)	
Data Management Responsible		Ivano Castelli (DTU)	
Industry Representative		Philippe Jacques (EMIRI)	
Representative of large-scale facilities		Marc Johnson (ILL)	
BATTERY 2030+ project coordinator		Kristina Edström (UU)	
WP2 leader	Kersti Hermansson (UU)	WP7 leader	Simon Clark (SINTEF)
WP3 leader	Wolfgang Wenzel (KIT)	WP8 leader	Alexis Grimaud (CNRS)
WP4 leader	Henning Lorrmann (FRAUNHOFER)	WP9 leader	Nicola Marzari (EPFL)
WP5 leader	Sandrine Lyonnard (CEA)	WP10 leader	Helge Stein (KIT)
WP6 leader	Isidora Cekic-Laskovic (FZJ)	WP11 leader	Ole Winther (DTU)

3.2.1.5 Advisory Board (AB)

An Advisory Board will be appointed to support in developing aspects of the research, dissemination of results and help achieve the impact goals in the project. The Advisory Board will convene once a year, three meetings total for the project period, the Advisory Board meetings are aligned with the GA meetings.

Table 3.2.1b: Members of BIG-MAP advisory board

No.	Stakeholder Organization	Representative	Stakeholder role
1	International MAP expert	Alan Aspuru-Guzik	International developments in MAP and QML
2	Batteries Europe	Stefano Passerini	Alignment of data standards and protocols
3	Mission Innovation/EERA	Holger Ihssen	Knowledge transfer with MAP activities in EC
4	Automotive rep. (Volvo Cars)	Hanna Brygnelsson	End-user needs and EV design specifications
5	EuroHPC JU/LUMI	To be named by GA	HPC resources and collaboration
6	LC-BAT-13 representative	Post award decision	Infrastructure and data alignment for sensing
7	LC-BAT-14 representative	Post award decision	Infrastructure and data alignment for self-healing

3.2.1.6 Research & innovation activities reporting

Technical and financial follow-up at the level of the whole project will be implemented on a 6 months basis and presented during GA meetings, which will assess the progress achieved by the project. Operational progress is

monitored by the PC and WP leaders at WP level every 3 months. Physical meetings gathering the GA will be organized on a 6-monthly basis in order to review and assess the project achievements. Project mid-term and final reviews will be implemented as stipulated in the GA. The GA will organize the mid-term meeting with all partners, and the EC if appropriate. The following criteria will be assessed:

- Degree of fulfilment of the work plan for the relevant period and of the related deliverables.
- Continued relevance of the Specific Objectives and breakthrough potential with respect to the scientific and industrial state-of-the-art.
- Resources planned and utilized in relation to the achieved progress, in a manner consistent with the principles of economy, efficiency and effectiveness.
- Management procedures and methods of the project and partners' contributions and integration within the project.
- Expected potential impact in economic, competition and social terms, and the partners' plan for the use and dissemination of results.

3.2.1.7 Decision making

The GA will be the ultimate decision making body for the project. The principles of the decision making mechanisms to avoid status-quo or blocking situations will be applied:

- Each consortium body requires 2/3 of its members to be present or represented (quorum). If the quorum is not reached, another meeting is convened. Each member has one vote (no vote for defaulting party).
- Decisions shall be taken by a majority of 2/3 of the votes cast. From an operational point of view, the project will strive as follows for conflicts resolution.
- If necessary, mediation will be conducted by the PC or an identified neutral party who will propose adequate timing for resolution.
- Otherwise, the rules of the CA will apply and decisions may be submitted to a vote.
- In extreme cases, a clear risk assessment will be realized and balance will be carefully weighed between the damages/solutions that can lead to defaulting partner exclusion.

3.2.2 Milestones

Important milestones have been identified (Table 3.2a) for the project implementation and will be carefully monitored by the corresponding WP leaders and at project level by the PC. When the date of milestones review is achieved the results verification will be conducted against the set objectives, a short report will be issued regarding the milestones assessment. When a milestone is delayed or is not achieved, the impact on the project and WP will be assessed and a back-up plan will be proposed by the concerned WP leaders. Such issues will be reviewed by the EB who report the status to the GA.

3.2.3 Risk and contingency plan

Quality monitoring and quality assurance: In addition to the measures taken in the project and the management structure definition, the project will monitor/supervise the quality through periodic controls. The PC supported by the MST and WP leaders, will be responsible for quality accomplishment in deliverables generation. The purpose is to describe the actions and measures that will be taken by the consortium, in order to ensure the quality of the project and its full conformance with the contractual requirements, issued in accordance to the ISO-9001 standard. The main quality goals will be (1) to provide to all concerned directives for the quality actions required by each partner, (2) to exhibit project's quality performance in accordance to contractual requirements and (3) to document the internal review, supervision procedures and roles. Specifically, WP1 is clearly tasked to ensure the quality of WP2 to WP11 in terms of development and demonstration results, validating the output and ensuring a smooth transfer of the developed methods and key demonstrators, minimizing the risks by detecting potential issues as early as possible. A quality culture will be instilled in the consortium such that every participant shares this commitment.

Management of knowledge and Intellectual Property Right (IPR) issues: The need for pre-existing know-how and the foreground associated to the project and its use is regulated in the CA. An active policy of IP protection will be adopted where applicable, with an emphasis on patents. See previous full section on IPR (section 2.3.1.6).

Risks have been assessed by breaking the work into an achievable set of smaller developments. The WPs have been structured in such a way to have easy tracking of milestones and objectives. A preliminary list of risks is given based on this analysis. The PC supported and the WP leaders will be responsible for this follow-up, as well as for proposing corrective measures, with a dedicated section in the consortium meetings. Each WP and task leader will review the status of each task's achievement for risks identification. The preliminary risks identified are shown in Table 3.2b.

3.2.4 Baseline for consortium agreement

A CA based on the DESCA Horizon 2020 Model will be elaborated and approved among partners. The ground-rules are the following:

- Ownership of Results: shall be the property of the partner/contractor generating it. Where several contractors have jointly carried out work generating the knowledge, a joint ownership of that knowledge shall be established by a Joint Ownership Agreement.
- Confidentiality: during the project execution, the partners shall treat any project information as confidential, which is designated as such by a disclosing partner. The partners shall apply the same obligations to their employees and suppliers.
- Dissemination: any publication or communication proposed by one of the parties, regardless of the media, in connection with all or part of the project and of the knowledge is required to be submitted for the prior written consent of the GA. Prior notice shall be given at least 45 calendar days before the publication, and any objection is to be formulated within 45 calendar days after receipt of the notice.
- Use and dissemination: as long as dissemination of results does not adversely affect its protection or use and subject to legitimate interests, the partners shall ensure further dissemination of their own results knowledge as provided under the Grant and the Consortium Agreement.
- Background knowledge: each partner is and remains the sole owner of its intellectual and industrial property rights over its background knowledge. A list of background knowledge over which they may grant access rights for the project is included in the CA.

3.3 Consortium as a whole

The **BIG-MAP** consortium truly **covers the whole battery discovery value chain** from **atoms to battery cells** totalling 34 partners from 15 countries, and spanning **world leading partners** in academia, research laboratories and industry. **BIG-MAP** is a joint European battery community effort, and as stated in the introduction, the large-scale European Research Initiative **BATTERY 2030+** stands united behind the **BIG-MAP** consortium for the LC-BAT-12-2020 call. To ensure and strengthen the close collaboration between the partners, an additional 100 k€ has been set aside (in the DTU budget, see Table 3.4b) to support longer stays of key researchers with a partner organization, e.g., to complete the development of key hard-/software modules. Allocation of extra mobility funds is based on a short application to the PC documenting the request; the PC then recommends to the EB for final approval of funding.

In addition to the 13 core partners from BATTERY 2030+, the **BIG-MAP** consortium includes an extra **21 leading European partners** with complementary battery skills and/or essential competences from critical research areas such as QML, deep learning and autonomous synthesis robotics to name a few.

Combined, the consortium unites **world leading European experts in all the core areas** needed to develop **BIG-MAP** for sustainable and ultra-performing battery materials and interfaces (details are found in Part B, Section 4-5):

- **Advanced characterization of battery interfaces**: e.g. Prof. Kristian Edström (UU), Prof. Clare Grey (UCAM) and Prof. Marnix Wagemaker (TUD).
- **Battery fundamentals and beyond Li-ion**: e.g. Profs. Jean Marie Tarascon (CNRS and RS2E), Peter Bruce (Oxford and The Faraday Institution), Robert Dominko (NIC and Alistore), Rosa Palacin (CSIC and Alistore) and Maximillian Fichtner (KIT, CELEST and POLIS).
- **Virtual multi-scale materials design**: Profs. Wolfgang Wenzel (KIT), Alejandro Franco (CNRS and RS2E) and Patrik Johansson (CTH and Alistore).
- **Accelerated HTS and formulation**: Prof. Martin Winter (WWU and MEET) and Oscar Miguel (CID).
- **Deep Learning in materials space**: Profs. Ole Winther (DTU), Gabor Csanyi (UCAM) and Anatole von Lilienfeld (UBAS).
- **Autonomous Materials Discovery**: Profs. Andy Cooper, Matthew Rosseinsky and Laurence Hardwick (ULIV and Materials Innovation Factory), Helge Stein (KIT) and Tejs Vegge (DTU)
- **Data-infrastructures and HPC**: Prof. Nicola Marzari (EPFL), Elisa Molinari (CNR and MaX); Dassault Systemes (3DS), Jesper Friis (SINTEF and EMMC).
- **European large-scale synchrotron/neutron facilities**: ESRF, ILL and SOLEIL.
- **Autonomous robotics**: Profs. Henning Lorrmann (FRAUNHOFER), Kasper Støy (ITU & Flow Robotics) and Alvo Aabloo (UT).
- **Industry production of advanced battery materials**: BASF, Solvay and Umicore.
- **Battery cell production**: SAFT and Northvolt.

In the ramp-up phase covered in the LC-BAT-12-2020 proposal period (year 1-3), important aspects in the development of future batteries have not been included, in order to keep focus on the development of the infrastructural backbone and to deliver a set of **acceleration and conceptual Key Demonstrators**. These areas include recyclability, smart functionality and end-users, e.g. the automotive industry, but these stakeholders will be included in later stages of the **BIG-MAP** implementation.

In addition to covering all critical segments of the value chain, **BIG-MAP** is **gathering leading national and international consortia**, e.g. RS2E, Alistore, CELEST, The Faraday Institution, MEET and POLIS, in a united effort giving critical mass to the initiative.

3.4 Resources to be committed

The total budget for **BIG-MAP** being requested from the EU is **19,998,025€.** The budget has been optimized to enable a maximum effort of the consortium as a whole, as well as for each of the WPs. The figures of the project are tabulated below.

Table 3.4b: other direct cost of BIG-MAP partners having more than 15% of their budget for non-personnel

1 – DTU	Cost (€)	Justification
Equipment	67,114	Purchase of and/or online services for CPU and GPU nodes (67k€)
Travel	40,000	Physical project management meetings every 6 month (10 k€) and technical meetings (30 k€)
Other	477,000	Consumables and supplies for the demonstrations (27 k€), additional support for extended research stays at another partners (100 k€), and support for BIG-MAP partners participating in Stakeholder Initiated Activities (350 k€)
Total	**584,114**	

3 – KIT	Cost (€)	Justification
Travel	30,000	12 projects meetings in Europe for 3 people (30k€)
Other	135,335	Consumables and supplies for WP3 (25 k€) and WP 10 (99,150€), dissemination costs (10 k€), and audit costs (1,185€)
Total	**165,335**	

4 – CNRS	Cost (€)	Justification
Equipment	180,000	Storage capability (400k€ purchase cost depreciated over 60 months, used 36 months and allocated at 75% for the project
Travel	35,000	10 meetings in Paris for 7 persons (5k€), consortium meeting in Europe (10 k€), dissemination conference (20k€)
Other	22,000	Consumables and supplies (14 k€) and dissemination costs (8k€)
Total	**237,000**	

6 – CEA	Cost (€)	Justification
Travel	14,850	6 person day travel / year
Other	10,450	Analysis costs (9k€) and audit costs (1,450€)
Large research infrastructure	91,040	Monthly operational costs for "Liten Battery" LRI (5036,63€) in WP2,3,5,6 for 25 months and "Liten Engineering" of 2661,40€ (22 months) at variable allocation fractions.
Total	**116,340**	

7 – NIC	Cost (€)	Justification
Travel	15,000	7 consortia meetings (3 persons 500 EUR/travel) and 3 conferences (1500 EUR/conference/person)
Other	37,000	Spare parts, chemicals, electrode fabrication tools (27k€) and open access publications and audit (10k€)
Total	**52,000**	

9 – PDT	Cost (€)	Justification
Travel	12,000	Project meeting nr 6, 2 days each travel, 2 people each travel (6k€) and Participation to Conference, Workshop,. For dissemination (in UE and extra UE) (6k€)
Other	13,700	Fees for Conference, Workshop, etc. (1.7k€) and Open Access Publications: fees (12k€)
Total	**25,700**	

10 – FRAUNHOFER	Cost (€)	Justification

Equipment	50,000	Lab equipment: rotary evaporator (25000€), pumps (24000€), filtration plant (25000€) and glassware (9333€) with eligible purchase cost depreciated over 60 months, used 36 months and allocated at 100% for the project, summing to 50000€.
Travel	10,000	Project meetings (4/yr) (7.2k€) and conferences (2.8k€)
Other	13,000	Diverse small parts for laboratory utensils and chemicals (10k€) and audit costs (3k€)
Total	**73,000**	

12 – WUT	**Cost (€)**	**Justification**
Equipment	30,000	Compact FT-IR Spectrometer (depreciation) (100k€ purchase cost depreciated in 30 months, used 30 months and allocated at 30% for the project)
Travel	11,000	Project meetings, 1 person, 7 meetings (9k€) and Scientific conference – 1 person, 1 travel (2k€)
Other	163,000	Printing costs, materials for publications, publishing costs (3k€), Glassware (3k€), Testing cells, sampling pans, vials, etc. (4k€), Raw materials for synthesis of salt (90k€), Raw materials for synthesis of additive (60k€), audit (3k€)
Total	**204,000**	

13 – CSIC	**Cost (€)**	**Justification**
Travel	16,000	Project meetings (1 general every 6 months + technical and dissemination meetings), 2 people per meeting
Other	38,120	Chemicals, labware, electrochemistry (16.5k€), Analysis & testing (diffraction, microscopy, etc) (6k€), Open Access fees (7.5 k€), computer access for SIESTA simulations (8,120€)
Total	**54,120**	

14 – TUD	**Cost (€)**	**Justification**
Travel	9,000	6 meetings, 2 persons
Other	37,500	Consumables (30k€) and Dissemination of results at international conferences (7.5k€)
Total	**46,500**	

15 – CNR	**Cost (€)**	**Justification**
Equipment	1,000	2 instrument laptops (1k€ purchase costs depreciated 60 months and used 30 months at 100% for the project)
Travel	15,000	Dissemination meetings (5k€), consortium meetings (6k€), technical meetings (4k€)
Other	13,242	Publications (7,242€) and software and consumables (6k€)
Total	**29,242**	

16 – EPFL	**Cost (€)**	**Justification**
Equipment	105,000	Computing infrastructure (105k€ purchase cost depreciated in 36 months, used 36 months at 100% for the project)
Travel	10,000	Consortium meeting every 6 months
Other	33,000	Consumables and supplies
Total	**148,000**	

17 – UCAM	**Cost (€)**	**Justification**
Equipment	44,508	Cycler chemistry (15k€ purchase cost depreciated in 12 months, used in 36 months at 100% for the project), and computer server (29,508€ purchase cost depreciated in 12 months and used 36 months at 100% for the project)
Travel	50,400	Engineering PI (12.6k€), Engineering PDRA x1 (12.6k€), Chemistry PI (12.6k€), Chemistry PDRA x1 (12.6k€)
Other	152,892	Consumables for engineering (58,746€), consumables for chemistry (58,746€), dissemination (30k€) and audit (5,400€)
Total	**247,800**	

18 – UOXF	**Cost (€)**	**Justification**
Travel	12,000	Travel to general meetings (4k€), Travel to WP partner sites and WP meetings (4k€), Travel to international meetings (4k€)
Other	85,330	Chemicals, materials and supplies (75,330€), audit (10k€)
Total	**97,330**	

19 – UT	**Cost (€)**	**Justification**
Travel	15,000	Travel to general meetings (1 person, twice per year) (3k€), Travel to WP partners site, work meetings (4 times per year) (6k€), Travel to international meetings (incl. fee) (3k€), Travel to robotics fairs (incl. fee) (3k€)
Other	28,000	Small scale prototyping details (20k€), Consumables and supplies for prototyping personnel (8k€)
Total	**43,000**	

20 – ULIV	Cost (€)	Justification
Equipment	50,000	Robotic equipment (50k€ purchase cost depreciated in 36 months, used 36 months at 100% for the project
Travel	10,000	Consortium meetings every 6 months
Other	16,519	Chemicals and lab consumables (13k€) and audit fees (3,519€)
Total	**76,519**	

23 – SOLEIL	Cost (€)	Justification
Equipment	37,500	Facility Standard Sample Environment (50k€ purchase cost depreciated in 24 months, used 24 months at 75% for the project)
Travel	10,000	WP meetings (5k€) and GA meetings (5k€)
Other	33,000	Sample preparation (13k€), dissemination (10k€) and open access fees (10k€)
Total	**80,500**	

25 – EMIRI	Cost (€)	Justification
Travel	10,000	Partner meetings every 6 months
Other	30,000	Events organization
Total	**40,000**	

28 – BASF	Cost (€)	Justification
Travel	21,000	Consortium and project meetings (5k€), technical meetings (6k€), conferences (10k€)
Other	180,160	Trials (65k€), material Analytics (SEM, HR-TEM, XRD) (80k€), administrative and financial project services (35,160€)
Total	**201,160**	

29 – NVOLT	Cost (€)	Justification
Travel	10,000	Consortium and project meetings (5k€), technical meetings and conferences (5k€)
Other	34,500	Consumables, materials and supplies (34,500€)
Total	**44,500**	

30 – UBAS	Cost (€)	Justification
Equipment	75,000	CPU/GPU nodes (75k€ purchase cost depreciated in 36 months, used 36 months at 100%)
Travel	15,000	Consortium meeting every 6 months
Other	15,000	Consumables and open access
Total	**105,000**	

34 – SAFT	Cost (€)	Justification
Travel	10,000	Partner meeting every 6 months
Other	60,000	cells components, fluids, solvents
Total	**70,000**	

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4 Members of the consortium

4.1 Participants

4.1.1 DANMARKS TEKNISKE UNIVERSITET (DTU)

DTU Danmarks Tekniske Universitet	**Name:** DANMARKS TEKNISKE UNIVERSITET (DTU)	**Partner no:** 1	**Country:** Denmark
	Type: UNI	**Number of R&D personnel:** 4 976 **Number of employees:** 6 053	**Turnover:** 703 M€

Interest in the project

The Department of Energy Conversion and Storage at the Technical University of Denmark (DTU Energy) share the vision of the BIG-MAP project described here, i.e., to inverse design and engineering of high-performance clean energy materials and interfaces, by combining physical and data-driven models trained on large data sets from multi-scale computer simulations and databases, operando characterization from large-scale research facilities, high-throughput synthesis and laboratory testing. BIG-MAP will allow us to develop new methodologies to automate the discovery of novel materials and integrate these methods with new artificial intelligence techniques and autonomous synthesis and characterization, bringing our competences to a new level of interoperability between theory and experiments.

Previous experience vs. main tasks in the project

The Atomic Scale Materials Modelling (ASM) section at DTU Energy is a leading centre in the development of electronic structure-based methods to model and understand the properties of materials and, aided by artificial intelligence, to use the insight to design new battery materials and interfaces. Our competences are within developing tools for computational prediction of materials properties and accelerated materials discovery through atomic-scale simulations, experimental data and machine learning methods. Among other state-of-the-art methodologies, we have developed advanced approaches to model electrochemical interface, cathode, anode and electrolyte materials for batteries, and to investigate transport and diffusion properties. Some of these tools have been implemented in the form of workflows to automate the design and discovery process. The section has a broad experience in participation and managing large EU projects and initiatives, not limited to battery applications. We also have two special initiatives (AiMade) targeted at integrating new computational tools, advanced experiments and artificial intelligence to accelerate and automate the discovery of new materials, and SURE (Self-correcting Unsupervised Reaction Energies) on the automated uncertainty-based prediction of chemical reaction networks.

The Section for Cognitive Systems at Department of Mathematics and Computer Science (DTU Compute) research information processing based on statistical machine learning and signal processing, on quantitative analysis of digital media and text, on mobility and complex networks, and on cognitive psychology. The main related contributions have been within deep unsupervised learning with generative models.

DTU's main tasks in the project are well-aligned with our core competencies, from the management of a large EU project (WP1) to contribute to establish of infrastructure for the accelerated and automation of the discovery of new materials (WP2 and WP9) and to develop state-of-the-art computational and AI/deep learning tools (WP11) applied to the grand challenges of batteries.

Description of legal entity and main tasks

The Technical University of Denmark (DTU) is a leading Scandinavian technical university and part of the Euro Tech University Alliance and Nordic Five Tech. DTU has extensive expertise within the areas of battery materials and mechanisms, heterogeneous and electro-catalysis, as well as computational materials design and autonomous synthesis and in-line characterization. The DTU activities are led by the Department for Energy Conversion and Storage (DTU Energy), focusing on the development of new technologies and materials for energy conversion and storage, including batteries. DTU Energy has core competencies within: electrochemistry; ion, defect and atomic transport in solids; functional ceramics and polymers; production and modelling processes; advanced testing; characterization of crystal, nano- and micro-structures; large facilities; as well as computer-based materials design, modelling and artificial intelligence.

CV or description of profile of key staff

- **Prof. Dr. Tejs Vegge** (M) is head of the ASM section at DTU Energy. He holds a PhD in computational materials physics from DTU and has subsequently worked as a postdoctoral fellow, senior researcher, and group leader as well as a visiting professor at SUNCAT@Stanford University and the Technical University of Munich. Prof. Tejs Vegge has been an innovator of clean energy materials for nearly 20 years, working on accelerating the clean energy materials discovery and innovation process. He is an internationally leading expert in the field of advanced battery materials and next-generation clean energy storage solutions. He has extensive management experience from several large national and international projects within computational and AI-assisted design of clean energy materials and batteries specifically. Among other things, he is an elected member of the Danish Academy of Technical Sciences (ATV), an appointed member of the Danish Government's Commission on Green Transportation and Mission Innovation Champion (2019), and an EU-US Frontiers of Engineering fellow (2016). Prof. Vegge is the author or co-author of >140 peer-reviewed scientific articles, which are cited more than 7,200 times, and he has an h-index of 42 (Google Scholar). His research interests include: Accelerated materials discovery, integrated computational and experimental design and development of novel materials for clean energy applications, first-principles theory of reaction mechanisms, integrated computational and experimental methods for reaction rates and kinetics, DFT-based design and modelling of electrochemical interfaces and nanoparticle catalysts. Finally, Prof. Vegge har supervised >20 PhD projects with an additional 10 still ongoing.
- **Prof. Dr. Ole Winter** (M) is Professor in data science and complexity at DTU Compute and professor MSO in Genomic bioinformatics at the Bioinformatics Centre, Department of Biology, Copenhagen University and Rigshospitalet. He is internationally renowned and a leading expert within machine learning, artificial intelligence and data science. He is part of two start-up companies that use natural language processing methods for aiding diagnosis of rare diseases and bringing better search to corporations. He has published 146 research articles (more than 7,400 citations, h-index 42, Google Scholar).
- **Assist. Prof. Dr. Ivano E. Castelli** (M) is Assistant Professor at DTU Energy. His expertise lies within big data and high-throughput material design. He has authored or co-authored 43 scientific articles, which are cited more than 2,800 times (h-index 21, Google Scholar). He is WP leader of the AiMade project, a competence centre at DTU Energy, focused on automate materials discovery and use of databases and artificial intelligence to speed up the design of novel materials. He is co-supervising three Ph.D. students, and main supervisor of a postdoc and two bachelor students.
- **Prof. Dr. Poul Norby** (M) He is Professor at DTU Energy. He is a leading international expert in in situ characterization of battery materials and the former coordinator of the EU project Hi-C, Novel in situ and in operando techniques for characterization of interfaces in electrochemical storage systems.

Relevant publications and/or products and/or services

- A. Bhowmik, **I.E. Castelli**, J.M. Garcia Lastra, P.B. Jørgensen, **O. Winther**, and **T. Vegge**, A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning, Energy Storage Materials 21, 446 (2019).
- F. T. Bölle, N. R. Mathiesen, A. J. Nielsen, **T. Vegge**, J. M. García Lastra, **I. E. Castelli**, Autonomous Discovery of Materials for Intercalation Electrodes, Batteries & Supercaps, DOI: 10.1002/batt.201900152 (2020).
- P. C. Jennings, S. Lysgaard, J. S. Hummelshøj, **T. Vegge**, T. Bligaard, Genetic Algorithms for Computational Materials Discovery Accelerated by Machine Learning, npj Comp. Materials 5, 46 (2019).
- D. Strmcnik, **I. E. Castelli**, J. G. Connell, D. Haering, M. Zorko, P. Martins, P. P. Lopes, B. Genorio, T. Østergaard, H. Gasteiger, F. Maglia, B. K. Antonopoulos, V. R. Stamenkovic, J. Rossmeisl, and N. M. Markovic, Electrocatalytic Transformation of Impurity HF to H_2 and LiF in Lithium Ion Batteries, Nature Catalysis 1, 255 (2018).
- S. Lysgaard, M. K. Christensen, H. A. Hansen, J. M. Garcia-Lastra, **P. Norby**, **T. Vegge**, Combined DFT and DEMS investigation of the effect of dopants in secondary zinc-air batteries, ChemSusChem 11, 1933 (2018).

Relevant previous project of activities connected to subject of proposal

- 2020-2022: Novo Nordisk Foundation "SURE: Self-correcting Unsupervised Reaction Energies", PI Tejs Vegge and co-PI Ole Winther (DTU), Duration: 2020-2022, task: develop a framework based on atomistic simulations and machine learning to predict uncertainty in chemical reactions.
- 2018-2022: Special Competence Initiative (SCI) "AiMade: Autonomous Materials Discovery", PI Tejs Vegge (DTU), task: establish a platform for autonomous materials discovery of clean energy materials through creation of a common data-infrastructure and ontology for materials data, connecting modelling and experiments.
- 2018-2022: H2020 FET Proactive "E-Magic: European Magnesium Interactive Battery Community", DTU is a partner, task: modelling and in-silico design of Mg-ion battery materials and interfaces.
- 2019-2020: H2020 CSA "Battery 2030+: A large-scale initiative on future battery technologies" DTU is a partner, task: development of a roadmap to enable Europe to take the lead for the discovery of new batteries.
- 2017-2020: H2020 FET Open "Salbage: Sulfur-Aluminium Battery with Advanced Polymeric Gel Electrolytes", DTU is a partner, task: modelling of the electrolyte and interfaces in Al-S batteries for the development of a more efficient, dendride free battery.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

DTU Energy is co-developer of the GPAW electronic structure code, which will be utilized in several tasks, and the Atomistic Simulation Environment (ASE) package, which will be one of the main platforms used to support the various implementations. The department contributes to the management of a powerful Linux cluster (Niflheim) with ~15000 CPU cores and a peak performance of >800 teraflops and GPU cluster with 78 GPUs. Both will be available for this project.

4.1.2 UPPSALA UPPSALA UNIVERSITET (UU)

UPPSALA UNIVERSITET	**Name:** UPPSALA UNIVERSITET (UU)	**Partner no:** 2	**Country:** Sweden
	Type: UNI	**Number of R&D personnel:** 4 782 **Number of employees:** 7 108	**Turnover:** 667 M€

Interest in the project

We want to augment the knowledge about battery-related interfaces and contribute to the goals put forward in the Battery 2030+ manifesto. We have expert knowledge, skills and track records in key experimental and modelling aspects of battery research. The objectives of Battery 2030+ and BIG-MAP are strongly supported by Uppsala University (UU).

Previous experience vs. main tasks in the project

Edström will contribute to large-scale facility research in WP5. UU pioneered synchrotron-based XPS research to explore the interfacial chemistry of Li-ion battery electrodes already in the 1990s. Since then, UU has worked with technology development through the exploration of HAXPES, operando techniques, and high-pressure XPS. Extensive research has also been carried out using neutron diffraction, and her group was pioneering in-situ diffraction techniques for batteries.
Brandell will mainly participate in WP8, "Standards and protocols". Having worked closely with computational-experimental research for several decades in the Li-ion battery area has made us well equipped to contribute to the task of communicating between different fields and disciplines in the area.
Broqvist will participate in WP3 and WP9 and related interacting WPs. Broqvist has a long experience in high-performance computing in materials science, including the development of models for material simulations at the electronic (high-level and approximate) and atomistic levels with a particular focus on redox chemistry.
Hermansson will be the WP leader of WP2. Hermansson has expertise in the fields of static and dynamic multi-scale modelling (sequential and hierarchical), model development, and, not least, the challenges of modelling ionics-molecular interfaces. Within the European Materials Modelling Council (www.emmc.org), Hermansson arranged international conferences to highlight synergies between physics-based and data-driven modelling in 2018 and 2019 (https://sites.google.com/site/emultiscale2019/).

Description of legal entity and main tasks

Founded in 1477, UU is the oldest University in the Nordic countries. UU is a comprehensive university with nine faculties and has been placed among the 100 best universities in the world in the three largest international rankings (THE, QS, ARWU/Shanghai). It has about 45,000 undergraduate students, 2,500 Ph.D. students and 6500 employees. The focus lies on both research and education.

The UU partner is embedded in the Department of Chemistry – Ångström Laboratory — one of Europe's best-equipped Materials Research Laboratories, where the Ångström Advanced Battery Centre (ÅABC) is an integral part. The Centre involves ca. 80 researchers and is the leading research environment for the development of electrochemical storage materials and advanced battery technology in the Nordic countries with a research focus on commercial and next-generation Li-ion batteries, as well as Na-ion, Li-S, organic electrodes, solid-state, etc. The expertise lies in the synthesis of electrode and electrolyte materials and electrochemical testing, but equally important are the development of in operando structural characterization techniques and surface science techniques. The Centre also has a vivid environment for multi-scale modelling, static and dynamical simulations of chemical interface systems, batteries and battery materials.

CV or description of profile of key staff

- **Prof. Kristina Edström** (F) received her PhD in Chemistry at Uppsala University in 1990, and today coordinates the Ångström Advanced Battery Center. Her research focus is on synthesis, structure, function and electrochemical characterization of novel nano-structured electrode and electrolyte materials. She is an expert on photoelectron spectroscopy and high energy spectroscopy studies of battery interfaces, as well as operando studies of battery cells, and thereby has extensive experience of development of synchrotron-based analytical tools for batteries. She has published more than 250 peer-reviewed papers in the battery field and her h-index is 59. She has supervised 28 PhD students (18 as first supervisor).
- **Prof. Daniel Brandell** (M) is Professor in Materials Chemistry and is responsible for the Structural Chemistry programme at UU since 2018, which hosts the ÅABC. Brandell has a background in several modelling techniques for batteries and battery materials, including DFT, MD simulations and Finite Element Methodology (FEM). His activities are often focused on bridging computational and experimental chemistry and materials science. Brandell has extensive experience in the field of polymer electrolytes, where he has an ERC Consolidator Grant, including MD simulations. Brandell has published >140 peer-reviewed research papers.
- **Senior lecturer Peter Broqvist** (M) possesses a comprehensive expertise in materials simulations: MSc degree in Chemical engineering, Ph.D. degree in Materials science (CTH UoT, 2005), research fellow position in Physics at EPFL (with Prof. A. Pasquarello) and now Inorganic Chemistry at UU, where he was recruited to the strategic e-science program eSSENCE in 2011. Broqvist has received the Göran Gustafsson Prize for young researchers and holds several computing-related commissions of trust. Research focus: multiscale models development at the electronic and atomistic levels with a focus on redox chemistry. > 70 peer-reviewed research papers.
- **Prof. Kersti Hermansson** (F) is Professor of Inorganic Chemistry. Her expertise lies in e-science for materials chemistry, namely the development of multiscale modelling strategies to bring chemical modelling closer to the complex dynamical systems of the real world. Her main applications are dynamical phenomena at metal oxide surfaces, redox chemistry at liquid/solid interfaces (mostly water) and computational vibrational spectroscopy. She is a member of the Royal Swedish Academy of Sciences (KVA), coordinator of the model development activities of the European Materials Modelling Council (www.emmc.info) and coordinator of CECAM-Sweden. > 220 peer-reviewed papers.

Relevant publications and/or products and/or services

- A.A. Franco, A. Rucci, D. Brandell, C. Frayret, M. Gaberscek, P. Jankowski, P. Johansson, "Boosting Rechargeable Batteries R&D by Multi-scale Modeling: Myth or Reality?", Chemical Reviews, 119 (2019) 4569.
- M. Ebadi, C. Marchiori, J. Mindemark, D. Brandell, C. Moyses Araujo, "Assessing Structure and Stability of Polymer/Lithium-Metal Interfaces from First-Principles Calculations", J. Mater. Chem. A, 7 (2019) 8394.
- V. Quaranta, M. Hellström, J. Behler, J. Kullgren, P. D. Mitev, and K. Hermansson. "Maximally resolved anharmonic OH vibrational spectrum of the water/ZnO(10-10) interface from a high-dimensional neural network potential, The Journal of Chemical Physics, 148 (2018) 241720. ("Editor's choice").
- J. Kullgren, M. J. Wolf, K. Hermansson, Ch. Köhler, B. Aradi, Th.Frauenheim, P. Broqvist. "Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Parameters for Ceria in 0D to 3D", J. Phys. Chem. C, 121 (2017) 4593.
- A. Mirsakiyeva, M. Ebadi, C.M. Araujo, D. Brandell, P. Broqvist, J.Kullgren, "Initial Steps in PEO Decomposition on a Li Metal Electrode", J. Phys. Chem. C, 123 (2019) 22851.

Relevant previous project of activities connected to subject of proposal

- **LiRichFCC – A new class of powerful materials for electrochemical energy storage: Lithium-rich oxyfluorides with cubic dense packing**. Funding organization: EU H2020 FET-OPEN. Duration: 2016-2019. Task: Multi-scale modelling and experimental research of bulk and interfacial transport and degradation processes. UU is partner.
- **FUN POLYSTORE – Functional Polymer Electrolytes for Energy Storage.** *Funding organization: European Research Council.* Duration: 2018-2023. Task: Synthesis of polymer electrolytes, MD modelling, Battery fabrication. UU is sole partner.
- **European Materials Modelling Council (EMMC-CSA).** *Funding organisation*: EU H2020 (LEIT) Coordinating and Support Action under Grant Agreement No 72386. Duration: 2016-2019 Task: To promote the use of materials modelling in European industry.
- **SintBat.** *Funding organization: EU H2020.* Duration: 2016-2020. Project on graphite/Si composite anodes. UU is responsible for interfacial characterization and electrolyte development, also involving solid-state electrolyte systems for stabilization of Si-based electrodes. UU is partner.
- **TriLi** and **ProLi.** *Funding organization*: Swedish Energy Agency. Duration: 2015-2019. Large-scale projects on utilization of Li-metal as anode material, also involving tailoring of electrolyte materials for stabilization and interfacial modelling.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Through the Swedish National Infrastructure for Scientific Computing (SNIC), UU has access to ample and advanced high-performance computing (HPC) resources, including CPU and GPU architectures (https://www.snic.se/resources/). In addition, SNIC makes available application experts to ensure proper use of the resources. Hermansson and Broqvist are the Pis of a running long-term large-scale project within SNIC and are both experienced HPC users.

4.1.3 KARLSRUHER INSTITUT FUER TECHNOLOGIE (KIT)

	Name: KARLSRUHER INSTITUT FUER TECHNOLOGIE (KIT)	**Partner no:** 3	**Country:** Germany
	Type: RTO	**Number of R&D personnel:** 5 046 **Number of employees:** 9 277	**Turnover:** 881 M€

Interest in the project

KIT is one of three partners in CELEST, the Center for Electrochemical Energy Storage Ulm-Karlsruhe which constitutes the largest battery research center in Germany as measured by its scientific output. CELEST is active in the fields of Li-ion and post-Li battery research. Materials discovery and design of tailored interfaces lie at the core of new battery technologies, and our existing activities in the areas of Na, Mg, Al, or Ca-based batteries align perfectly with the goals of Battery 2030+. By connecting with the European partners within Battery 2030+, we intend to create synergies for the development of novel paradigms in materials discovery and design of interfaces for new, powerful, and sustainable electrochemical energy storage technologies.

Previous experience vs. main tasks in the project

Led by experienced personnel and specialized infrastructure, KIT will provide full scientific-technical know-how from the Cluster of Excellence "POLiS" (Energy Storage Beyond Lithium). Moreover, KIT will provide a unique setup and approach for BIG-MAP. We designed two autonomy enabled high-throughput MAP-Agents that investigate early to intermediate lifetime SEI formation and processes. Extension to bulk materials testing is planned.

- The *52nravellin scale battery high-throughput battery research* (**MISCHBAR**) system that utilizes sequential experimentation to investigate the SEI by electrochemistry, XPS, UPS, FTIR, Raman and other methods
- The *manufacturing for ultraparallel long-term testing* of batteries (**MULLET**) system that assembles batteries with varied electrolyte formulation to study SEI effects at intermediate to late lifetime
- Early design plans for **parallel pre-aging of SEIs** for MISCHBAR

Combining our expertise in battery research and development, novel battery chemistries, and virtual materials design with that of the Battery 2030+, partners are anticipated to lead to a deeper understanding and discovery of design rules for battery interfaces and interphases and eventually to the development of full batteries which perform equal or better compared to existing technology and provide sustainable solutions for the energy storage of the future.
KIT will lead WP 5 "AI-Accelerated Materials Discovery". In this WP, KIT will lead or contribute to the following tasks: "5.1: Accelerating experiments with active learning", "5.2: Latent experiment and materials representation for translational learning and new fundamental insights", "5.3: An automated data analysis framework", "5.4: Automatic reasoning and materials funnel"

Description of legal entity and main tasks

KIT is a higher education and research organization with more than 9,000 employees, over 25,000 students, and a total annual budget of about 900 million €. At KIT, 17 institutes with 42 Pis have united in the joint initiative VirtMat aiming at virtual materials design. VirMat develops information-driven approaches towards predictive material simulations that will enable experimental breakthroughs in physics, chemistry, biotechnology and materials science. VirtMat is involved in many international projects addressing novel data infrastructures, data analysis and infrastructures, and machine learning.

The Battery Technical Center (BaTeC) pools the competencies of KIT along the battery research chain under one roof and constitutes an open technology platform for future electric energy storage systems. BaTeC

focusses on the development and production of new materials and cells as well as the development of full batteries and system integration. Simultaneously, new manufacturing processes for the cost-efficient battery production are being developed and demonstrated. In collaboration with Ulm University as well as the Deutschen Zentrum für Luft- und Raumfahrt (DLR) and the Center for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW) as associate partners, KIT founded the Helmholtz Institute Ulm (HIU), which pursues fundamental questions in electrochemical energy storage as a basis for vital new material and cell concepts.

CV or description of profile of key staff

- **Prof. Maximilian Fichtner** (M) is a director at KIT. He is also Professor at Ulm University (Uulm) for Solid State Chemistry and Head of Materials-I at the Helmholtz Institute Ulm for Electrochemical Storage (HIU). He has published more than 250 research and conference papers on energy storage materials and systems and is (co-)author of 20 patents and patent applications. His h index is 48. On the European level, he has been coordinator of a FET-OPEN project (LiRichFCC), an EU-RTD (NANOHY), and has participated in 8 other EU RTDs, MCRTs, and KIC InnoEnergy projects. He has been coordinating a joint proposal of KIT and Uulm in the framework of the German Excellence Strategy ("Energy Storage Beyond Li"), is co-author of the current SET-Plan Materials for Low Carbon Energy Technologies Roadmap. Since 2018 he is also spokesperson of CELEST and spokesperson of the Cluster of Excellence "Energy Storage Beyond Lithium" (budget 65 Mio EUR over 7 years).
- **Prof. Wolfgang Wenzel (M)** is head of department in the Institute of Nanotechnology at KIT. He is Professor at the Department of Physics since 2010 and Research Group Leader Nanoscale and Biomolecular Simulation at the Institute of Nanotechnology since 2001. He is also Speaker of the KIT Center for Materials in Technology and Life Sciences and also Speaker of the Joint Lab Virtual Materials Design and of the Virtmat Initiative. He has published more than 220 research papers on Multiscale Materials Modelling and Virtual Design. His h-index is 41. On the European level, he is member of the EU-NSF Committee Nanotechnology 2020 and Member of the European Materials Modelling Council. He is also on Extended Management Board of the Helmholtz Research Area Information and on Scientific Advisory Board of the von Neumann Center of the Research Center Jülich. He is part of the new excellence cluster 3D Matter Made to Order (3DMM2O), which is a collaboration of Karlsruhe Institute of Technology (KIT) and Heidelberg University (Uni HD).
- **Prof. Helge S. Stein (M)** is the appointed W1 Professor of Applied Electrochemistry (starting Spring 2020) and head of the Autonomous Robotics group at the Helmholtz Institute Ulm for Electrochemical Storage (HIU). He is a distinguished expert in the field of high-throughput electrochemistry, autonomous feedback loops, and machine learning for experimental materials science. He has published over 20 research items during his PhD and Postdoc time with a h-index of 10. As part of his appointment at KIT/HIU he is in charge of building up a robotic infrastructure capable of characterizing early interfacial effects and long term battery performance. Previous to his appointment at KIT/HIU he worked at Caltech on the establishment of a data science infrastructure, deployment of data management of millions of materials experiments, 53nravelling of fundamental insight through explainable AI, and acceleration of research by means of active learning.

Relevant publications and/or products and/or services

- P. Friederich, W. Wenzel, et al., Machine learning of correlated dihedral potentials for atomistic molecular force fields, Scientific Reports 8, 2018, doi.org/10.1038/s41598-018-21070-0
- P. Friederich, W. Wenzel, et al., Rational In Silico Design of an Organic Semiconductor with Improved Electron Mobility, Adv. Mater. 29, 2017, doi.org/10.1002/adma.201703505
- D. Bresser et al., Perspectives of automotive battery R&D in China, Germany, Japan, and the USA. 2018. Journal of Power Sources, 2018, doi.org/10.1016/j.jpowsour.2018.02.039
- Z. Zhao-Karger et al., A new class of non-corrosive, highly efficient electrolytes for rechargeable magnesium batteries. 2017. Journal of Materials Chemistry A, doi.org/10.1039/C7TA02237A
- Z. Li, M. Fichtner, et al., Towards stable and efficient electrolytes for room-temperature rechargeable calcium batteries, Energy & Environm. Sci., 2019, doi.org/10.1039/C9EE01699F

Relevant previous projects or activities connected to subject of proposal

- Cluster of Excellence POLiS: 65 Mio. € project on post-lithium electrochemical energy storage in collaboration with Ulm University, ZSW Ulm, and Giessen University, 2019-2025, coordinator
- LiRichFCC: H2020 FET-OPEN project on high-energy density cathode materials for Li-ion battieries, 2016-2019, coordinator
- VirtMat, Platform with 42 Pis on information-driven materials research, since 2016, KIT
- Mag-S, Development and production of rechargeable magnesium-sulphur batteries, 2016, BMBF (Germany), DLR
- Mat4Bat, Advanced Materials for Batteries, 2013 – 2017, EU FP7, CEA

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

All involved research facilities and institutes at KIT house state-of-the art equipment for materials synthesis & characterization as well as cell or battery testing. Special infrastructures include: HEMF: Pilot plant for the synthesis of battery storage materials up to 10 kg; ERWIN (Energy Research with Neutrons): Dedicated beamline at the Neutron Research Reactor FRM II, Garching, Production line for electrodes for lab cells to industrial format cells (mixers, 2 roll-to-roll coaters, 3 calenders), Semi-automated assembly line for 50 mAh lab pouch cells to 20 Ah cells.

KIT has the entire computational and laboratory infrastructure available that is necessary to successfully conduct the proposed work. This includes access to computer clusters, data management and sharing facilities, materials processing and characterization equipment, as well as cell and battery testing facilities with hundreds of test channels. Particularly for the work in this project, KIT is currently setting up a fully automated, robot-assisted test facility for autonomous materials discovery at Helmholtz-Institute Ulm. This facility includes the automated, combinatorial formulation, synthesis, assembly and characterization of electrochemical energy storage systems which is coupled with an AI-based analysis system that autonomously decides about process variations and optimization.

4.1.4 CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS)

	Name: CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS)	**Partner no:** 4	**Country:** France
	Type: RTO	**Number of R&D personnel:** 11 000 **Number of employees:** 32 000	**Turnover:** 3400 M€

Interest in the project

The CNRS network is already fully engaged at the French level into the development of better electrochemical energy storage and conversion devices such as Li- and Na-ion batteries. Joining the Battery2030+ consortium will allow the CNRS to join forces at the European level for the acceleration of discoveries of better chemistries for batteries, for that the network will bring its expertise and existing infrastructure for the design, modelling and testing of batteries while taking advantages of the new capabilities and expertise built in the project (AI for batteries, etc.)

Previous experience vs. main tasks in the project

RS2E lab of CNRS is composed of 17 research laboratories with complementary expertise in materials science, electrochemical devices, modelling (molecular dynamics and density functional theory) as well as upscaling and prototyping. More specifically, the CNRS has previous experience regarding multiscale modelling of batteries (existing teams working on this topic with Prof. Franco, Prof. Salanne, Dr. Doublet etc.), the development of platforms for batteries prototyping and testing (platform already existing in LRCS Amiens), development of characterizations techniques such as XPS, NMR, TEM as well as a strong collaboration with SOLEIL with two permanent researchers from the network being full-time at the synchrotron (J. Sottman and A. Iadecolla) and the standardization of data (electrochemical and characterization) at the French level with recent data mining experiences (Prof. Franco and Dr. Grimaud).
Combining this experience as well as using the strong collaborative environment provided by such existing network, CNRS will lead the efforts regarding WP8 (Standards and Protocols) where close relationship between experimentalist, theoretical chemists as well as battery testing will be critical. Furthermore, CNRS will participate to WP5 with the development of multi-techniques electrochemical cells for synchrotron/neutron measurements owing to our strong collaborative experience with synchrotron SOLEIL. CNRS/UPJV (described below) will also contribute to WP3 for the development of multiscale modelling capabilities as well as to the Battery Interface Genome (WP11) for the integration of multi-fidelity data to the definition of descriptors for the physical phenomena at the interface.

Description of legal entity and main tasks

CNRS (legal entity)
The Centre National de la Recherche Scientifique (CNRS, National Centre for Scientific Research) is a state-funded science and technology establishment placed under the authority of the French Minister for Research with around 32,000 agents. The mission of CNRS is to assess and conduct any research of utility to the advancement of science and to the economic, social and cultural progress of France through its laboratories located throughout France. In the field of *electrochemical storage systems (namely rechargeable batteries and supercapacitors)*, CNRS decided to create in 2010 together with the French Ministry of Higher Education and Research the **French Network on Electrochemical Energy Storage (RS2E)** so as to put France at the cutting-edge of research and tech-transfer activities.

CNRS-RS2E
RS2E is a federative structure without any legal personality, coordinated by CNRS and created in 2010 in the purpose of fostering relationship between the main research laboratories working in France in the field of rechargeable batteries and supercapacitors. Labelled in 2011 “Laboratoire d’Excellence” (LABEX “STORE-EX”), RS2E is headed to date by Prof. Jean-Marie Tarascon (CNRS-CSE) and Prof. Patrice Simon (CNRS-CIRIMAT)

and reunites 17 research laboratories having complementary and world-class expertises in the field as decribed below:

- **Solid-state Chemistry-Energy, Paris (CNRS-CSE)**: This laboratory led by Prof. Jean-Marie Tarascon is a joint-research unit between CNRS, College de France and Sorbonne Université. Created within the facilities of College de France (Paris) after Jean-Marie Tarascon was appointed as Professor at College de France in June 2013, it consists of 20 staff members including 4 permanent staff, the remainders being Post-Doc and PhD students. The main research areas herein developed focus on solid state/soft chemistry, crystallography, electrolyte formulation and electrochemistry applied to electrochemical storage devices such as Li-ion batteries and alternative technologies dealing with Oxygen Evolution Reaction (OER) or Oxygen Reduction Reaction (ORR) both in aqueous and non-aqueous media.
- **Laboratory of reactivity and solid-state chemistry, Amiens (CNRS-LRCS)**: The laboratory was founded in 1968 and became a joint Research Institute between the CNRS and the University of Picardie Jules Verne (UPJV will be a Linked Third Party (LTP) in the project, Amiens (UMR 7314) in 2000. It consists of 85 researchers, of whom 35 are permanent; the remainders are PhD students and postdocs. The laboratory has a strong expertise in the design/development of tailored materials for batteries (active material and electrolyte as well) both at the lab and prototyping scale, in interface characterization through in situ microscopy techniques with a recent and strong emphasis on modeling and safety aspects of battery components.
- **Physico-chemistry of electrolytes and interfacial nanosystems, Paris (CNRS-PHENIX):** The Laboratory is a joint research unit between CNRS and Sorbonne Université created in 2014. Research activities are mainly focused on colloidal systems and porous materials dedicated to energy, health and environmental applications. One of the main worldwide-known expertise at PHENIX is the strong coupling between lab experiences and modeling. In the field of electrochemical storage systems, PHENIX is active on modeling and experimental characterisation of transport and retention properties of confined fluids and charged species together with chareactization of rechargeable energy systems at synchrotron facilities. PHENIX currently gathers ca. 90 people including 40 permanent researchers.
- **Interuniversity center of materials research and engineering, Toulouse (CNRS-CIRIMAT):** CIRIMAT is a joint research unit between Université Paul Sabatier (Toulouse 3) and CNRS labelled since 2006 as Carnot Institute due to its wide connection with industries. There are 8 research groups at CIRIMAT, representing 204 people (ca 100 permanent staff and 84 PhDs and Post Doc) including the "Materials for Energy Storage" team activity which, led by Prof Patrice Simon, involves 16 people. The world-class team has sound knowledge of the (electro)chemical modifications and the electrochemical characterizations of materials for energy storage (sodium ion and supercapacitors).
- **Institute of chemistry and condensed matter, Bordeaux (CNRS-ICMCB):** the laboratory is a joint research unit between CNRS, University of Bordeaux and Institut National Polytechnique de Bordeaux (Bordeaux-INP). It gathers 7 research groups in the field of Solid State Chemistry, Materials Science and Molecular Science. It is strongly associated to the University of Bordeaux and to the Graduate Engineering School of Chemistry, Biology and Physics (ENSCBP). The group "Energy: Materials and Batteries" of ICMCB headed by L. Croguennec from 2004 develops researches mainly devoted to material synthesis, transport properties and electrochemistry, as well as characterization of mechanisms involved within the materials during their use in electrochemical systems (from alkaline batteries to Li(Na)-ion batteries, microbatteries and more recently supercapacitors).
- **Institute of material science, Mulhouse (CNRS-IS2M):** the laboratory is a mixed research unit between CNRS and University of Haute Alsace (UHA) and an international leading Institute in the field of materials focused on polymers, carbon, oxides, ceramics and semi-conductors. IS2M is specialized in the development of innovating synthesis processes, functionalisation methods, characterizations tools and the study of interaction mechanisms between a surface and its environment. The French government attributed the Label 'Institute Carnot' to our Institute recognizing our capacity to conduct upstream research capable of renewing their scientific and technological skills, and an ambitious academic and industrial partnership research policy to the benefit of the socio-economic world. IS2M employs around 150 staff included tenured researchers, engineers and support staff.
- **Institute of analytical Sciences and physico-chemistry for environment and materials (CNRS-IPREM):** IPREM is a joint Research Institute between CNRS and the University of Pau. It consists of about 200 researchers including 110 permanent staff. It is a multi-field research center dedicated to research on environment and materials, organised in four teams. The Physical Chemistry Team (ECP) develops a specific expertise in research on materials surfaces and interfaces (inorganic and hybrid compounds) and theoretical chemistry. A group of 16 people including 8 permanent people is working in the field of energy storage systems and is a world-class research group in the investigation of interfaces in various systems.
- **Institute of materials Jean Rouxel, Nantes (CNRS-IMN)**

- **Institute Charles Gerhardt, Montpellier » (CNRS-ICGM)**
- **Laboratory of extreme conditions and materials : high temperature and irradiation » (CNRS-CEMHTI)**
- **Laboratory of chemistry of condensed matter, Paris » (CNRS-LCMCP)**
- **Research institute of chemistry, Paris (CNRS-IRCP)**
- **Institute of radical chemistry, Marseille (CNRS-ICR)**
- **Institute of electronics, microelectronics and nanotechnology, Lille (CNRS-IEMN)**
- **Laboratory of analysis and modeling for biology and environment, Evry (CNRS-LAMBE)**

CV or description of profile of key staff

- **Prof. Jean-Marie Tarascon** (M): Director of the RS2E lab of CNRS network since 2011, Director of the UMR8260 laboratory since 2013 (Collège de France, Paris). Prof. Tarascon has more than 30 years of experience in the domain of batteries. He has been the coordinator of European and French projects related to the topic. Prof. Tarascon has published more than 700 publications and holds more than 100 patents (20 were licensed and 7 are commercialized). ERC Advanced Grant 2015, Recipient of the 2011 ENI Award, the 2015 Yeager Award, the 2015 Centenary Prize from the RSC, the 2017 Samson Prize, the 2017 Galvani Prize etc.
- **Prof. Patrice Simon** (M): Vice-Director of the RS2E network since 2011. Prof. Simon has been working on capacitors and batteries since early 2000. He has been the coordinator of European and French projects related to the topic. Prof. Simon has published more than 200 publications in the field of electrochemistry. ERC Advanced Grant 2012, Recipient of the 2009 Tajima Prize (ISE), the RUSNANOPRIZE 2015, the CNRS Silver Medal 2015, Elected Fellow of the ISE in 2016.
- **Dr. Alexis Grimaud** (M): CNRS researcher since 2014 and member of the RS2E. Dr. Grimaud has been working in the field of electrocatalysis and electrochemical interfaces since 2012, and is part of European projects as well as coordinator of French project in the field of Energy conversion and storage devices. Dr. Grimaud has published more than 50 publications in the field of electrochemistry. Prize from the French Society of Chemistry 2018 (Energy division), recipient of the Young carrier award from the French National Funding Agency (ANR) 2017.
- **Prof. Alejandro A. Franco** (M): Full professor at Université de Picardie Jules Verne (Amiens, France). Main expertises: multiscale modeling and A.I. applied to electrochemical energy devices. Leader of the Theory Open Platform at the ALISTORE-ERI. Grantee of an ERC Consolidator Grant (project "ARTISTIC": multiscale modeling of Lithium Ion Battery fabrication). >80 peer-reviewed articles, 20 patents, >60 invited keynotes/invited oral presentations in international conferences. He has been PI/Work package leader in several national and EU projects as well as in collaborative projects with industry.

Relevant publications and/or products and/or services

- Profs. Tarascon and Simon are funders and Board Members of TIAMAT (http://www.tiamat-energy.com/en/)
- P. Simon et al, Materials for Electrochemical Capacitors, Nature Materials 2008 (> 10000 citations)
- P. Simon et al, Where do Batteries end and Supercapacitors begin, Science 2014 (> 2000 citations)
- J.M. Tarascon et al, Issues and Challenges Facing Rechargeable Batteries, Nature 2001 (> 12000 citations)
- M. Armand and J.M. Tarascon, Building Better Batteries, Nature 2008 (> 10000 citations)

Relevant previous project of activities connected to subject of proposal

- ERC Advanced Grant 2015 - ARPEMA, coordinator Prof. Tarascon, Anionic redox processes for better electrochemical energy storage devices
- ERC Advanced Grant 2012 – IONACES, coordinator Prof. Simon, Ion transport in nanoporous carbons for energy storage and sustainable development
- H2020 project 2015 – NAIADES, participant Prof. Tarascons and Simon, Development of Na-ion batteries
- H2020 project 2019 – NAIMA, participant Prof. Tarascon, Development of Na-ion batteries
- ERC Consolidator Grant 2017 – ARTISTIC, coordinator Prof. Alejandro Franco (part of the CNRS), Multiscale modelling and reverse engineering for the formulation and fabrication of Li-ion batteries

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work
The RS2E/CNRS, network which is made of 17 academic laboratories and which gathers 15 industrial partners as well as 3 government funding organizations is specialized in the transfer of technologies related to electrochemical energy storage and conversion devices. The network possesses its own prototyping platform of 5500 m², located at the HUB in LRCS Amiens, for the development of Li- and Na-ion batteries. This platform comprised clean room as well as equipment for the scaling up of battery materials as well as the assembly of 18650 batteries. Furthermore, the academic laboratories comprising the CNRS possess a wide variety of materials characterization equipment such as HRTEM (LRCS, Amiens), XPS (IPREM, Pau), high field NMR (CEMHTI, Orléans) etc. as well as computational clusters (PHENIX, Paris and ICGM, Montpellier). Furthermore, the network is comprised of research laboratories with synthesis and battery testing capabilities. These platforms will be fully open to other participants to this European project. Furthermore, the tools and testing protocols currently developed within the network will also be shared with other members in order to create a productive scientific environment.

4.1.5 WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER (WWU)

	Name: WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER (WWU)	**Partner no:** 5	**Country:** Germany
	Type: UNI	**Number of R&D personnel:** 145 **Number of employees:** 165	**Turnover:** 600 M€

Interest in the project

The participation in this project will provide a detailed understanding of transport and reaction mechanisms at battery interfaces and interphases across multiple scales. Our strongholds in high-throughput sampling (HTS), the broad range of physicochemical, electrochemical, analytical, spectroscopic, and structural methods, and high-level multiscale simulation methods fit well to the scope of the BIG-MAP concept.

Previous experience vs. main tasks in the project

Three key fields of expertise are supplied: (1) Modelling ion transport phenomena in various electrolytes via classical and *ab initio* Molecular Dynamics (MD) simulations, Monte Carlo (MC) simulations, as well as hybrid MD/MC schemes addressing the initial SEI formation, the latter enabling the treatment of chemical reactions in classical MD simulations, as well as the development of analytical transport models. (2) Identification of advanced active and inactive battery materials, including their incorporation in the battery cell. (3) A fully operational HTS system for liquid electrolytes, comprising their formulation, cell assembly, and preselected electrochemical methods serving as filter. The tight exchange of multiscale simulation and HTS experiments facilitates the validation, understanding, and prediction of advanced electrolyte formulations for given cell chemistry. Furthermore, via the HTS approach lead electrolyte formulations can be identified for the BIG-MAP consortium. The resulting data pool from simulations and HTS experiments have to be included in standardized data formats to be developed within BIG-MAP.

Description of legal entity and main tasks

The University of Münster (WWU), with 45,500 students, is one of Germany's leading universities. Electrochemical energy storage research at WWU is taking place at multiple groups. MEET Battery Research Center (Münster Electrochemical Energy Technology) works on R&D of innovative electrochemical energy storage materials and devices. As MEET aspires to build bridges between fundamental research and practical application, it cooperates not only with other scientific institutions but also with industry. MEET pursues holistic, systemic R&D, which, in addition to synthesis and production, characterization and analysis of materials, components and cells, naturally also covers the various aspects of application, including environmental impact, economic efficiency, and social impact. MEET has outstanding state-of-the-art equipment and laboratories. The facilities include the modules functional material synthesis, electrode and cell production, cell testing and electrochemical measurement techniques, supplemented by a large technical center, including a dry room and a clean room. Of particular relevance for the BIG-MAP proposal is the HTS system and the broad portfolio of methods for post-mortem analysis of aged lithium-ion cells. The current focus is on research into lithium-ion batteries; in addition, future battery generations and alternative electrochemical storage devices and converters are under intensive development. In the Institute of Physical Chemistry at WWU in the working group "Theory of Complex Systems" computer simulations are performed on very different scales, contributing significantly to the better understanding of electrolytes, interphases and electrolyte/electrode interfaces.

CV or description of profile of key staff

- **Prof. Dr. Andreas Heuer** (M) is full professor at WWU (Institute of Physical Chemistry) since 1999 and, at the same time, responsible for the theory activities at HI MS. He obtained his PhD (Physics) at the University of Heidelberg and his Habilitation (Theoretical Physics) at the University of Mainz. In strong interaction with a large network of experimental groups, in his group computer simulations are applied to many complex systems, in particular to systems, containing electrolytes. Due to the multitude of methods, established in his group, material properties can be analysed for a large range of length and time scales. Whenever possible, computer simulations are supplemented by analytical calculations. The work is published in more than 200 papers.
- **Prof. Prof. h.c. mult. Dr. Martin Winter** (M) is Director of the Helmholtz-Institute Muenster (FZJ-IEK 12) and MEET Battery Research Center of WWU Münster, Member of the National Academy of Science and Engineering, Member of the National Platform E-Mobility (NPE9), Chairman of the Advisory Board of German Battery Research by the Federal Ministry of Education and Research (BMBF), President of the International Meeting on Lithium Batteries (IMLB), Chairman of the International Battery Materials Association (IBA). He received more than 50 awards and recognitions, among them: Fellow of the International Society of Electrochemistry (ISE) and of the Electrochemical Society (ECS) and German Federal Cross of Merit-1st Class. He has been involved in the field of energy electrochemical energy storage and conversion for almost 30 years, with a focus on materials, components and cell design for Li-ion batteries and Li metal batteries, >600 articles, h=82 (Google), 'Highly cited researcher' 2008-2017 (Web of Science). Martin Winter holds a professorship for "Materials Science, Energy and Electrochemistry" at the Institute of Physical Chemistry at the University of Münster.
- **Dr. Tobias Placke** (M) is head of the division "Materials" at the MEET Battery Research Center (University of Münster) in Münster, Germany. In this division, the synthesis, optimization and characterization of advanced anode and cathode active materials as well as inactive components for the next generation of lithium ion batteries (LIBs) is investigated. Besides LIBs, the group also focusses on the development of alternative advanced battery storage technologies. Tobias Placke studied chemistry at the University of Münster and received his diploma in the group of Prof. Martin Winter in the field of physical chemistry in 2010. He finished his doctorate (Dr. rer. nat.) at MEET in 2014 in the field of graphite-based anode materials for LIBs and dual ion batteries.

Relevant publications and/or products and/or services

- Schmuch, R.; Wagner, R.; Hörpel, G.; Placke, T.; Winter, M., Performance and cost of materials for lithium-based rechargeable automotive batteries. Nature Energy 2018, 3, (4), 267-278.
- Betz, J.; Bieker, G.; Meister, P.; Placke, T.; Winter, M.; Schmuch, R., Theoretical versus Practical Energy: A Plea for More Transparency in the Energy Calculation of Different Rechargeable Battery Systems. Advanced Energy Materials 2019, 9, 1803170-1803187.
- S. Nowak, M. Winter, The Role of Cations on the Performance of Lithium Ion Batteries: A Quantitative Analytical Approach, Acc. Chem. Res. 2018, 51, 2, 265-272.
- Smiatek, J., Heuer, A.; Winter, M., Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective. Batteries 2018, 4, 62.
- Diddens, D.; E. Paillard, E.; Heuer, A., Improving the Lithium Ion Transport in Polymer Electrolytes by Functionalized Ionic-Liquid Additives: Simulations and Modeling. J. Electrochem. Soc. 2017, 164 (11), E3225-E3231.

Relevant previous project of activities connected to subject of proposal

- **FestBatt** Topics: solid electrolytes and solid state batteries, 2018-2020, German Federal Ministry of Education and Research (BMBF)
- **Elektrolytlabor** (4E) Topics: synthesis of new materials, the High Throughput Screening (HTS) for fast, automated substance evaluation and the analysis for the establishment and realization of the necessary quality standards as well as the investigation of the mechanisms of action; 2013-2017, German Federal Ministry of Education and Research (BMBF)
- **Go3** Topics: High-capacity anode materials (Si/C) and high-capacity cathode materials for lithium ion batteries; pre-lithiation), Federal Ministry for Economic Affairs and Energy (BMWi)
- **BenchBatt** Topics: Evaluation of lithium- and post-lithium-ion technologies (Li//air and Li//sulfur), energy density, cost- and resource analysis), 2016-2018, German Federal Ministry of Education and Research (BMBF)
- **MEET - High End II** Topics: Study of materials based on metallic anode materials. (2016-2019), German Federal Ministry of Education and Research (BMBF)

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Automated high throughput screening (HTS) approach for effective optimization in liquid electrolyte MEET has outstanding state-of-the-art equipment, technology and laboratories. There is an extensive amount of synthesis equipment for anode and cathode active material synthesis, including e.g. Couette-Taylor-Flow reactor (CTFR), muffle furnaces, tube furnaces, carbonization and graphitization furnaces, ball mills and mixer mills, hydrothermal synthesis reactor, etc. This further includes instruments for analysing active and inactive materials as well as electrolyte components (IC, IC/ICP-MS, ICP-OES, IC/ESI-MS, GC-MS), devices for microscopic (SEM-EDX-FIB, AFM, OM) and spectroscopic analyses (XPS, Raman, IR, MS, UV-VIS, liquid and solid-state NMR), and facilities for particle/material and thermal analyses (XRD, PSA, BET, pycnometry, Hg-porosimetry, DSC, TGA, TGA-MS, TGA-IR) With its battery cyclers (Maccor, Digatron), MEET also has about 1,500 channels.

Two large High-Performance Computer (HPC) clusters are directly accessible to WWU/MEET. (1) HPC cluster of the WWU (also on the TOP 500 list after installation in 2018). (2) HPC cluster of the simulation group at the Institute of Physical Chemistry with more than 100 nodes.

4.1.6 COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES (CEA)

	Name: COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES (CEA)	**Partner no:** 6	**Country:** France
	Type: RTO	**Number of employees:** 19 925	**Turnover:** 5.3 B€

Interest in the project

The French Alternative Energies and Atomic Energy Commission (CEA) is very active in research & innovation on electrochemical energy storage and has established over the years a large network of academic and industrial partners in this field. CEA is thus highly interested in participating in the current project, which will enable us to make the best use of research data and establish strong links between numerical simulation, material synthesis and characterization to accelerate the discovery and optimization of battery materials and interfaces.

Previous experience vs. main tasks in the project

CEA will participate to research & innovation activities related to numerical simulation, material characterization and high-throughput material synthesis.

CEA will rely on the skills and expertise of its research teams dedicated to batteries: 200+ staff, 30+ industrial partners, 350+ patents, covering the full value chain (from battery materials to cells, modules, packs, BMS, and recycling, including multi-scale modelling and characterization).

Description of legal entity and main tasks

CEA is a key player in research, development and innovation in four main areas: defense and security, low carbon energy, technological research for industry, and fundamental research in the physical sciences and life sciences. Drawing on its widely acknowledged expertise, CEA actively participates in collaborative projects with a large number of academic and industrial partners.

CEA will be involved in the project through its **Liten** (technological research in the field of renewable energy) and **Irig** (fundamental research) institutes.

CV or description of profile of key staff

- **Dr. Sandrine Lyonnard** (F) received her Ph.D. in Solid State Physics from the University of Orsay (France) in 1997. She was developing neutron techniques for the analysis of atomic hopping mechanisms. In 2000, she was appointed at the Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) in Saclay as a soft matter physicist, responsible of X-rays spectrometers. In 2002 she joined Grenoble's CEA center to develop neutron and X-rays techniques for the characterization of the morphology, structure and dynamics in nanostructured/complex materials used as electrodes/electrolytes for energy conversion and storage. In recent years, her focus is on operando studies of lithium ion batteries at Large Scale Facilities (synchrotron and neutrons). She served as WP leader in H2020 projects (BACCARA, SINTBAT, ECO2LIB) related to the multi-scale operando characterization of Li-ion batteries. She is involved in national/bilateral projects on solid state electrolytes (MoveYourIon ANR, MOLIBE BMBF-ANR). She is/has been serving as expert in neutron panels at LLB (Saclay), ILL (Grenoble), MZL (Munich), ISIS (England); she was member of the SOLEIL users committee and member of the ILL scientific council. She is deputy group leader at the Fundamental Research institute (CEA-Irig) of CEA in Grenoble.
- **Dr. Mathias Gérard** (M) is the head of the fuel cell and battery multi-scale and multi-physics modelling and performance analyses lab at CEA-Liten. He received a MSc degree in 2007 (INSA Lyon) and a PhD degree in 2010 in science engineering (University of Franche-Comté). His main research activities include multi-scale

modelling of fuel cells and batteries with upscaling methodologies to include degradation mechanisms into the system level (bottom-up approach) for energy management and mitigation strategies. Co-inventor of more than 10 patents, author of more than 20 publications and supervisor of 8 PhDs.

- **Dr. Frédéric Le Cras** (M): Master in Electrochemistry and in Engineering, PhD in Physics, Habilitation to supervise research. Senior researcher and expert in lithium(-ion) batteries at CEA-Liten, with a 25-year experience in the development of batteries and battery materials. Author/co-author of 65 peer reviewed papers (h-index 30) and patents dealing with the synthesis, characterization of electrode and solid electrolyte materials, and the design of batteries for specific applications (automotive, microelectronics, healthcare). Supervisor/co-supervisor of > 15 PhD theses. Most recent research focuses on all-solid-state thin-film Li(-ion) microbatteries prepared by sputtering and the characterization of electrodes/solid electrolyte interfaces: Bilateral developments with STMicroelectronics (2007-2017), European projects E-STARS (Efficient Smart sysTems with enhAnced eneRgy Storage, FP7-ICT, 2008-2011), EnSO (Energy for Smart Objects, H2020-ECSEL, 2014-2018), ENABLES (European Infrastructure Powering the Internet of Things, H2020 EU.1.4.1.2., 2018). Currently on secondment at the Institute for Condensed Matter Chemistry (ICMCB), Bordeaux, France.

Relevant publications and/or products and/or services

- Tardif, S.; Pavlenko, E. ; Quazuguel, L. ; Boniface, M. ; Maréchal, M. ; Micha, J-S. ; Gonon, L. ; Mareau, V. ; Gebel, G; Bayle-Guillemaud, P. ; Rieutord, F. ; Lyonnard, S. "Operando Raman Spectroscopy and Synchrotron X-ray Diffraction of Lithiation/Delithiation in Silicon Nanoparticle Anodes". *ACS Nano* (2017) 11 (11), pp 11306–11316.
- Berhault, C. L.; Zapata-Dominguez D. ; Kumar, P. ; Jouneau, P-H. ; Porcher, W. ; Aradilla, D. ; Tardif, S.*; Pouget, S.* ; Lyonnard, S. "Multiscale Multiphase Lithiation and Delithiation Mechanisms in a Composite Electrode Unraveled by Simultaneous Operando Small-Angle and Wide-Angle X-ray Scattering". *ACS Nano* (2019)
- M. Chandesris et al., "Thermodynamics and Related Kinetics of Staging in Intercalation Compounds", *The Journal of Physical Chemistry C* (2019) 123 (38), 23711-23720
- N. Dufour, M. Chandesris et al., "Lithiation heterogeneities of graphite according to C-rate and mass-loading: A model study", *Electrochimica. Acta* 272 (2018) 97-107
- T. Famprikis, J. Galipaud, O. Clemens, B. Pecquenard, F. Le Cras, "Composition dependence of ionic conductivity in LiSiPO(N) amorphous thin-film electrolytes for solid-state batteries", *ACS Appl. Energy Mater.* 2 (2019) 4782-4791

Relevant previous project of activities connected to subject of proposal

- Horizon 2020 project **BATTERY 2030+** (*BATTERY 2030+: At the heart of a connected green society*), **project deputy coordinator**
- Horizon 2020 project **TEESMAT** (*OPEN INNOVATION TEST BED FOR ELECTROCHEMICAL ENERGY STORAGE MATERIALS*), **project coordinator**
- Horizon 2020 project **SPIDER** (*Safe and Prelithiated hIgh energy DEnsity batteries based on sulphur Rocksalt and silicon chemistries*), **project coordinator**
- Horizon 2020 project **SINTBAT** (*Silicon based materials and new processing technologies for improved lithium-ion batteries*), **project partner**
- FP7 project **MAT4BAT** (*Advanced materials for batteries*), **project coordinator**

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

In the project, CEA will use the **BATTERY PLATFORM** (3,000 sq. m of facilities, including 1,000 sq. m of dry rooms), which is a **large research infrastructure** gathering all the tools required to develop, manufacture and test small series of lithium-ion batteries at the pilot scale. R&D at the platform starts with identifying and synthesizing materials to optimize battery performance, and encompasses manufacturing the battery cells, assembling the battery packs, and integrating them into complete systems. Battery safety and performance are assessed via a range of tests, including abuse tests. The platform has around 20 pieces of heavy equipment, including coating and filling machines and a test assembly line. The platform can address lithium-ion batteries of all sizes, from tiny hearing-aid batteries weighing in at just a few grams to 300-kg electric-bus batteries. With a strong commitment to industrial R&D partnerships, the platform collaborates with several leading companies across the value chain.

CEA will also use the **NANO-CHARACTERIZATION PLATFORM**, which houses around 40 pieces of heavy research equipment operated by a staff of experienced researchers and technicians. The platform studies samples for CEA research programs and conducts research on characterization techniques and protocols to prepare appropriate responses to tomorrow's characterization needs. The platform possesses certain equipment that exists at just a handful of other locations worldwide—this is the case for the platform Titan Ultimate transmission electron microscope, which offers resolutions of 50 picometers. Researchers at the platform can characterize material morphological, physico-chemical, and electrical properties, depending on partner needs, providing 2D and, increasingly, 3D images of the materials studied. These tests provide valuable insight into nanomaterials and nanocomponents. The platform also works with large research instruments ESRF and ILL, leveraging their synchrotron and neutron capabilities. The platform is used by scientific equipment manufacturers that wish to improve their products, as well as by other manufacturers from startups to corporations like IBM and STMicroelectronics.

CEA operates (with CNRS) some CRG beamlines at the **ESRF** and **ILL European facilities**, CEA staff being beamline scientists and local contacts on several types of spectrometers and instruments, including X-rays micro-diffraction, X-rays reflectivity, neutron inelastic scattering.

CEA will also use the modelling platform called **MUSES**. MUSES is a multi-scale and multi-physics modeling and simulation platform dedicated to the study of PEMFC, PEMWE and lithium-ion batteries focusing on performances, safety and durability aspects. The different models of the platform, from materials to systems, are developed with a common material and physical database and a multi-scale methodology. The versioning and test cases for no regression of the platform allow model co-developing. In particular, for lithium-ion batteries, **the**

atomistic and meso-scales are focused on the upscaling of *ab-initio* properties to the thermodynamics and kinetics of the electrochemical reactions; **the microscale** is focused on linking performances and durability, including mechanical swelling, at the agglomerate scale based on real or virtual images**; the electrode scales** are dedicated to couple electrochemical with complex transport phenomena in the different phases, with degradation mechanisms, to understand and optimize electrode design; **the cell level** is focused on cell design optimization and understanding with thermal runaway reactions; **the module and pack design** are dedicated to lifetime prediction and optimization based on optimized management, and to thermal runaway propagation.

4.1.7 KEMIJSKI INSTITUT (NIC)

	Name: KEMIJSKI INSTITUT (NIC)	**Partner no: 7**	**Country: Slovenia**
	Type: RTO	**Number of R&D personnel: >250** **Number of employees:~330**	

Interest in the project

NIC has a long tradition in battery research. Our focus is mainly on material design, interface understanding and development of special operando mode characterization techniques.

Previous experience vs. main tasks in the project

WP3 - Multiscale modeling: We have proprietary multi-scale simulation suits covering the entire chain from reaction kinetics and crystal lattice structure level over continuum models to observer models. In the WP3, we propose several innovative approaches for more consistent coupling between the scales that will contribute to a paradigm shift in multi-scale modelling. WP4 – Based on our experience in organic chemistry, we are in charge for the synthesis of optimized molecules and coatings defined from computational chemistry. Molecules will be characterized in WP5 and ontology tests will be performed in WP7. Finally, NIC is a task leader in WP11 for the transferability of developed methodology to other materials due to long-term experience working on multivalent batteries.

Description of legal entity and main tasks

NIC, Ljubljana, Slovenia has over 330 employees working on basic and applied research towards fields that are of long-term importance to both Slovenia and EU. NIC's employees publish more than 200 scientific papers per year and have established ties with the top global engineering research centres and universities. NIC currently runs 18 Horizon 2020 projects. The Institute offers high-level research equipment, allowing researchers to engage in even the most cutting-edge research challenges at the world level. Some acquisitions are: AR STEM –atomic resolution scanning transmission electron microscope (HR TEM, HAADF, EELS, etc.), a high resolution powder x-ray diffractometer, and an 800 MHz NMR spectrometer. The battery group within the Department of Materials Chemistry works mainly on modern battery systems with a focus on post-Li-ion technologies. Equipment available in the group is based on needs for laboratory-scale battery research.

CV or description of profile of key staff

- **Prof. Dr. Robert Dominko (M)**, Ph.D. in chemical technology in 2002 from University of Ljubljana. He is a scientific councillor (research position equivalent to full professor) with his laboratory within the Department of Materials Chemistry at NIC. He is an experienced team leader at the international level with coordination of HELIS (H2020), EUROLIS (FP7) projects, ALISTORE-ERI (deputy director), MNT ERA-NET, collaborative project with CEA, co-shared PhD students. His research topics are new systems and materials for energy storage, where he is specialized in the preparation and optimization of materials and systems, including different in situ characterisations. He has several contracts with domestic and international industrial partners. He is an associate professor at the University of Ljubljana and member of Slovenian engineering academy. He has more than 130 per reviewed scientific publications (H index 49 with approximately 63 citations per publication), 3 chapters and 7 granted patents.
- **Prof. Dr. Miran Gaberscek (M)**, Ph.D. in Chemistry, University of Ljubljana in 1994. He is head of Laboratory for Materials Chemistry at NIC, Director of Centre of Excellence for Low-Carbon Technologies and Professor of materials science at University of Ljubljana. His research is focused on solid ionic conductors, electrochemical

interfaces, batteries, fuel cells, and corrosion systems. He has been involved in various EU research projects (NATO SfP 971837, Lithium batteries, Slovenian co-director; ALISTORE, Advanced lithium energy storage systems based on the use of nano-powders and nano-composite electrodes; "Advanced PEM Fuel Cells" (APOLLON); NANOBIOPHARMACEUTICS, FP6-2004-NMP; APOLLON B, IP project, (PEM fuel cells); EUROLION, High energy density Li-ion cells for traction; EUROLIS (CONOT is project partner). He has about 155 publications (H index=35), 12 patents.

- **Prof. Dr. Tomaž Katrašnik (M)**, Ph.D. (2004), MSc (2001) in mechanical engineering and BSc (1999) in physics, all at University of Ljubljana and 2 Postdoc projects. He is a full professor and head of the Laboratory for Internal Combustion Engines and Electromobility at the University of Ljubljana, Faculty of Mechanical Engineering. His research focuses on conventional, hybrid, electric and fuel cell powertrains, heat and mass transfer, fluid mechanics as well as numerical simulations of powertrains. He is an expert in the development of vehicle-powertrain-related simulation and modelling tools with more than 12 years of continuous international industry-funded engagements in development of professional commercial powertrain modelling tools including libraries for modelling electrified powertrains, batteries and fuel cells. He has also been involved in various internationally funded projects on sustainable mobility, e-mobility and fuel cells: FP7 Civitas Elan, FP7 ASTERICS, H2020 OBELICS, FFG (Austria) MEA Power and SOH4PEM. He is author of 71 per reviewed papers, 2 independent scientific chapters in a monograph and 4 patents. Beside other awards, he received also the 2004 Siegfried Marcus international award of the ÖIAV, Austria (Österreichischer Ingenieur- und Architekten-Verein) for his PhD thesis. Member of EGVIA and EARPA.

Relevant publications and/or products and/or services

- Vižintin, Alen, BITENC, Jan, Kopač Lautar, Anja, Pirnat, Klemen, Grdadolnik, Jože, Stare, Jernej, Randon-Vitanova, Anna, Dominko, Robert. Probing electrochemical reactions in organic cathode materials via in operando infrared spectroscopy, *Nat. Commun.,* (2018), 9, Art. No. 661
- Kopač Lautar, Anja, Kopač, Drejc, Rejec, Tomaž, Bančič, Tanja, Dominko, Robert. Morphology evolution of magnesium facets: DFT and KMC simulations. *PCCP*, 21, 2434-2442
- Dreyer, Wolfgang, Jamnik, Janko, Guhlke, Clemens, Huth, Robert, Moškon, Jože, Gaberšček, Miran. The thermodynamic origin of hysteresis in insertion batteries. *Nature materials,* 2010, 9, 448-453.
- Sirisopanaporn, Chutchamon, Masquelier, Christian, Bruce, Peter G., Armstrong, A. Robert, Dominko, Robert. Dependence of Li2FeSiO4 electrochemistry on structure. *Journal of the American Chemical Society*, 2011, 133, 1263-1265.
- Zelič, Klemen, Katrašnik, Tomaž. Thermodynamically consistent derivation of chemical potential of a battery solid particle from the regular solution theory applied to LiFePO4. *Scientific reports*, ISSN 2045-2322, Feb. 2019, vol. 9, f. 1-13

Relevant previous project of activities connected to subject of proposal

- 2019-2020: H2020 CSA "Battery 2030+: A large-scale initiative on future battery technologies"
- 2015-2019: H2020 "HELIS: High energy lithium sulphur cells and batteries"
- 2012-2016: EU FP7 "EUROLIS: Advanced European lithium sulphur cells for automotive applications"
- 2017-2020: H2020 "OBELICS: Optimization of scalable realtime models and functional testing for e-drive concepts"
- 2016-2019: H2020 FET Open "LiRichFCC: Lithium-rich oxyfluorides with cubic dense packing"

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

- AR STEM –atomic resolution scanning transmission electron microscope (HR TEM, HAADF, EELS etc.);
- FIB-SEM and Cryo TEM microscopes;
- X-Ray Powder Diffractometer PANalytical X'Pert PRO HTK;
- Ex-situ testing of morphology, structure, chemical environment: FE-SEM and HR-TEM investigation combined with local chemical characterization (EELS etc.); AFM measurements (imaging, force measurements);
- High resolution NMR spectrometers (800 and 600 MHz);
- Linux and HPC computer clusters with 4000 cores;
- 120 channels for battery cycling (Bilogical VMP3 equipped with EIS, Maccor, Arbin);
- Climate chambers for battery cycling
- in-situ combined spectroscopical-electrochemical measurements (XRD, Mossbauer, UV-Vis, Raman/FTIR; EXAFS/XANES); ex-situ electrical measurements (conductivity); impedance measurements;
- Ansys and AVL simulation suits including relevant 3D and 1D continuum battery models as well as other open sources and relevant pre- and post-processing;
- Proprietary multi-scale simulation suits (developed during several international and national as well as industrial funded projects) based on sequential linking covering the entire chain from reaction kinetics and crystal lattice structure level over continuum models to observer models.

4.1.8 SINTEF AS (SINTEF)

SINTEF	**Name:** SINTEF AS (SINTEF)	**Partner no:** 8	**Country:** Norway
	Type: RTO	**Number of R&D personnel:** 1 400 **Number of employees:** 2 000	**Turnover:** 323 M€

Interest in the project

SINTEF is a key player in many of the on-going battery research initiatives in Europe. We bring experience in many different post-Li-ion chemistries to the BIG-MAP, including metal-air, multivalent metal-ion, and model-based materials screening and design. We hope to apply some of the recent advances in relevant fields, including ontology, materials modelling, battery cell modelling, and artificial intelligence made in our various research groups.

Previous experience vs. main tasks in the project

WP7: Battery Interface Ontology (WP Leader)

SINTEF is a key player in the European Materials Modelling Council (EMMC) and one of the core authors of the European Materials Modelling Ontology (EMMO). As such, SINTEF is well-positioned to lead the WP on Battery interface ontology development and integrate the results of the project into the existing EMMO framework.

WP2: Accelerated Atomic-Scale Simulations

SINTEF is working to develop FCIQMC (Full-CI Quantum Monte Carlo) simulations, a novel method to give more accurate materials modelling simulations. As the name indicates, it is a method to find a Configuration Interaction wavefunction by optimizing the coefficients of the Slater determinants by stochastic means, giving it much better scaling than traditional CI methods. The method is more expensive than DFT but can deal with multireference systems, which is an objective of WP2.

WP3: Multi-Scale Modelling

Multi-scale modelling of complex systems is a core competence at SITNEF. We have research groups working at all levels of the multi-scale chain, including atomistic and molecular (DFT, MD, FCIQMC), mesoscale (Phase field theory and lattice-Boltzmann method) and continuum (finite volume and finite element). SINTEF also specializes in the use of AI-supported multi-physics modelling, which we recently applied to model and predict highly turbulent airflows. In addition, our researchers are working on new theory development for post-Li-ion batteries and interfaces, a key aim for the BIG-MAP.

Description of legal entity and main tasks

SINTEF is a broadly based, multidisciplinary research foundation that possesses top-level expertise in technology, medicine and the social sciences. SINTEF is an independent, non-commercial organization. The contract research covers all scientific and technical areas that range from fundamental research through applied research to commercialization of results into new products. The profits of our contract research projects are invested in new research, scientific equipment and competence development. SINTEF has a close collaboration with the Norwegian University of Science and Technology (NTNU) in Trondheim and the University of Oslo (UiO). SINTEF Industry has long term specialization and a proven track record in delivering complex research projects in rechargeable zinc-air batteries, Li-ion batteries, post-Li-ion batteries and hydrogen technologies.

CV or description of profile of key staff

- **Dr. Jesper Friis** (M): Ph.D. in Physics, NTNU in 2003. Dr. Friis joined SINTEF in 2007 and is a Senior Research Scientist. He is author of several publications. His main fields of competence include: microstructure modelling of aluminium alloys (precipitation, flow stress, recrystallization, recovery...), first principles modelling (VASP), thermodynamical and diffusion modelling (Thermo-Calc, DICTRA, FactSage), Monte Carlo simulations, charge density and electron distribution, quantitative convergent beam electron diffraction, crystallography and diffraction theory, programming (C, Fortran, Python, Unix shell, etc.). Dr. Friis is also one of the core authors of EMMO and a main contributor to the EMMO-python package for working with EMMO.
- **Dr. Espen Sagvolden** (M): Ph.D. in Physics, Tulane University in 2007. Dr. Sagvolden joined SINTEF in 2010 and is a Research Scientist. His main research focus is the development and application of physics-based theory to discover new functional materials. He is a leader in the development of materials modelling, having pioneered an advanced method to more accurately calculate the electronic behavior of battery materials. His research has also included the application of machine learning with DFT to discover new materials, a key aim of BIG-MAP.
- **Dr. Simon Clark** (M): Dr. rer. nat in Computational Electrochemistry, Ulm University in 2019. Dr. Clark joined SINTEF in 2019 and is a Research Scientist. He is an expert in multi-physics modelling, which he has applied across a wide range of fields in both industry and research. In his recent work, he derived a new framework for modelling advanced aqueous electrolytes in metal-air batteries. He is currently developing both Li-ion and next-generation batteries based on Zn, Mg, and Al. Dr. Clark leads SINTEF's Battery Modelling Platform, a cross-disciplinary initiative to apply model-based methods to discover new battery materials and improve battery design. He is the author of several publications and has recently filed a patent application in the field of model-based electrolyte design.

Relevant publications and/or products and/or services

- Z. Hang, K. Hippalgaonkar, T. Buonassisi, O. M. Løvvik, E. Sagvolden, and D. Ding, “Machine Learning for Novel Thermal-Materials Discovery: Early Successes, Opportunities, and Challenges,” ES Energy Environ., vol. 2, pp. 1–8, 2018.
- S. Clark, A. Latz, and B. Horstmann, “Rational Development of Neutral Aqueous Electrolytes for Zinc-Air Batteries,” ChemSusChem, vol. 10, no. 23, pp. 4735–4747, 2017.
- S. Clark et al., “Towards rechargeable zinc–air batteries with aqueous chloride electrolytes,” J. Mater. Chem. A, vol. 7, pp. 11387–11399, 2019.
- J. P. Perdew, L. A. Constantin, E. Sagvolden, and K. Burke, “Relevance of the Slowly Varying Electron Gas to Atoms, Molecules, and Solids,” Phys. Rev. Lett., vol. 97, no. 22, p. 223002, Nov. 2006.
- X. Chen, F. L. Bleken, O. M. Løvvik, and F. Vullum-Bruer, “Comparing electrochemical performance of transition metal silicate cathodes and chevrel phase Mo6S8 in the analogous rechargeable Mg-ion battery system,” J. Power Sources, vol. 321, pp. 76–86, 2016.

Relevant previous project of activities connected to subject of proposal

- Partner – Battery2030+ CSA, 2019, EU H2020. Battery2030+ is an EU large-scale research initiative on advanced battery technologies.
- Partner – European Materials Modelling Council (EMMC-CSA), 2016-2019, EU H2020. The goal of EMMC-CSA is to establish current and forward looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe.
- Coordinator - Zinc-air secondary innovative nanotech-based batteries for efficient energy storage (ZAS), 2015-2018, EU H2020. Development of new materials for rechargeable zinc-air batteries, a low-cost, safe, and sustainable alternative to Li-ion.
- Partner- Building an attractive European R&I ecosystem on batteries (Batteries Europe ETIP), 2019-2022, EU. Batteries Europe is the forum bringing together all relevant stakeholders in the European batteries research and innovation ecosystem in order to develop and support a competitive battery value chain in Europe.
- Coordinator – Modelling of interfaces for high performance solar cell materials (Hipersol), 2009-2012, EU FP7. HiperSol is an ambitious project with the main objective to build up a multi-scale modelling framework based

on first principles, and to use this framework to describe and understand the interfaces between the metal contact and passivation layer with the silicon substrate in solar cell devices
Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work
SINTEF has access to all relevant modelling software that will be needed for BIG-MAP.

4.1.9 POLITECNICO DI TORINO (PDT)

	Name: POLITECNICO DI TORINO (PDT)	**Partner no:** 9	**Country:** Italy
	Type: UNI	**Number of R&D personnel:** 1 000 **Number of employees:** 900	**Turnover:** 267 M€

Interest in the project

This project represents a unique opportunity for applying multiscale modelling techniques, which have been developed for different applications, including batteries. We expect to rely on a wide range of experts covering different features of this challenging problem. Hence, this project can provide a very promising platform for increasing the impact of what Politecnico di Torino (PDT) has already been doing.

Previous experience vs. main tasks in the project

PDT will be mainly involved in the WP on Multiscale Modelling (WP3), with a leading responsibility of the sub-task 1.1 "Development and validation of mesoscale mode", within the Task 1 "Development of an interphase morphology model (SEI/CEI)". Moreover, PDT will contribute to the Work Package about Multi-fidelity Data (WP9). Finally, PDT will collect in-house experimental data about battery performance and degradation for validating the numerical simulations and investigating specific phenomena. For performing these tasks, PDT can rely on many years of experience on materials modelling and multiscale simulations of transport phenomena, including all-atoms and coarse-grained molecular dynamics simulations, Dissipative Particle Dynamics (DPD), mesoscopic simulations by Lattice Boltzmann Method (LBM), solving population balance equations and computational fluid dynamics (CFD). This experience represents a quite unique modelling asset, which spans from molecular effects to macroscopic implications. Moreover, PDT has solid experience in experimental characterization of batteries, which is ideal for validating the numerical simulations.

Description of legal entity and main tasks

PDT is an Engineering and Architecture University based in Turin: Established in 1859, it is the oldest Technical University in Italy. Two departments will be involved in the project: the Department of Energy and the Department of Applied Science and Technology. Within the Department of Energy, the multi-Scale Modeling Laboratory (SMaLL) will contribute to the project by relying on many years of experience in multiscale modeling and numerical simulations of energy devices. Within the Department of Energy and the Department of Applied Science and Technology, two research groups will contribute: the Multiphase Systems and Chemical Engineering (MuSyChEn) group and the Electrochemistry group. The MuSyChEn group has a strong expertise in multiscale modelling and simulation of transport phenomena. The Electrochemistry group has more than 80 years of experience in the materials synthesis, characterization and testing for electrochemical power sources application.

CV or description of profile of key staff

- **Prof. Eliodoro Chiavazzo** (M): Associate Professor, Director of the multi-Scale Modeling Laboratory (SMaLL), Member of the Faculty Board of the PhD in Energetics, Deputy Coordinator of the Degree Programme in Mechanical Engineering, entered into the organization as a faculty member on late 2014. He has been active in securing research funds for a total amount around 1 million euros during the last 4 years (since 2016), from EU (H2020) and national programs, about materials modelling and energy technologies. Prof. Eliodoro Chiavazzo has published over 70 articles in international journals with peer-review (2007-2020, 13 years of experience), including Nature Sustainability, Science Adv., Nature Comm. and PNAS about energy and environmental sustainability, materials modelling and the use of AI-aided engineering computations.

- **Prof. Daniele Marchisio** (M): Ph.D. in Chemical Engineering from Politecnico di Torino in collaboration with Iowa State University in 2001. Full Professor in Chemical Engineering since 2016 (joined Politecnico di Torino in 2004), member of the MuSyChEn research group, Coordinator of the PhD program in Chemical Engineering (2017-2019), Member of the Academic Senate (2019-2023). He is a principal investigator for Politecnico di Torino of numerous research projects funded by the Italian Ministry of Higher Education and Scientific Research, European Commission, Region of Piedmont and industrial partners (e.g.: BASF, ENI, Solvay, Cargill, Rockwood). Prof. Daniele Marchisio is an expert on multiscale modelling of chemical processes (with particular attention to reacting systems and flows), author of a book for Cambridge University Press and of 148 papers that resulted in 4516 citations and H-index of 35 (source Scopus).
- **Assoc. Prof. Silvia Bodoardo** (F): Ph.D. in Materials Engineering. Associate Professor in Chemistry since 2015 (entered in Politecnico in 1991). She is coordinating the Electrochemistry group. She is Responsible for the group of Chemistry professors and she is in charge of the Battery Task Force in Politecnico di Torino. Silvia Bodoardo participated as principal investigator for PDT in several EU funded projects (coordinator of STABLE project) and also national and regional ones. She is actually participating in Battery2030+ initiative and she is co-chair of WG3 on advanced materials in ETIP BatteRIesEurope and she is also expert in ETIP SNET. Silvia organized many conferences and workshops on materials with electrochemical applications and was Chairwoman at the launch of the Horizon Prize on Innovative Batteries.

Relevant publications and/or products and/or services

- Alberghini, M., Morciano, M., Fasano, M., Bertiglia, F., Fernicola, V., Asinari, P., Chiavazzo, E., Multistage and passive cooling process driven by salinity difference (2020), *Science Adv.*, vol. 6, p. eaax5015;
- Chiavazzo, E., Covino, R., Coifman, R.R., Gear, C.W., Georgiou, A.S., Hummer, G., Kevrekidis, I.G., Intrinsic map dynamics exploration for uncharted effective free-energy landscapes (2017), *PNAS*, vol. 114, p. E5494-E5503;
- Chiavazzo, E., Fasano, M., Asinari, P., Decuzzi, P., Scaling behaviour for the water transport in nanoconfined geometries (2014), *Nature Comm.*, vol. 5, p. 3565;
- Bazzano, M., Marchisio, D., Sangermano, M., Wörner, M., Pisano, R. A molecular dynamics approach to nanostructuring of particles produced via aerosol cationic photopolymerization (2019) *Chemical Engineering Science*, 195, 1021-1027.
- V. Pellegrini, S. Bodoardo, D. Brandell, K. Edström, Challenges and perspectives for new material solutions in batteries, (2019) *Solid State Communications* 113733.

Relevant previous project of activities connected to subject of proposal

- 2016-2019: H2020 LEIT "EMMC-CSA: European Materials Modelling Council"
- 2018-2021: H2020 "OYSTER: Open characterisation and modelling environment to drive innovation in advanced nanoarchitectured and bio-inspired hard/soft interfaces"
- 2019-2023: H2020 "SimDOME: Digital Ontology-based Modelling Environment for Simulation of materials (with focus on cathode materials for Li-ion batteries)"
- 2018-2022: H2020 "VIMMP: Virtual Materials MarketPlace"
- 2019-2020: H2020 CSA "Battery 2030+: A large-scale initiative on future battery technologies"

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

- The HPC initiative of the Politecnico di Torino is a center of Academic Computing, that is, it provides computing resources and technical support for academic and didactic research activities (http://hpc.PDT.it/).
- Center for Multiscale Process Simulation
- Nanoparticle synthesis and characterization laboratory
- Microscopy, Spectrometry & Diffraction: FESEM, XRD, XPS
- Physical-Chemical Analysis: ICP, BET (porosity, surface)
- Synthesis, Manufacturing & Assembly: All facilities for the realization of lithium cells as coin cells and coffee bags, Dry room 10m2 for preparation of electrodes, cells in controlled atmosphere, 1000ppm, MODULAR GLOVE BOX JACOMEX, in stainless steel, 1200x900x725mm, vacuum pump 21m3/h), Savatec S.r.l. / Buchi, B-585, Miller (micromulino a vibrazione MM400, codice RE207450001/Verder Scientific S.r.l.); Film deposition facility (Noselab ATS), Dry room (SOIMAR), UV lamp (UV CURING LAMP HELIOS ITALQUARZ), HotPress DGTS PM 20/2000 DG UGOV 529/2010.
- Electrochemistry: Up to 50 channels for the electrochemical characterization of cells, Coin cell/crimper, Swagelok, El-Cell, pouch cell, ARBIN INSTRUMENTS, 50 channels 5A MODELLO BT2000, ARBIn instrument 16 channel 200A.
- Aging: calendar aging, cycling aging
- Abuse tests: Accelerating Rate Calorimeter (ARC), Nail Test, Crush Test

4.1.10 FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V. (FRAUNHOFER)

Fraunhofer ISC	**Name:** FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V. (FRAUNHOFER)	**Partner no:** 10	**Country:** Germany
	Type: RTO	**Number of R&D personnel:** 18 913 **Number of employees:** 26 648	**Turnover**: 2.6 B€

Interest in the project

Fraunhofer ISC (FRAUNHOFER) is one of a dozen institutes within the Fraunhofer-Gesellschaft dedicatedly focusing on advanced functional materials and one of only a few targeting new materials for battery applications. Preceded first by our expert group for glass development and then for lab automation at our Fraunhofer Translation Center for Regenerative Therapies, our institute develops turnkey robotic systems for material synthesis and testing with now three systems installed on-site.

Besides collaborating in a unique and top-class consortium, our scientific/technological interest in the project follows two general strategies of FRAUNHOFER: 1. Transfer of existing know-how for the material synthesis and screening for battery applications (liquid and polymer syntheses) and 2. Evolution along our internal R&I roadmap from automated systems today to semi-autonomous, AI-controlled synthesis platforms within the project.

Previous experience vs. main tasks in the project

FRAUNHOFER has a solid track record of more than 25 years in R&I projects for electrochemical storage devices and developed unique material- and process-related know-how for the development of state-of-the-art cell components and battery cells. One of the core competencies of the batteries group FZEB at FRAUNHOFER is the development of tailor-made inorganic-organic hybrid polymers and their application within different parts of a battery cell.

Website: www.fzeb.fraunhofer.de

The TLC-RT project group at FRAUNHOFER develops devices such as bioreactors as well as specific incubator systems. In addition, TLC-RT provides the construction of an automated laboratory in which nanoparticles (NPs) for medical applications and test systems can be produced, substance tests carried out and, in the medium term, implants can be produced under the required technical conditions.

TLC-RT established a flexible robot-based platform for the automated production of diagnostic and therapeutic NP systems. Interactive robotics implements synthesis steps in a precise, efficient and quality-controlled manner under GMP-compliant conditions. This allows reproducible manufacturing of NPs with narrowly defined specifications and short development cycles while meeting the requirements of personalized medicine. The results are tailor-made products that are used in individualized diagnostics and therapy.

Website: https://www.regenerative-therapien.fraunhofer.de/en/fields-of-activity/lab-automation-and-bioreactor-technologies.html

Description of legal entity and main tasks

The Fraunhofer Institute for Silicate Research ISC is one out of 72 institutes and research units of the Fraunhofer-Gesellschaft the largest European institution for applied research [2.6 billion euros annual research budget totalling. Of this sum, 2.2 billion euros generated through contract research. 2,500 staff (qualified scientists and engineers)]. In December 2017, the Fraunhofer-Gesellschaft was awarded the "HR Excellence in Research" logo from the European Commission in recognition of its outstanding Integrated Human Resources Management. The award is based on the 40 principles of the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers (EU-Charta & Code). As Europe's leading organization for applied research and as project partner of many EU-projects, Fraunhofer fulfils these principles. Fraunhofer is one of the first organizations for applied research in Germany to receive the logo.

FRAUNHOFER has become one of the leading R&D centres on energy and resource efficiency. With a permanent staff of about 400 scientists and technicians, the Institute works to develop innovative materials for today's and tomorrow's products. As part of the Fraunhofer-Gesellschaft, the Institute is crosslinked with its sister institutes and a number of other R&D institutions in and outside Europe. It is involved in a multitude of joint projects on a national and international scale.

The proposed project will be carried out within two departments at Fh-ISC, the Fraunhofer Translation Center for Regenerative Therapies TLZ-RT with its expert group for Lab automation and the Fraunhofer R&D Center Electromobility FZEB with its expert group for materials for Lithium-ion batteries. One of the core competencies of the batteries group at FRAUNHOFER is the development of tailor-made inorganic-organic hybrid polymers and their application within different parts of a battery cell.

CV or description of profile of key staff

- **Dr. Henning Lorrmann** (M): Ph.D. in Chemistry. Head of Fraunhofer R&D Center Electromobility. Dr. Henning Lorrmann is head of the Fraunhofer R&D Center Electromobility. Henning is working in the field of electrochemical energy storage since more than ten years, with a focus on lithium-ion batteries for over eight years. Henning has over ten years of experience in the application and management of contract research projects on energy storage and was involved in a large amount of collaborative projects on battery development, with several of them as coordinator. With over 35 scientist and technicians, his group is collaborating in various public and industry funded collaborative projects from the basic research to the industrialization. The focuses of his group are the material and process development of state-of-the-art and next-generation lithium-ion batteries and analytical services (aging, post-mortem) for lithium-ion and lead-acid batteries.
- **Thomas Schwarz** (M): Dipl.-Ing. (FH) in Mechanical Engineering (product development). Head of expert group Lab Automation and Bioreactor Technologies at Fraunhofer Translation Centre Regenerative Therapies TLC-RT. Thomas Schwarz has studied mechanical engineering with a focus on product development at the University of Applied Sciences Wuerzburg-Schweinfurt. After his studies, he worked at the Musculoskeletal Center Wuerzburg (MCW) in the project "Development, construction and distribution of modular Bioreactors for biomedical research". In 2010, he moved to the Translational Center for Regenerative Therapies and since then has gained wide experience in incubator and bioreactor design for tissue engineering applications. In addition, a large part of his work is in the field of laboratory automation.
- **Dr. Sofia Dembski** (F): Ph.D. in Chemistry. Head of expert group Biomaterials at Fraunhofer Translation Centre Regenerative Therapies TLC-RT. Dr. Sofia Dembski, senior researcher and head of business unit biomaterials at FRAUNHOFER/TLC-RT, has more than 10 years' experience in biomaterial research, especially as project manager in the field of theranostic nanoparticles and regenerative medicine. One focus of her work is Good Manufacturing Practice (GMP)-compliant automated production of therapeutic and diagnostic (nano)particles. She is responsible for acquisition and coordination of projects (public and industrial) and the professional development of the team (e.g. supervision of bachelor, master and PhD students, technicians and scientists).

- **Dr. Simone Peters** (F): Ph.D. in Chemistry. Researcher at Fraunhofer R&D Center Electromobility. Dr. Simone Peters is a chemist and works at Fraunhofer Institute for Silicate Research since 2015. She is an expert in material syntheses, especially in polymer syntheses and a professional in the design and synthesis of multifunctional precursors systems. Due to her experience in industry prior to her career at Fraunhofer, she has gained experiences in material development and their potential application in chemical industry.

Relevant publications and/or products and/or services

- Schmid, F. F, et al., Applicability of a Dual-Arm Robotic System for Automated Downstream Analysis of Epidermal Models, Applied In Vitro Toxicology. 2016, 2, 2. DOI: 10.1089/aivt.2015.0027
- N. Boaretto, et. al., Highly Conducting 3D-Hybrid Polymer Electrolytes for Lithium Batteries Based on Siloxane Networks and Cross-Linked Organic Polar Interphases. Chem. Mater. 2014, 26, 6339. DOI: 10.1021/cm5024647
- N. Boaretto, et al.; Property-Relaxation Correlations in 3D-Siloxane/Polyether Hybrid Polymer Electrolytes. Electrochim. Acta 2017, 241, 477. DOI: /10.1021/acs.jpcc.6b01631
- Diegler, A., Screening apparatus for glass development - FRAUNHOFER, https://www.isc.fraunhofer.de/content/dam/isc/de/documents/Publikationen/Screening_apparatus_for_glass_development.pdf

Relevant previous project of activities connected to subject of proposal

- 2015 - 2017; H2020, NMP-01-2014, Project no. 645993; Flexible Pilot Scale Manufacturing of Cost-Effective Nanocomposites through Tailored Precision Nanoparticles in Dispersion CO-PILOT: The project aims to develop an open access infrastructure for SMEs interested in the production of high quality (multi-)functional nanocomposites on a pilot scale.
- 2016 - 2018; EIT RawMaterials, KIC Up-scaling projects (D4.2); ECO COM'BAT Ecological Composites for High-Efficient Li-Ion Batteries: Materials development and application of functional coatings for LiB. Upscaling activities
- 2017 - 2019; StMWi, BayFor; 3D-RoboMuk Robotbased production of personalized organoid test systems for the in vitro testing of CFTR mutation-specific cystic fibrosis active substances: Process automation and high-throughput testing
- 2017 - 2020, BMBF, KMU-NetC; APRONA Flexible robotic platform for the automated production of nanoparticles: Implementation of two-arm robot system in the automation process for the automated production of therapeutic nanoparticles.
- 2020-2023; H2020, LC-BAT-1-2019, Project no.875029; ASTRABAT All Solid-state reliable battery for 2025: Materials development and cell design for next-gen solid state batteries.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

- SPS-Controlstadion technology (Siemens SIMATIC) with necessary Software (TIA- Portal) for
- CAD-Software SolidWorks for the construction of complex setups
- Dual-Arm Robot application for automatical manufacturing of nano particles

4.1.11 CHALMERS TEKNISKA HOEGSKOLA AB (CTH)

CHALMERS UNIVERSITY OF TECHNOLOGY	**Name:** CHALMERS TEKNISKA HOEGSKOLA AB (CTH)	**Partner no:** 11	**Country:** Sweden
	Type: UNI	**Number of R&D personnel:** 3 000 **Number of employees:** 5 000	**Turnover:** 380 M€

Interest in the project

We are pursuing both experiments (in-house and at large scale facilities) as well as modelling efforts to rationally understand features underlying the macroscopic performance observed for LIBs and Next Generation Batteries (NGBs). Here we offer our expertise in accurate computational basic property predictions and measurements incl. operando set-ups and will gain from a wider expertise and materials availability including various commercial level electrodes and electrolytes.

Previous experience vs. main tasks in the project

Johansson contributes with experience and capacity of electrolytes – both experimentally (operando spectroscopy) and computationally (SEI formation and reactions, solubility calculations – including method development).
Matic contributes with experience of large-scale facilities, access and development projects and operando experiments.

Description of legal entity and main tasks

CTH performs leading research in the areas of life sciences, materials science, information technology, micro-and nanotechnology, environmental sciences and energy. CTH is continuously involved in approx. 200 projects within different EU programmes and is a coordinator of the EU Graphene Flagship. CTH also hosts the Swedish Electromobility Centre - an academic/industry network which includes the theme Energy storage. The Division of Condensed Matter Physics at the Department of Physics has since >25 years been heavily involved in research on electrolytes for both lithium batteries (liquids, gels, polymers, ionic liquids) and since >7 years also for next-generation batteries. The expertise in ab initio/DFT calculations and (in situ/operando) spectroscopic measurements are successfully applied to speciation in electrolytes, to suggest and explain new materials, to determine transport limiting factors, and to optimize performance, using both model systems and working cells.

CV or description of profile of key staff

- **Prof. Patrik Johansson** (M): Permanent position, Department of Physics, 95% research. Prof. Johansson has a Ph.D. in Chemistry and is Full Professor of Physics. He runs many research projects within the area of materials for energy applications and especially next generation batteries. At CTH since 1999, Prof. Johansson has directed 7 finalized PhDs, mentored 23 postdocs, and currently mentors 3 postdocs and supervises 7 PhD students. He has >25 years of experience of battery research and training, >145 peer-reviewed publications, and has written 5 book-chapters. Total number of citations is >7100 and h-index is 44 (Google Scholar, Oct. 2019). He currently attracts research funding of ca. 1.2 M€/ year, mainly from the EU and major Swedish research agencies. Apart from the recent H2020 projects listed below he has been involved in 4 more FP6/FP7 projects: EUROLIS, Hi-CONDELEC, DECODE, and STORAGE. He was the Chief Investigator of CTH Battery Initiative 2015-2018 and is/has been evaluator/expert for research councils in Sweden, France, Germany, the Netherlands, Slovenia, Poland, Norway, USA, and Israel, and acts as referee for several scientific journals of high repute. He is since January 1st 2018 co-director of ALISTORE-ERI (CNRS FR 3104); Europe's largest industry-academia network within the field of modern batteries. In 2015, he won the BASF Creator Space Energy Storage Contest for his new ideas on Al-battery technology (prize sum 100,000 €).
- **Prof. Aleksandar Matic** (M): Permanent position, Department of Physics, 70% research. Prof. Matic has a Ph.D. in Physics, Full Professor of Physics and head of the Condensed Matter Physics Division. His research interests

cover from fundamental aspects of soft matter to applications of advanced and nanostructured materials in battery technology. He has expertise in characterization of structure and interactions of materials using e.g. operando Raman spectroscopy of next generation batteries, neutron and x-ray scattering of electrolyte and electrode materials. He has so far graduated 7 PhDs and mentored 11 postdcos and has so far published > 125 peer-reviewed publication (>3950 citations, h-index is 37 on Google Scholar, Oct. 2019). He is currently supervising 3 post-docs, 3 PhD-students and 2 MSc-students. He is involved in the development of the ForMax beamline at the MAXIV synchrotron source and also leading the ForMAX-portal for access to advanced experiments for applied research. He is on the board of the neutron source Institut Laue Langevin and leads the panel for High technology laboratories materials science, life science and subatomic physics at the Swedish Research Council.

Relevant publications and/or products and/or services

- Functional Ionic Liquids: Cationic SEI-formers for Lithium Batteries, P. Jankowski, W. Wieczorek and P. Johansson, Energy Storage Materials, 2019, 20, 108-117
- Impact of sulfur-containing SEI-forming additives on lithium-ion battery performance – from DFT predictions to full cell assessments, P. Jankowski, N. Lindahl, J. Weidow, W. Wieczorek and P. Johansson, ACS Applied Energy Materials, 2018, 1, 2582-2591.
- Fluorinated ether based electrolyte for high-energy lithium–sulfur batteries: Li+ solvation role behind reduced polysulfide solubility, S. D. Talian, S. Jeschke, A. Vizintin, K. Pirnat, I. Arčon, G. Aquilanti, P. Johansson and R. Dominko, Chemistry of Materials, 2017, 29, 10037-10044.
- Free-standing 3-D sponged nano-fibre electrodes for ultrahigh-ate energy storage devices, M. Agostini, D-H. Lim, S. Brutti, N. Lindahl, J. H. Ahn, B. Scrosati, and A. Matic, Applied Materials and Interfaces 10, 34140-34146 (2018)
- Rational design of low cost and high energy lithium batteries through tailored fluorine-free electrolyte and nanostructured sulfur/carbon composite, M. Agostini, D-H. Lim, M. Sadd, J-Y. Hwang, S. Brutti, J. Heo, J-H. Ahn, Y-K. Sun, and A. Matic, ChemSusChem 11, 2981-2986 (2018)

Relevant previous project of activities connected to subject of proposal

- EU-H2020 project (H2020-NMP-GV-2014): HELIS - High Energy Lithium Sulphur Cells and Batteries, partner & WP Leader, Grant n° 666221, 2015-2019.
- EU-H2020 project (H2020-LCE-2014-3): NAIADES - Na-ion battery demonstration for electric storage, partner & WP leader, Grant n° 646433, 2015-2018.
- EU-H2020 project (H2020-FETOPEN-1-2016-2017): CARBAT - Calcium rechargeable battery technology, partner & WP leader, Grant n° 766617, 2017-2020.
- EU-FP7 Advanced, High Performance, Polymer Lithium Batteries for Electrochemical Storage (2011-2013)
- EU-FP7 LISSEN – Lithium Sulfur Super Battery Exploiting Nanotechnology (2012-2015)

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

CTH has a wide set-up of light scattering experimental equipment (PCS, FT-IR incl. ATR inside glove-box, FT-Raman, in situ Raman, temperature and climate cells), thermal characterisation set-ups (TGA (with EGA-FTIR add-on), DSC), dielectric spectrometers (Novocontrol), a densitometer coupled with a viscosimeter (Anton Paar),

several different battery testers for both coin cells and Swagelok cells including a climate chambers, and general lab facilities (several Ar glove-boxes, Karl-Fischer titration, potentiostats, spin-coater). We also have access to the vast instrument park of CTH by the joint CMAL. For any large-scale computational chemistry studies, we have grants on Swedish National Supercomputing facilities (>40.000 coreh/month) as well as nodes at the local supercomputer. Access and licenses to commercial softwares as well as implemented home-written codes to several platforms.

4.1.12 POLITECHNIKA WARSZAWSKA (WUT)

	Name: POLITECHNIKA WARSZAWSKA (WUT)	**Partner no: 12**	**Country: Poland**
	Type: UNI	**Number of R&D personnel: 2 651** **Number of employees: 4 970**	**Turnover: 18 M€**

Interest in the project

WUT group is expecting the results of the pillar to accelerate the advance of electrolytes and other components of Li-ion cells. This acceleration would be due to a faster analysis of the results and faster feedback to synthesis development. The automated high-throughput analysis may provide an interesting insight and hopefully will deliver an additional point of view for new possible structures for main electrolyte and/or functional additives. Such quick advance will provide the advantage of the European battery technology, for which WUT hopes to be a provider of the key electrolyte technology.

Previous experience vs. main tasks in the project

Our group is the leading lab in the field of design and development of new electrolytes and their components for lithium-ion and post-lithium-ion batteries with over 160 papers published gaining over 5600 citations with more than 4600 independent citations, 22 patents with 12 international patents. Participation in 4 European Framework Projects. Our Major scientific achievements are: development of the concept of composite polymeric electrolytes; use of organic anion receptors to enhance lithium conductivity in electrolytes; development of concept of nonaqueous proton conducting gel polymeric electrolytes for application in electrochromic devices and supercapacitors; development of novel family of Huckel type salts for application in electrolytes used in lithium and (or) sodium-ion batteries - licensed in 2018 to the French Chemical Company –Arkema; development of new sulfur-based SEI forming additives.

The expertise and know-how within this task are related to the smartly tailored synthesis of electrolyte components, namely conducting salts and functional additives/co-solvents for lithium and post-lithium chemistries. The proprietary conducting salts are based on weakly-coordinating anions that weaken the interactions between anion and cation in the structure, thus resulting in increased ionic conductivity and cation transference number values, lower tendency towards formation of associates and high tolerance to moisture. These conducting salts containing novel, proprietary anions, are in addition functional as SEI modifiers and moisture absorbent/inside desiccants, present in electrolyte as single additive or in a mixture. The synthesis aspects will additionally be related to new sulfur-containing aliphatic aromatic functional additives as well as to the fluorine-free and multivalent anions. The overall approach will comprise small scale synthesis, optimization aspects, preliminary compatibility studies and material up scaling up to 1kg in a batch.

Description of the legal entity and main tasks

Innovations in battery technologies at WUT include both materials and concepts, efficient usage (incl. recycling and 2nd use) and diverse applications and are also focused on designing new materials for post-Li-ion batteries. In 2004 WUT was a founder of the European Network of Excellence Alistore, established in the frame of 6th European Framework Program, which in 2008 transformed into a self-supporting organization known as Alistore European Research Institute. Since the beginning, WUT is a coordinator of electrolyte and interface research carried out in the Alistore. The international cooperation results in the participation in the 4 European research projects within the 6th European Framework Program. On the national level, WUT is a founder and a leader of the POL-STOR-EN scientific consortium comprising 7 leading Polish scientific institutions working in the field of batteries. High international recognition of WUT research groups in the field of solid-state ionics led WUT to organize the most

prestigious and important conference in the field in 2011 – 18th International Conference on Solid State Ionics, SSI-18, with almost 700 participants from all over the world.

- **CV or description of profile of key staff**

- **Prof. Władysław Wieczorek PhD, DSc, Distinguished professor of chemistry** (M): Leader in the field of design and development of new electrolytes and their components for lithium – ion and post lithium –ion batteries in the frame of Alistore ERI and Battery 2030+ initiatives. One of co- funders of the Alistore European Research Institute responsible for task on electrolyte design and formulation. Over 15 years experience as a member of didactic committee of the Erasmus Mundus Program Materials for Energy Conversion and Storage – MESC. He works on design and development of new electrolytes and their components for lithium – ion and post lithium – ion batteries in particular sodium –ion , lithium sulphur as well as fuel cells, supercapacitors and electrochromic devices. Main scientific achievements: development of the concept of composite polymeric electrolytes, use of organic anion receptors to enhance lithium conductivity in electrolytes, development of concept of nonaqueous proton conducting gel polymeric electrolytes for application in electrochromic devices and supercapacitors, and development of novel family of Huckel type salts for application in electrolytes used in lithium and (or) sodium ion batteries - licensed in 2018 to the French chemical company -Arkema

- **Prof. Marek Marcinek** (M): PhD, DSc Professor of Chemistry. Prof. Marcinek is a full professor of technical sciences. He is Polish scientist specializing in energy storage systems (Li-ion, Na-ion ...) and entrepreneurship/ management education. Marek Marcinek is an alumnus of the Faculty of Chemistry at Warsaw University of Technology, Warsaw School of Economics (Marketing and Management) and Law Department of Warsaw University / University of Poitiers (European Law). He worked in USA (Lawrence Berkeley National Laboratory, CUNY), Canada, France and Germany. He is a member of the European Research Institute Alistore and Electrochemical Society. He was one of initiators of PolStorEn University joint initiative. Prof. Marcinek is the author of a total of 51 scientific publications with the total Impact Factor of 152.563. The mentioned theses were cited in total 1209 times (as of November 2017 according to the Web of Science Core Collection database and JCR calculated by the Main Library of the University of Technology) of which 1116 citations (over 92%) are independent quotes. The value of the Hirsch index is 18 (17 without taking into account self-citations). The number of oral domestic and foreign conference contributions: 80. In total, Marek Marcinek is a co-author 7 European and American patents; Know -how: 1; Marcinek was a grant researcher in 10 research grants. He ran a single Polish grant (Homing) and one foreign (FP7 Sirbatt). He was also the leader of the task package in the FP7 EuroLiion project. As part of teaching activity Marek Marcinek have promoted two PhD students. For organizational achievements Prof. Marcinek was honored with the Rector's Award in 2011 and the Bronze Medal of the Centenary of the Warsaw University of Technology for Science-Industry cooperation in 2016. For educational achievements in cooperation with the Industry he received in 2016 the team award of the Rector of the Warsaw University of Technology for educational achievements in the years 2014-2015 along with business leaders of BASF, DOW and Merck, co-organising the classes. For science achievements he was awarded by Spot Recognition Award 2006 and Rector’s Award in 2012 and 2018

- **Leszek Niedzicki** (M): PhD, DSc Associate Professor of Chemistry. Prof. Niedzicki has 13 years of experience in the synthesis and electrochemical investigation of novel anions and electrolytes for lithium-ion, sodium-ion and other types of galvanic cells. He has been participant of 4 EU projects (leader of two and main contractor in one) and 2 Domestic projects, with all but one connected to electrolytes. His patent portfolio includes 7 granted patents (including one with US, EU, JP and CN extensions) on electrolyte-related technologies (anions and additives synthesis and electrochemical applications), and 2 patent applications. 5 patents have been commercialized, including one application on multi-tonnage scale. Prof. Niedzicki, although still a young researcher (35 years old), has published 29 JCR-listed articles on electrolyte materials (over 600 independent citations, H-index 15). For his achievements in the electrolytes' field he has been awarded with Siemens Award (2011), Prime Minister of Poland Award (2012), WUT President award (twice, 2011 and 2018) and Ignacy Moscicki Award for the Best Industrial Application of Research (2019).

Relevant publications and/or products and/or services

- P. Jankowski, M. Dranka, W.Wieczorek, P. Johansson, “TFSI and TDI anions: probes for solvate ionic liquid and disproportionation –based lithium battery electrolytes”, J. Phys. Chem. Lett. 8(2017) 3678-3682
- P. Jankowski, W.Wieczorek, P. Johansson, “SEI forming electrolytes additives for lithium-ion batteries: development and benchmarking of computational approaches” J. Molecular Modeling 23 (2017) 6
- P. Jankowski., N. Lindahl, J. Weidow, W.Wieczorek, P. Johansson, “Impact of Sulfur-Containing Additives on Lithium-Ion Battery Performance: From Computational Predictions to Full-Cell Assessments” ACS Applied Energy Materials, 1 (6), (2018) pp. 2582-2591.
- P. Jankowski, M. Poterała, N. Lindahl., W. Wieczorek, P. Johansson, “Chemically soft solid electrolyte interphase forming additives for lithium-ion batteries” Journal of Materials Chemistry A, 6 (45), (2018) pp. 22609-22618.
- F. Lindgren, C. Xu, L. Niedzicki, M. Marcinek, T. Gustafsson, F. Björefors, K. Edström, R. Younesi, “SEI formation and Interfacial Stability of Si Particles in a LiTDI-salt Based Electrolyte with FEC and VC Additives, ACS Applied Materials & Interfaces, 815758-15766

Relevant previous project of activities connected to subject of proposal

- 2020-2023 ASTRABAT: "All Solid-sTate Reliable BATtery for 2025"- Project no.875029, Horizon 2020, Partner
- 2019 – Faraday Institute - Partner
- 2011-2015 EuroLiion (High energy density Li-ion cells for traction)- FP7 WP Leader
- 2012-2015 Sirbatt – Stable Interfaces for Rechargeable Batteries - FP 7WP Leader
- 2007-2010 Facess- Flexible Autonomuus Cost efficient Energy Source and Storage - FP7 - Partner2004-2008 – ALISTORE NOE –FP6 – WP Leader

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

We have a standard electrochemical, x-ray and spectroscopic equipment necessary to perform studies regarding the synthesis of materials and electrochemical tests. Our specialty is up scaling synthesis facility in which we can perform synthesis of the chosen material up to several kilograms (typically around 1 kg in batch).

4.1.13 AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS (CSIC)

	Name: 4.1.13 AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS	**Partner no:** 13	**Country:** Spain
	Type: RTO	**Number of R&D personnel:** >4 000 **Number of employees:** >10 000	**Turnover:** 737 M€

Interest in the project

Contribute to the integration of fundamental research in the industrial value chain for new battery technologies and contribute to standardization and experimental validation of data/trends.

Previous experience vs. main tasks in the project

Participation in WP11 (Electrode and electrolyte materials): All previous research on batteries is based on fundamental understanding of electrode and electrolyte materials. Our recent emphasis on post Li-ion technologies comes as an added value to the project.
Co-leadership of WP1 (Education, Exploitation and outreach): Participation and coordination of European projects and networks (ALISTORE-ERI, CARBAT FET-Open, etc.). Member of the Governing Board of Batteries Europe ETIP. Secretary of the International Battery Association.
CSIC will also contribute to BIG-MAP through the Siesta computational team belonging to the MaX Centre of Excellence(*). In particular it will contribute to:

- Ab initio benchmarking of multiscale calculations for selected sub-systems (WP3).
- Dynamic fidelity assessment of calculations (WP11)

(*) See description in CNR section

Description of legal entity and main tasks

The Spanish National Research Council (CSIC) is Spain's largest public research institution, ranks third among Europe's research organizations, produces 20% of the Spanish national scientific output and remains the first institution in Spain in the generation of patents. The CSIC is a major player in the development of the European Research Area (ERA) and, therefore, a significant contributor to the European integration process. As of May 2019, the CSIC has obtained 575 projects in H2020, with a total EU financial contribution of 239 million euros and is listed as the 1st organization in Spain and the 4th participant by the number of projects (E-CORDA).

ICMAB-CSIC (www.icmab.es) is a CSIC research institute in Advanced Functional Materials in the fields of energy, electronics and nanomedicine. It has outstanding international competitiveness, with a large number of high impact articles and citations (about 220 scientific articles per year in journals with an average IF > 6) and European research projects participation (9 ERC grants at present), with the strongest international leadership position in the specific domains of Functional molecular, supramolecular and oxide materials. The center has been recently awarded the label of Center of Excellence "Severo Ochoa" by the Spanish Ministry (only 22 research centers in Spain hold this award, ICMAB being the only one related to Materials Science). The Strategic Research Program includes five mission-oriented Research Lines to face three social grand-challenges: clean and secure energy, smart and sustainable electronics and smart nanomedicine. One of the strategic Research Lines specifically focuses on energy storage and conversion, which is the field of application of the current proposal.

CV or description of profile of key staff

- **Dr. M. Rosa Palacín (**F, > 130 publications, h=35): holds a Ph.D. in Chemistry (1995) from UAB (Spain) and is a staff researcher (since 1998) and deputy director (since September 2014) at ICMAB-CSIC. She has >20 years of research experience in the battery field. Her focus is mainly on crystal chemistry, electrode materials and structure-property correlations. Main past achievements concerned electrode materials for nickel and lithium-based batteries. More recently the research has expanded to a much wider scope (technological aspects) with specific emphasis on post-Li battery technologies; sodium-ion and multivalent (calcium, magnesium) chemistries (7 patents and 37 articles published since 2012) with >1500 citations (self-citations excluded). She has a wide international recognition, being scientific director of the ALISTORE-ERI (www.alistore.eu) between 2010 and 2017. She is presently project coordinator of the CARBAT FET-Open (2017-2020, contract #766617) for the development of calcium metal battery demonstrator and was also one of the main scientific actors in the H2020 project NAIADES (2015-2018, contract #646433) for the development of sodium-ion batteries.
- **Dr. Alexandre Ponrouch** (M, > 45 publications, h=23): holds a Ph.D. in Chemistry (2010) from the National Institute of Scientific Research (INRS-EMT, Canada) and is a staff researcher (since 2010) at ICMAB-CSIC. Dr. Ponrouch is a young expert in electrochemistry and was awarded with an ERC Starting Grant (CAMBAT Project) in 2016 to develop new sustainable battery chemistries based on Ca or Mg metal anodes. His research focus on the formulation of new non-corrosive electrolytes via fundamental electrochemistry approaches.
- **Dr. Carlos Frontera** (M, > 190 publications, h=36): holds a Ph.D. in Physics (1997) from UB (Spain) and is a staff researcher (since 2007) at ICMAB-CSIC. Dr. Frontera is an expert in structural characterization, especially using X-ray and neutron scattering techniques and will be in charge of these aspects for the prepared cathode active materials.
- **Dr. Alberto García** (M): Member of the "Laboratory of Electronic Structure of Materials" at the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC). He is a member of the development group of SIESTA and one of his most active contributors. He has a wide experience in the development of ab-initio simulation methods and their applications in physics, materials science, and geophysics and has participated in international initiatives in scientific data management and computational frameworks. He is author of around 80 scientific publications in international peer-reviewed scientific journals (with around 12,800 citations, h-index=32, source: Web of Science, Jan. 2020)

Relevant publications and/or products and/or services

- "Towards a calcium-based rechargeable battery", *Nature Materials* 2016, 15, 169. A. Ponrouch, C. Frontera, F. Bardé, and M. R. Palacín. Impact Factor: 38.8; Citations (Scopus): 188
- "Why do batteries fail?", *Science* 2016, 351, 1253292. M. R. Palacín and A. de Guibert. Impact Factor: 41.1; Citations (Scopus): 173
- "Achievements, Challenges, and Prospects of Calcium Batteries", *Chem. Rev.* 2019, https://doi.org/10.1021/acs.chemrev.9b00339. M. E. Arroyo-de Dompablo, A. Ponrouch, P. Johansson, and M. R. Palacín. Impact Factor: 54.3
- "High capacity hard carbon anodes for sodium ion batteries in additive free electrolyte" *Electrochem. Commun.* 2013, 27, 85. A. Ponrouch, A.R. Goñi, and M. R. Palacín. Impact Factor: 4.4; Citations (Scopus): 304
- "In search of an optimized electrolyte for Na-ion batteries" *Energy & Environmental Science* 2012, 5, 8572. A. Ponrouch, E. Marchante, M. Courty, J.M. Tarascon, and M. R. Palacín. Impact Factor: 33.2; Citations (Scopus): 394.

Relevant previous project of activities connected to subject of proposal

- H2020 Project: (FETOPEN-01-2016-2017, #766617). Acronym: "CARBAT: CAlcium Rechargeable BAttery Technology", October 2017 - September 2020. Coordinator: Rosa Palacín (ICMAB-CSIC, Spain).
- ERC Project (ERC-2016-STG, PE8, #715087). Acronym: "CAMBAT: Calcium and magnesium metal anode based batteries", January 2017 - December 2021. PI: Alexandre Ponrouch (ICMAB-CSIC, Spain).
- H2020 Project: (FETPROACT-01-2018, #824066). Acronym: "E-MAGIC: European Magnesium Interactive Battery Community", January 2019 - December 2022. Coordinator: Alberto Blasquez (CIDETEC, Spain).
- H2020 Project: (LCE-10-2014, #646433). Acronym: "NAIADES: NA-Ion bAttery Demonstration for Electric Storage." January 2015 – December 2018. Coordinator: Loic Simonin (CEA, France).
- Research contract with Toyota Motor Europe on the development of Calcium based batteries (April 2013-March 2017).

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

The Solid-State Chemistry Department at ICMAB-CSIC has all the necessary laboratory equipment to carry out activities on new electrodes and electrolytes development: horizontal and vertical furnaces for O2, Ar, Ar/H2, N2, NH3; gloveboxes for manipulation of air-sensitive materials, equipment for conductivity and viscosity measurements, laboratory battery assembly equipment, potentiostats for electrochemical characterization under different conditions and temperatures, carbon evaporator for thin films or particles. The scientific and technical services at the Institute include the Electron Microscopy Laboratory; Spectroscopic Techniques Laboratory; Thermal Analysis Laboratory and X-ray diffraction Lab; in-situ cell developed in collaboration with ALBA synchrotron. These are further complemented by facilities in the UAB Campus, within walking distance, which are open to ICMAB members.

4.1.14 TECHNISCHE UNIVERSITEIT DELFT (TUD)

	Name: TECHNISCHE UNIVERSITEIT DELFT (TUD)	**Partner no: 14**	**Country: Netherlands**
	Type: UNI	**Number of R&D personnel: 650** **Number of employees:900**	**Turnover:** 370 M€

Interest in the project

TU Delft (TUD) is participating because of its activities and interests in research towards next-generation batteries, and to collaborate on this with European partners. The expected benefits are the involvement in a coordinated European research effort, the use of local expertise by funded resources, network building, progress in resolving the challenges in batteries.

Previous experience vs. main tasks in the project

The group of Prof. Marnix Wagemaker will contribute to the project in the work package WP6 Characterization as a co-lead. Our experience is on battery research investigating fundamental processes using a broad range of (operando)characterization techniques, that are expected to play an important role for the project, acting as vital input for the AI strategies to discover new materials/interface chemistries and solutions. We have developed operando approaches for several of these techniques, and especially our know-how on Operando Neutron Depth Profiling, Neutron and X-ray Diffraction, Operando Neutron Reflectometry, (Operando) Solid State NMR (as well as several XAS techniques), provide unique know-how relevant to the task. We have direct access to the neutron facilities of the reactor institute delft, including Neutron Diffraction, Neutron Reflectometry, Neutron Depth Profiling and Solid State NMR, directly relevant for the project. (and to other potentially relevant techniques in including Small angle Neutron Scattering and Positron Annihilation and XRD techniques).

Description of legal entity and main tasks

Delft University of Technology (TUD) is a multifaceted institution offering education and research in the technical sciences at an internationally recognized level. TUD comprises eight faculties, unique laboratories, research institutes and schools.

The Faculty of Applied Sciences is the largest faculty of TUD, with around 650 scientists, 250 support staff and 1,800 students. The faculty conducts fundamental, application-oriented research and offers scientific education at the bachelor, master and doctoral levels. The faculty is active in the fields of Life and Health Science & Technology, Chemical Engineering, Radiation Science & Technology and Applied Physics.

The department Radiation Science & Technology (RST) is specialized in the application of radiation in material sciences and has direct access to the neutron facilities of the hosting Reactor Institute Delft, enabling rapid and efficient execution of experiments for the project, and operando method development.

CV or description of profile of key staff

- **Prof. Dr. Ir. Marnix Wagemaker** (M) is full professor on the chair Storage of Electrochemical Energy (fundamental processes in batteries). His main field of expertise is next generation batteries, revealing the fundamental bottleneck processes with a range of experimental approaches (based on neutrons, X-rays and solid state NMR) as well as modeling approaches (DFT, Phase Field, Thermodynamics). For his fundamental battery research, which is directly related to the project, he received prestigious Dutch personal grants (Veni/Vidi/Vici) and an ERC-Consolidator grant. He published many results on fundamental processes in batteries of direct relevance for the project, and several patents that are potentially relevant.

Relevant publications and/or products and/or services

- Clarifying the role between redox activity and electrochemical stability for solid state electrolytes, https://arxiv.org/abs/1908.10144, Tammo Schwietert, Violetta Arszelewska, Chao Wang, Chuang Yu, Alexandros Vasileiadis, Niek J.J. de Klerk, Jart Hageman, Thomas Hupfer, Ingo Kerkamm, Yaolin Xu, Eveline van der Maas, Erik M. Kelder, Swapna Ganapathy and Marnix Wagemaker, Nature Materials, Accepted.
- Operando monitoring the lithium spatial distribution of lithium metal anodes, Lv, S., Verhallen, T., Vasileiadis, A., Ooms, F., Xu, Y., Li, Z., Li, Z. & Wagemaker, M., 2018, *Nature Communications.* 9, 1, 2152.
- Accessing the bottleneck in all-solid state batteries, lithium-ion transport over the solid-electrolyte-electrode interface. Yu, C., Ganapathy, S., van Eck, E. R. H., Wang, H., Basak, S., Li, Z. & Wagemaker, M., 1 Dec 2017, *Nature Communications.* 8, 1, 1086.
- Review of Recent Development of In Situ/Operando Characterization Techniques for Lithium Battery Research, Liu, D., Shadike, Z., Lin, R., Li, H., Liu, M., Ganapathy, S., Qin, X., Wagemaker, M., Yang, X. Q. & More Authors, 2019, *Advanced Materials.* 31, 28, 57 p., 1806620
- Lithium-Ion BatteriesSh, arma, N. & Wagemaker, M., 2015, Neutron Applications in Materials for Energy. Kearley, G. J. & Peterson, V. K. (eds.). Zwitserland: Springer, p. 139-203 308 p.

Relevant previous project of activities connected to subject of proposal

Current:

- VICI national personal grant, reference grant number 16122, Spying on Batteries, development and application of operando techniques for next-generation batteries. Role: coordinator.
- Materials for Energy, reference project number 739.017.012, national project grant on solid state battery research, Role coordinator
- HTSM project, reference project number 15788, Development of hybrid solid electrolytes and stable interfaces to Li-metal, Role coordinator.

Past:

- 2013-2017: EU FP7 “HiPerBat: Hunting for high performance energy storage in batteries Fundamental”
- VIDI, national personal talent, reference project number 700.57.421, Storage and dynamics of Li-ions in nanostructure electrode materials, Role: Coordinator

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Operando Neutron Depth Profiling (Li-distribution at interfaces)

Operando Neutron Reflectometry (Structure changes at interfaces)

(Operando) Solid State NMR (Ion transport and chemistry at interfaces)

Neutron Diffraction (Structure Characterization)

4.1.15 CONSIGLIO NAZIONALE DELLE RICERCHE (CNR)

	Name: CONSIGLIO NAZIONALE DELLE RICERCHE (CNR)	Partner no:15	Country: Italy

Consiglio Nazionale delle Ricerche	**Type:** RTO	**Number of R&D personnel: 5 338** **Number of employees: 8 319**	**Turnover: 1,150 M€**

Interest in the project

The CNR team is leading in the development of first-principles methods, codes and applications of high performance (HPC) and high throughput (HTC) computing in materials research. The design of new battery materials involves key challenges where such methods, combined with HPC and HTC on the forthcoming (pre)exascale supercomputers, can demonstrate their impact. We expect strong interactions with computational teams working at multiple (larger) scales, as well as experimental teams in industry and academia, to identify specific subsystems of relevance (input to our calculations) and for validation of results at various levels.

Previous experience vs. main tasks in the project

CNR will contribute electronic structure calculations of interfaces/interphases/defects at the level of Density Functional Theory (DFT), and beyond when needed. In WP3, these will constitute the smallest-scale extreme of multiscale calculations and will be the basis for validation for selected sub-systems. In WP2, CNR will contribute to the prediction of spectroscopies. In WP11 it will contribute to the dynamic fidelity assessment of calculations. In this context, CNR will also develop frontier pre-exascale calculation(s) as a demonstrator of the impact and potential of extreme HPC in battery materials research towards 2030. Furthermore, CNR will contribute to the prediction of spectroscopies (WP2), the development of automated simulation workflows (WP9) and the uncertainty quantification and dynamic fidelity assessment of calculations (WP11).

The CNR team is leading in the development of first-principles methods, codes and applications of high performance computing (HPC) in materials research, with focus on surfaces, interfaces and nanostructured systems and their computational spectroscopies. CNR is especially involved in the development of Quantum Espresso and Yambo code suites, and in their porting to the new heterogeneous supercomputing architectures that will be made available in Europe in the next years. This know-how will be essential to take advantage of the performance of future (pre)exascale HPC architectures, required for battery materials simulations in BIG-MAP and in the Battery2030+ evolution.

The CNR team coordinates MaX – "Materials design at the exascale" (www.max-centre.eu), the European Centre of Excellence for HPC which enables frontier development and automated use of simulation codes based on quantum-mechanical description of electronic properties of complex materials.

Importantly, the MaX European Centre of Excellence as a whole contributes to BIG-MAP. Beside the CNR team, it participates through the CSIC, EPFL and CEA partners, with its flagship codes Quantum Espresso, Yambo, Siesta, and the AiiDA and the Materials Cloud platforms.

Description of legal entity and main tasks

CNR is the main public research institution in Italy, gathering over 100 institutes distributed along the entire country in all fields. CNR Nano is devoted to frontier research in nanoscience and nanotechnology and counts about 200 research staff and associates over its two sites (Pisa and Modena).

CNR Nano Modena has a strong emphasis on computational materials research, with a team of over 15 involved senior scientists. Their activities in first principles simulations range from the prediction of structural, electronic, vibrational properties in the ground state, to the study of excitations and space- and time-resolved spectroscopies. They address a broad range of materials and devices, from organic, inorganic and Carbon-based nanostructures to low-dimensional systems, surfaces, interfaces and defects. CNR Nano Modena leads the MaX European Centre of Excellence for HPC in the materials domain.

CV or description of profile of key staff

- **Prof. Elisa Molinari** (F) is associate researcher at CNR-Nano Modena and full professor of Condensed Matter Physics at the University of Modena and Reggio Emilia (UniMoRe). She is the Director of the MaX European Center of Excellence for HPC in the materials domain. She is a member of the EuroHPC JU Advisory Board (RIAG); of the EU H2020 High Level Group of EU Member States and Associated Countries on Materials, and the NMBP Program Committee. She has pioneered the field of first-principles computational materials science: particularly active in the study of fundamental properties of low-dimensional systems, in the simulation of nano-structures and devices, and in the development of related methods and computational applications. More info on publications: ORCID ID 0000-0002-0692-6096 (h-index 52, 9373 citations, Scopus).
- **Dr. Deborah Prezzi** (F) is researcher at CNR-Nano Modena since 2011. Her activity is mainly devoted to the ab-initio investigation of structural, electronic and optical properties of materials, in collaboration with world-renowned experimental groups. Special emphasis is on simulation of spectroscopies for low-dimensional systems (e.g. CNTs, graphene nanoribbons, TMDs) and hybrid interfaces. She has been local coordinator/PI of National projects devoted to spectroscopy simulations and modeling of light harvesting materials, and co-PI of an Italy-US bilateral action on materials for energy (Mae Italy-US Nanolab: "Nanoscience for energy: a joint Italy-US laboratory", 2013-2015). More info on publications: ORCID ID 0000-0002-7294-7450 (h-index: 20, Scopus).
- **Ivan Marri** (M) is a researcher at the CNR-Nano Modena. The main focus of his research activity is on the ab-initio study of electronic and optical properties of interface, surfaces and nanostructures of metal oxides and of organic molecules on surfaces. He also expert in the study of Auger recombination and Carrier Multiplication processes in both extended and low dimensional systems. He is currently a developer of the Many Body code Yambo. More info on publications: ORCID ID 0000-0002-1192-8790 (h-index:15, Scopus).

Relevant publications and/or products and/or services

- S. M. Falke et al, Coherent ultrafast charge transfer in an organic photovoltaic blend, Science 344, 1001 (2014).
- D. Sangalli et al, Many-body perturbation theory calculations using the yambo code, J. Phys Cond Mat 31, 325902 (2019).
- P. Ruffieux et al, Electronic Structure of Atomically Precise Graphene Nanoribbons , ACS Nano 6, 6930 (2012).
- A. Batra et al, Probing the mechanism for graphene nanoribbon formation on gold surfaces through X-ray spectroscopy, Chemical Science 5, 4419 (2014).
- M. Govoni et al, Carrier Multiplication Between Interacting Nanocrystals for Fostering Silicon-Based Photovoltaics, Nature Photon. 6, 672 (2012).
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Relevant previous project of activities connected to subject of proposal

- MaX - Materials design at the exascale, European Centre of Excellence for HPC (CNR-Nano is the Coordinator. Call: H2020-EINFRA-2015-1, H2020-INFRAEDI-2018-1; Grant agreement ID: 676598, 824143; Dates: 2015-2018, 2018-2021). It involves the 5 main European HPC Centres, the main developers of key codes for first principles materials HTC and HPC simulations (Quantum Espresso, Siesta, Yambo, BigDFT, Fleur, Cp2k, and Aiida) –based at SISSA, ICN2, CNR, CSIC, CEA, ETH, and EPFL—, as well as several technology and training/dissemination partners.
- INTERSECT - Interoperable Material-to-Device simulation box for disruptive electronics (CNR-Nano is the Coordinator. Call: H2020-NMBP-TO-IND-2018; Grant agreement ID: 814487; Dates: 2019-2022). It develops interoperability among materials modeling codes to advance multiscale simulations and accelerate the process of materials selection and device design and deployment. Software and teams of relevance for BIG-MAP are included (Quantum Espresso, Siesta, Aiida).
- Si-DRIVE. Silicon Alloying Anodes for High Energy Density Batteries comprising Lithium Rich Cathodes and Safe Ionic Liquid based Electrolytes for Enhanced High VoltagE Performance (Call: H2020-NMBP-ST-IND-2018; Grant agreement ID: 814464; Dates: 2019-2023, CNR-ISC Partner).
- NFFA Europe. A platform for comprehensive multidisciplinary research projects at the nanoscale from synthesis to nanocharacterization to theory and numerical simulation https://www.nffa.eu. (H2020 Grant agreement ID: 654360, Dates: 2018-2020, CNR-Iom Coordinator)
- Graphene Flagship - Graphene-based disruptive technologies http://graphene-flagship.eu (CNR-Nano Partner)

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

CNR contributes to the development and evolution of the Quantum Espresso and Yambo codes, of relevance to many BIG-MAP applications. The planned calculations require High Power Computing (HPC) resources.. Smaller scale preparatory studies will be performed on local computational facilities which include a local medium-size HPC cluster [> 24-node Linux cluster (Intel Xenon, 12/16 cores, 48/64 Gb shared memory] and in-campus hardware and technical assistance.

4.1.16 ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

EPFL	**Name:** ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)	**Partner no:** 16	**Country:** Switzerland
	Type: UNI	**Number of R&D personnel:** 4 025 **Number of employees:** 6 060	**Turnover:** 965 M€

Interest in the project

Nicola Marzari directs the Swiss National Centre for Computational Design and Discovery of Novel Materials, a 12-year effort (2014-26), http://nccr-marvel.ch, with around 25 groups participating, and a budget of ~5M$/year.

Previous experience vs. main tasks in the project

The group has unique capabilities in discovering and characterizing novel materials with quantum-mechanical simulations (see e.g. http://materialscloud.org), and developing complex workflows for interoperable software using the AiiDA (http://aiida.net) materials' informatics infrastructure.

Description of legal entity and main tasks

The Ecole Polytechnique Federale de Lausanne (EPFL) is one of two federal technical universities in Switzerland. It has three missions: education, research and technology transfer at the highest international level. EPFL, in its location on the shores of Lake Geneva, brings together a campus of more than 10,000 people with more than 250 laboratories and research groups. With 120 nationalities represented on campus and more than 50% of the professors coming from abroad, the School is one of the world's most cosmopolitan universities. The EPFL School of Engineering (STI) consists of more than 50 laboratories organised within 5 institutes at the intersection of mechanics, electrical engineering, micro-technology, and materials science. EPFL is member and hosting institution of CECAM.

CV or description of profile of key staff

- **Prof. Nicola Marzari** (M): PhD, University of Cambridge (1997). Full Professor (2011-onwards), Director (2014-onwards) of the National Centre for Competence in Research MARVEL on computational design and discovery of novel materials (http://nccr-marvel.ch)
- **Dr. Giovanni Pizzi** (M): senior (permanent) researcher in the EPFL group led by Prof. Marzari. He is the lead developer of the AiiDA code and architect of the Materials Cloud.

Relevant publications and/or products and/or services

- N. Bonnet and N. Marzari, First-principles prediction of the equilibrium shape of nanoparticles under realistic electrochemical conditions, Physical Review Letters 110, 086104 (2013), Editors' Suggestion.
- A. Cepellotti and N. Marzari, Thermal transport in crystals as a kinetic theory of relaxons, Phys. Rev. X 6, 041013 (2016) (featured in Physics: http://physics.aps.org/articles/v9/118).
- N. L. Nguyen, N. Colonna, A. Ferretti, and N. Marzari, Koopmans-compliant spectral functionals for extended systems, Phys. Rev. X 8, 021051 (2018).
- N. Mounet at al., Novel two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds, Nature Nanotechnology 13, 246 (2018). News and Views, and Journal Cover.

- L. Kahle, A. Marcolongo, and N. Marzari, Modeling lithium-ion solid-state electrolytes with a pinball model, Physical Review Materials 2, 065405 (2018), Editors' Suggestion.

Relevant previous project of activities connected to subject of proposal

Coordinator, http://nccr-marvel.ch

Partner, http://max-centre.eu

Partner, http://nffa.eu

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

http://quantum-espresso.org

http://aiida.net

http://materialscloud.org

4.1.17 THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE (UCAM)

	Name: THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE (UCAM)	**Partner no:17**	**Country: UK**
	Type: UNI	**Number of R&D personnel: 8 000** **Number of employees: 11 000**	**Turnover: 2 Bn**

Interest in the project

Cambridge University (UCAM) is a research and teaching institution. With respect to this proposal, we have expertise in atomic scale simulation and machine learning (Csanyi) and battery technologies (Grey). Grey has a particular interest in connecting experimental measurements with theoretical predictions and developing theoretical methods to aid this. We hope to contribute to the science objectives in BIG-MAP.

Previous experience vs. main tasks in the project

The group of Csanyi, together with a handful of others, were the first to apply machine learning to develop interatomic potentials, and he has lead this field in the past 10 years. Recent success include a potential for carbon that is able to realistically describe processes involving amorphous carbon (formation by quenching, CVD, film growth, Li+ diffusion) and this is transformative in terms of what is possible to simulation computationally on the atomic scale. Similar breakthroughs followed for amorphous and crystalline silicon. Csanyi is co-leading the WP on “Accelerated atomic-scale Simulations”, WP2 in which potentials will be constructed for describing electrodes and electrolytes.

Grey is contributing significantly to “Characterisation”, WP5, and also WP3 and WP6. She is aiding in materials choice, assisting with characterization and critically working on methods for experimentally validating predictions that arise from theory.

Description of legal entity and main tasks

UCAM has a reputation as one of the top Research Institutes in the world, and is routinely ranked in the top 5 in international academic rankings such as ARWU and Shanghai Ranking, and has a longstanding history of educational and scientific excellence. Over 90 affiliates of University of Cambridge have won Nobel Prizes for their significant advances. Cambridge is also a major participant in European projects and is one of the top recipients of FP7 funding. The departments contributing are Chemistry (Grey) and Engineering (Csanyi). The Department of Chemistry is consistently ranked amongst the top departments worldwide. The department included 50+ internationally recognized, diverse research teams in a wide range of chemistry-related fields. The scientists in the Department work in many leading areas and have collaborators at academic and industrial institutions across the world. Each year the Department hosts around 200 postdoctoral research staff, over 250 postgraduate students, and around 60 academic staff.

CV or description of profile of key staff

- **Prof. Clare Grey** (F): Clare P. Grey, FRS is the Geoffrey Moorhouse-Gibson Professor of Chemistry at UCAM (from 2009) and a Fellow of Pembroke College Cambridge. She holds a Royal Society Professorship (from 2018). She was the director of the Northeastern Chemical Energy Storage Center, a Department of Energy, Energy Frontier Research Center (2009-2010) and Associate director (2011-2014). She is currently the director of the EPSRC Centre for Advanced Materials for Integrated Energy Systems (CAM-IES) and a member of the Expert Panel of the Faraday Institution. Recent honours and awards include Honorary PhD Degrees from the Universities of Orleans (2012) and Lancaster (2013), the Research Award from the International Battery Association (2013), the Royal Society Davy Award (2014), the Solid State Ionics Galvani-Nernst-Wagner Mid-Career Award (2017), and the RSC John Goodenough Award (2019). She has published more than 425 peer-reviewed papers. Her H-index (WOS) is currently 79, (89, Google Scholar) and she is included in the list of most highly cited scientists (e.g., https://recognition.webofsciencegroup.com/awards/highly-cited/2019). She has been awarded a second EU ERC Advanced grants.
- **Prof. Gabor Csanyi** (M): Professor of Molecular Modelling, Department of Engineering. He is an expert in atomistic simulation, particularly in multi scale modelling that couples quantum mechanics to larger length scales. He is currently engaged in applying machine learning techniques to materials modelling problems e.g. deriving force fields (interatomic potentials) from ab initio data. He is also interested in statistical problems in molecular dynamics, e.g. in enhanced sampling algorithms that can be used to automate the calculation of phase diagrams from atomistic models.

Relevant publications and/or products and/or services

- "Electrodes with high power and high capacity for rechargeable lithium batteries", K Kang, YS Meng, J Bréger, CP Grey, G Ceder, Science 311 (5763), 977-980
- "Fluoroethylene carbonate and vinylene carbonate reduction: Understanding lithium-ion battery electrolyte additives and solid electrolyte interphase formation", AL Michan, BS Parimalam, M Leskes, RN Kerber, T Yoon, CP Grey, et al. Chemistry of Materials 28 (22), 8149-8159
- "Towards an atomistic understanding of disordered carbon electrode materials, VL Deringer", C Merlet, Y Hu, TH Lee, JA Kattirtzi, O Pecher, G Csányi, SR Elliott, CP Grey, Chem. Comm., 54, 5988-5991
- "Machine learning unifies the modeling of materials and molecules", AP Bartók, S De, C Poelking, N Bernstein, JR Kermode, G Csányi, et al. Science advances 3 (12), e1701816
- US Patent US8843509B2, "Method and system for estimating properties of atoms and molecules", Method and system for estimating properties of atoms and molecules

Relevant previous project of activities connected to subject of proposal

Grey leads the "Extending Battery Life" a 12M research programme of the Faraday Institution

Csanyi is a member of the UKCP consortium, major users of the UK's national High Performance Computing facility.

4.1.18 THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD (OXFORD)

UNIVERSITY OF OXFORD	**Name:** THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD (OXFORD)	**Partner no:** 18	**Country:** United Kingdom
	Type: UNI	**Number of R&D personnel:** 6 700 **Number of employees:** 14 000	**Turnover:** 2.5 B€

Interest in the project

This project will bring together world-leading researchers from across Europe and will result in a platform that will accelerate development of new battery techniques, at a rate not possible by individual groups or nations. Combining our work on materials and characterization with modeling, simulation and AI from our partners will result in greater understanding of processes and identification of new chemistries. The large datasets involved in this project will enable us to identify trends in a way not currently possible.

Previous experience vs. main tasks in the project

The Department of Materials at the University of Oxford has the experience and know-how to contribute to several of the work packages:

WP5: Electrode & Electrolyte materials

WP8: Characterization

WP11: HTS and Testing

We have published extensively on Li and Na-ion materials. The group's expertise is in synthesizing new materials and detailed characterization, using a range of techniques, to understand how a material's properties affect its performance. We have world-leading facilities and researchers in materials synthesis and discovery, including electrochemical screening. We have developed techniques to study as-prepared materials and changes during cycling. We also lead a national project on solid-state batteries, with a particular focus on the interfaces between the anode/cathode and the electrolyte. We use in-operando and ex-situ measurements in the lab and at large-scale facilities (e.g. XRD, NPD, NMR, XPS, SEM/TEM, XAS, RIXS and tomography). For example, we have used neutron and synchrotron techniques, such as diffraction and PDF to study changes in structure and XAS/RIXS to probe changes in oxidation states. In addition to the techniques listed above, we use a range of electrochemical techniques to understand the changes taking place in materials and at interfaces, e.g. three electrode cells, EIS, cycling and CV.

Description of legal entity and main tasks

The Department of Materials is part of the University of Oxford (OXFORD). The University has an outstanding reputation and is world-leading in both teaching and research – ranked first in the Times Higher Education world rankings for the last four years. The work on Li-ion batteries for which Goodenough was recently awarded the Nobel Prize in Chemistry was carried out at the University.

The Department of Materials is research intensive and offers undergraduate and PhD degrees in Materials Science. World-leading research is carried out in the Department in the areas of energy storage, structural and nuclear materials, nanomaterials, manufacturing, characterization and computational modelling. The Department has close links to other departments in Oxford and international collaborators. Energy storage research in the Department is rapidly growing and this has been made possible by a significant investment by the University.

CV or description of profile of key staff

- **Prof. Peter G. Bruce** (M):

Education: BSc, PhD Chemistry, University of Aberdeen, UK

Current Position: Isaac Wolfson Professor of Materials, University of Oxford, UK (2014 – present)

Lead a research group of 30 people (PhD students and postdocs) working on electrochemical energy storage projects, including Li and Na ion, solid-state and Li-air batteries. Principal Investigator of a consortium (SOLBAT – six UK universities) tackling the fundamental challenges in solid-state batteries. PI or Co-I on a number of other large UK grants.

Co-founder and Chief Scientist of the Faraday Institution (UK national institute for electrochemical energy storage research) (2017 – present)

Vice President and Physical Secretary of the Royal Society (2018 – 2023)

Core Area Champion (Energy Storage), Sir Henry Royce Institute (UK national institute for advanced materials research and innovation.

Previous experience / background (like projects) related to the activities of the project:

Over 40 years of research on materials for electrochemical energy storage

PI of over 30 energy storage projects funded by research bodies, both UK and EU

15 industry funded projects

Professor of Chemistry at the University of St Andrews, UK

Over 350 publications and 500 invited talks in the field of energy storage.

Fellow of the Royal Society (Scientific academy of the UK)

Fellow of the Royal Society of Chemistry

Fellow of the Royal Society of Edinburgh

Web of Science Highly Cited researcher 2015-18

Relevant publications and/or products and/or services

- Nature of the "Z"-phase in layered Na-ion battery cathodes. J. W. Somerville, A. Sobkowiak, N. Tapia-Ruiz, J. Billaud, J. G. Lozano, R. A. House, L. C. Gallington, T. Ericsson, L. Häggström, M. R. Roberts, U. Maitra & P. G. Bruce. Energy & Environmental Science, 12, 2223-2232 (2019).
- Critical stripping current leads to dendrite formation on plating in lithium anode solid electrolyte cells. J. Kasemchainan, S. Zekoll, D. Spencer Jolly, Z. Ning, G. O. Hartley, J. Marrow & P. G. Bruce. Nature Materials, 18, 1105-1111 (2019).
- What Triggers Oxygen Loss in Oxygen Redox Cathode Materials? R. A. House, U. Maitra, L. Jin, J. G. Lozano, J. W. Somerville, N. H. Rees, A. J. Naylor, L. C. Duda, F. Massel, A. V. Chadwick, S. Ramos, D. M. Pickup, D. E. McNally, X. Lu, T. Schmitt, M. R. Roberts & P. G. Bruce. Chemistry of Materials, 31, 3293-3300 (2019).
- 7Li NMR Chemical Shift Imaging To Detect Microstructural Growth of Lithium in All-Solid-State Batteries. L. E. Marbella, S. Zekoll, J. Kasemchainan, S. P. Emge, P. G. Bruce & C. P. Grey. Chemistry of Materials, 31, 2762-2769 (2019).
- Enhanced Li-O2 Battery Performance in a Binary "Liquid Teflon" and Dual Redox Mediators. M. Balaish, X. Gao, P. G. Bruce & Y. Ein-Eli. Advanced Materials Technologies, 4, 1800645 (2019).

Relevant previous project of activities connected to subject of proposal

Recent projects:

SOLBAT, Faraday Institution, UK – Addressing the challenges in all solid-state batteries, Coordinator

CATMAT, Faraday Institution, UK – Next generation cathode materials, Partner

LiBatt, EPSRC, UK – Next generation lithium batteries, Coordinator

SUPERGEN, EPSRC, UK – Addressing challenges blocking commercialization of energy storage, Coordinator

PALIS, EPSRC, UK – Protected anodes for Li-S batteries, Partner

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

The Department has well-equipped laboratories for battery research. This includes general purpose lab space, instrumentation (e.g. XPS, XRD, NMR, ICP, BET, DEMS, TGA, DSC, SEM/TEM and tomography), a suite of gloveboxes (>20), electrochemical test facilities and furnaces.

4.1.19 TARTU ULIKOOL (UT)

	Name: TARTU ULIKOOL (UT)	**Partner no:**	**Country: Estonia**
	Type: UNI	**Number of R&D personnel: 1517** **Number of employees: 3602**	**Turnover: 166 M€**

Interest in the project

IMS Lab is interdisciplinary research unit in University of Tartu since 2003. Our expertise in area of batteries are mostly theoretical, based on computational materials science, however our group has extensive expertise on robotics and automation. We like to combine our previous knowhow in area of batteries with our knowhow in area of automation and robotics

Previous experience vs. main tasks in the project

The IMS lab has been working in basic research and modelling of polymer battery interfaces more than 20 years. We have been involved in industrial robotics projects since 2016. We have in-house competence of robotics and manufacturing technology and have dedicated sub-team of manufacturing engineering and human collaborative robotics. Currently, we are member of EIT Manufacturing consortium.

Description of legal entity and main tasks

UT is Estonia's leading centre of research and training. It preserves the culture of the Estonian people and spearheads the country's reputation in research and provision of higher education. UT belongs to the top 1.2% of world's best universities.

As Estonia's national university, UT stresses the importance of international co-operation and partnerships with reputable research universities all over the world. The robust research potential of the university is evidenced by the fact that the University of Tartu has been invited to join the Coimbra Group, a prestigious club of renowned research universities.

University of Tartu Institute of Technology (TUIT) is a science and development institution established in 2001 and is part of the Faculty of Science and Technology. Our goal is to lay the foundation for novel technological solutions and therefore be the leader of innovation.

Institute of Technology is a multidisciplinary research institution that gives broad-based education. It gives a strong advantage in Estonian and also in the world job market. Institute unites computer engineering, robotics, electronics, material science, biosciences and environmental technologies, therefore our students have a broad opportunity to work with scientists who are creating novel solutions in all fields. Practical courses give students the opportunity to gain necessary skills in order to work in industry during and after the studies.

CV or description of profile of key staff

- **Prof. Alvo Aabloo** (M)
  - PhD, in Solid State Physics, University of Tartu
  - Professor of polymer materials technology since 2007, University of Tartu, Head of the IMS Lab (www.ims.ut.ee), ORCID 0000-0002-0183-1282
  - Has been active in ion conductive polymer material membranes for ion-polymer battery since 2015.
  - Coordinator of MSCA-ITN project MICACT, coordinator of H2020 project TWINNIMS. WP leader in 5+ FP7/H2020 projects.
  - H-index 29. More than 200 publications, 2500+ citations
- **Dr. Vahur Zadin** (M)
  - PhD in Computer Engineering, University of Tartu
  - Senior Scientist, University of Tartu, ORCID 0000-0003-0590-2583
  - Working on polymer battery electrode materials since 2012, materials in hazardous environment and high local electromagnetic fields
  - Coordinator of MATTER EraChair H2020 prject
  - H-index 7, 27 publications.
- **Tauri Tätte** (M)
  - Chief Engineer
  - Has been responsible more than engineering and automation prjects, including FP 7 project SHEE automation workpackage.

Relevant publications and/or products and/or services

- Vigonski, S., Jansson, V., Vlassov, S., Polyakov, B., Baibuz, E., Oras, S., Aabloo, A., Djurabekova, F., Zadin, V. (2018) Au nanowire junction breakup through surface atom diffusion, Nanotechnology.
- Priimägi, P., Kasemägi, H., Aabloo, A., Brandell, D., Zadin, V. (2017) Thermal Simulations of Polymer Electrolyte 3D Li-Microbatteries, Electrochimica Acta.
- Nelson, J.V., Osborne, B., Imhof, A.B., Weiss, P., Taillebot, V., Aabloo, A., Doule, O., Gancet, J., Ransom, S., Saleny, V. (2016) Results of the Self Deployable Habitat for Extreme Environments (SHEE) project, Proceedings of the International Astronautical Congress, IAC.
- Imhof, B., Hoheneder, W., Ransom, S., Waclavicek, R., Weiss, P., Taillebot, V., Gobert, T., Osborne, B., Nelson, J., Gancet, J., Rodriguez, G., Salini, J., Aabloo, A., Kull, P., Ševčík, D., Gajdoš, P., Vajdák, M., Doule, O. (2015) Building the test-bed SHEE – a self-deployable habitat for extreme environments lessons learnt and exploitation opportunities for the scientific community, AIAA SPACE 2015 Conference and Exposition.
- Punning, A., Kim, K.J., Palmre, V., Vidal, F., Plesse, C., Festin, N., Maziz, A., Asaka, K., Sugino, T., Alici, G., Spinks, G., Wallace, G., Must, I., Põldsalu, I., Vunder, V., Temmer, R., Kruusamäe, K., Torop, J., Kaasik, F., Rinne, P., Johanson, U., Peikolainen, A.-L., Tamm, T., Aabloo, A. (2014) Ionic electroactive polymer artificial muscles in space applications, Scientific Reports. http://doi.org/10.1038/srep06913

Relevant previous project of activities connected to subject of proposal

- 2015-2018: H2020 Marie Sklodowska Curie ITN project MICACT- Microactuators (coordinator)
- 2019-2022: H2020 Twinning project TWINNIMS (coordinator)
- 2011-2014: FP7 RADINTERFACES - Multiscale Modelling and Materials by Design of interface-controlled Radiation Damage in Crystalline Materials
- 2013-2015: FP7 project SHEE - Self-deployable Habitat for Extreme Environments
- 2019-2022: CHIST-ERA project Robot In-hand Dexterous manipulation by extracting data from human manipulation of objects to improve robotic autonomy and dexterity

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

University has state of the art analytical tools, for battery characterization, mechanical and electronical workshop, also several robotics labs.

4.1.20 THE UNIVERSITY OF LIVERPOOL (ULIV)

UNIVERSITY OF LIVERPOOL	**Name:** THE UNIVERSITY OF LIVERPOOL (ULIV)	**Partner no: 20**	**Country: UK**
	Type: UNI	**Number of R&D personnel:** **Number of employees:**	**Turnover: 680 M€**

Interest in the project

The group at the University of Liverpool (ULIV) has been working on materials discovery, robotic synthesis and Li based battery interfaces (FP7 SIRBATT, 608502, https://www.liverpool.ac.uk/sirbatt) and electrode degradation for several years and has published a wide range and number of papers on these subject areas. The Materials Innovation Factory (MIF) at Liverpool is a state-of-the-art centre for materials science and robotics offering important underpinning instrumentation to support the activities within this project

Previous experience vs. main tasks in the project

The group at ULIV combines expertise in battery science, electrochemistry, materials synthesis and discovery, robotics, machine learning that are critical to its role within the project in WP4 and WP10.

Description of legal entity and main tasks

University of Liverpool (ULIV) was founded in 1881. Chemistry Department is the ideal host for this leading research as evidenced by its very high ranking in REF 2014 (first for outputs and third for impact) and the award of a Regius Chair of Chemistry in November 2016 "in recognition of outstanding research and teaching". The recent Liverpool City Region and Science and Innovation Audit, commissioned by the Department for Business, Energy and Industrial Strategy, has also substantiated its reputation for world class science and innovation in materials chemistry and related areas. In 2013 the Stephenson Institute for Renewable Energy was opened within the Departments of Chemistry and Physics, as a £10m interdisciplinary research institute playing a leading role in renewable energy research (https://www.liverpool.ac.uk/renewable-energy/).

Recent investments include the £82 M Materials Innovation Factory (MIF), opened in late 2017 (https://www.liverpool.ac.uk/materials-innovation-factory/). The MIF is a state-of-the-art centre for materials science offering important underpinning instrumentation to support a very wide range of scientific research. This facility greatly enhances the Department's characterisation tools and academic engagement with industry, ensuring research results can be made widely available to industrial partners and providing an ideal opportunity to exploit the discoveries and develop impact.

The research group within ULIV brings a combination of expertise in robotics, materials discovery, electrochemistry, spectroscopy and battery chemistry, and understanding of battery management. Liverpool is well equipped for research into electrode interfaces with high integrity argon filled gloveboxes for handling air-sensitive materials, a range of electrochemical equipment (Biologic and Maccor cycling and AC impedance equipment,) and a variety of spectroscopic and analytical tools including state-of-the-art Raman, infrared and atomic force microscopy, X-ray photoelectron spectroscopy.

Main task within the projects:
WP4 - Modular Lab Automation Infrastructure
WP10 – AI Accelerated Materials Discovery (on active learning and software platform for controlling robotics)

CV or description of profile of key staff

- **Prof. Laurence Hardwick** (M) is Professor of Electrochemistry and Director of the Stephenson Institute for Renewable Energy (SIRE). He has been actively researching in the battery field for 16+ years with an international profile in alternative battery chemistries to Li-ion and has pioneered the use of operando spectroscopic techniques to monitor battery electrode electrochemistry including shell-isolated nanoparticles for enhanced Raman spectroscopy (SHINERS) and surface enhanced infrared absorption (SEIRAS) and Raman (SERS) spectroscopies. He has published major contributions in the field of metal-air in understanding the role of interface and electrolyte on the metal oxide discharge product as well as contributing to leading review articles and book chapters. He has 65 publications (h-index = 32, >11000 citations) and presented over 50 invited talks. Since 2012 he has been PI or Co Investigator (CoI) on 11 EPSRC and Innovate UK grants > £4m, which have been mostly related to beyond Li-ion batteries. He has previous experience of managing large multisite grants through coordination of €4.5m EU FP7 project SIRBATT (Stable Interfaces for Rechargeable Lithium-ion Batteries, www.liverpool.ac.uk/sirbatt). LJH is CoI on four Faraday Instituion Projects: Chararaterisation, Degradation, Li-ion Cathodes and Solid State Batteries. He is an Editor of the International Society of Electrochemistry journal Electrochim. Acta.
- **Prof. Andy Cooper** (M) FRS – AIC (ULIV) is the Director of the £82 M MIF in Liverpool, the Leverhulme Research Centre for Functional Materials Design and Champion for the Chemical Materials Discovery theme in the Sir Henry Royce Institute. He is the inventor of three influential classes of materials, all with demonstrated or potential relevance to battery technology: conjugated microporous polymers (ACIE 2007 8574), porous organic cages (Nature Materials 2009 973, Nature 2011 367) and porous liquids (Nature 2015 216), AIC is also a cofounder and Director of a spin-out, Porous Liquid Technologies Ltd. (www.porousliquidtechnologies.com), which is an industry partner in this proposal. He was named in 2011, 2014 and 2017 Thomson Reuters lists as one of the Top 100 Materials Scientists of the last decade.
- **Prof. Matthew Rosseinsky** (M) FRS – MJR (ULIV) is a Fellow of the Royal Society and a Royal Society Research Professor. He received the inaugural De Gennes Prize of the RSC in 2009, a lifetime achievement award in materials chemistry open internationally, and the Royal Society's Hughes Medal in 2011, and its Davy Medal in 2017. He brings expertise in the design and discovery of new materials (Science 2013 847, Nature 2017 280, 2019 213), in controlling the structure of materials for function (Nature 2015 420) and in the role of crystal chemistry at interfaces (Nat. Chem. 2016 347) in mixed conducting electrode materials (Nat. Energy 2017 16214).
- **Dr. David Marquez-Gamez** (M) PhD in Robotics & Artificial Intelligence, LAAS-CNRS, Toulouse, France. Dr. Marquez-Gamez is research fellow and robotics and intelligent automation theme leader at the Leverhulme Research Centre for Functional Materials Design (ULIV) where he is currently involved in the development of a self-driving autonomous scientific laboratory powered by artificial intelligence and robotics and participate in the definition of robotics and intelligent systems in the laboratory of the future. His main research work cover multi robot systems, trajectory planning and control for robot manipulation, perception and navigation for autonomous robots, localization and recently has shifted to higher-level decision-making processes, especially within distributed robotics systems.

Relevant publications and/or products and/or services

1. Z.N. Taylor, A.J. Perez, J.A. Coca-Clemente, F. Braga, N.E. Drewett, M.J. Pitcher, W.J. Thomas, M.S. Dyer, C. Collins, M. Zanella, T. Johnson, S. Day, C. Tang, V.R. Dhanak, J.B. Claridge, L.J. Hardwick and M.J. Rosseinsky Stabilization of O-O bonds by d^0 cations in $Li_{4+x}Ni_{1-x}WO_6$ ($0 \leq x \leq 0.25$) rocksalt oxides as the origin of large voltage hysteresis J. Am. Chem. Soc., 141 18 (2019), 7333
2. J. Gamon, B. Duff, M. Dyer, C. Collins, L. Daniels, T. Surta,, P. Sharp, M. Gaultois, F. Blanc, J.B. Claridge, M.J. Rosseinsky Computationally Guided Discovery of the Sulfide Li_3AlS_3 in the Li-Al-S Phase Field: Structure and Lithium Conductivity. *Chem. Mater*, 31. (2019) 9699 – 9714
3. R. J., Kearsey, B. M., Alston, M. E Briggs, R. L. Greenaway, A. I. Cooper, Accelerated robotic discovery of type II porous liquids, *Chem. Sci*., 10, 2019, 9454-9465
4. R. L. Greenaway, V. Santolini, M. J. Bennison, B. M. Alston, C. J. Pugh, M. A. Little, M. Miklitz, E. G. B. Eden-Rump, R. Clowes, A. Shakil, H. J. Cuthbertson, H. Armstrong, M. E. Briggs, K. E. Jelfs, A. I. Cooper High-throughput discovery of organic cages and catenanes using computational screening fused with robotic synthesis, *Nature Commun*.9, 2849 (2018)
5. C. Collins, M. S. Dyer, M. J. Pitcher, G. F. S. Whitehead, M. Zanella, P. Mandal, J. B. Claridge, G. R. Darling & M. J. Rosseinsky, Accelerated discovery of two crystal structure types in a complex inorganic phase field Nature 546, (2017) 280-284

Relevant previous project of activities connected to subject of proposal

- Faraday Institution Project: Next Generation Li-ion Cathode Material (CATMAT) (at Liverpool) (EP/T012315/1) £2.16M
- Faraday Institution Project: Quantitative Imaging of Multi-Scale Dynamic Phenomena at Electrochemical Interfaces (EP/T007745/1) £1.0M
- Faraday Fast Start Project: SOLBAT - The Solid-State (Li or Na) Metal-Anode Battery (at Liverpool) (EP/R042047/1) £1.46M
- Faraday Fast Start Project: Towards a Comprehensive Understanding of Degradation Processes in EV Batteries (at Liverpool) (EP/R042012/1) £0.39M
- ERC Synergy Grant: Autonomous Discovery of Advanced Materials 10M€

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Glove box for Li-ion cell assembly

96 Maccor Li-ion Cell Cyclers for electrochemical testing of materials

4.1.21 EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF)

	Name: EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF)	**Partner no:** 21	**Country:** France
	Type: RTO	**Number of R&D personnel:** 250 **Number of employees:** 700	**Turnover:** 90 M€

Interest in the project

After the conclusion of a pluri-annual upgrade effort, with the implementation of the EBS, the ESRF will become the most brilliant synchrotron source in the world. The new source will enable groundbreaking scientific opportunities, in particular in the domain of operando and in-situ characterisation, and of the interface science. These families of experiments are particularly important to guarantee disrupting advancements in the crucial field of batteries. The ESRF intend to team up with the most qualified scientific community in this field to obtain the best from the new source, for a robust return both in terms of scientific excellence and of accelerating innovation.

Previous experience vs. main tasks in the project

WP1: the ESRF has a well-established industrial programme worth 2.5MEuro income, matured in the context of proprietary project with industry, and a set of further collaboration with industry in the context of pre-competitive publishable research. Based on this expertise the ESRF possess a strong expertise in the activities of valorisation of the know-how and in general about the bridging between industry and academia.

WP5: once the needs are well specified by the battery experts, the ESRF will contribute to the definition of the experimental workflows, also in the role of leader of the task 5.3. The synchrotron can offer also his expertise in data reduction and data analysis, and also in FAIR data policy.

WP8: the ESRF can bring to this action the experience matured in other context, like the NFFA project and the TEESMAT project.

WP9: for sure the ESRF have a proven track record in its capability to plan, launch and conduct innovative instrumentation programmes, which could bring to the construction novel equipment and infrastructure. The topic of interoperability has been also addressed, both on the point of view of data and of sample environment.

WP11: the ESRF is involved as a leader of task 11.1 and will bring all his experience about the possibility to use synchrotron light to optimise the fidelity cost, both on modeling and on experimental methodologies.

Description of legal entity and main tasks

The ESRF is the world's most intense X-ray source and a centre of excellence for fundamental and innovation-driven research in condensed and living matter science. Located in Grenoble, France, the ESRF owes its success to the international cooperation of 22 partner nations, of which 13 are Members and 9 are Associates. Thanks to the brilliance and quality of its X-rays, the ESRF functions like a "super-microscope" which probe the chemical, structural and morphological properties of condensed and living matter.

The Experiments Division staff will be in charge for the execution of the project. The beamline scientists will contribute to define the best experimental design to guarantee the collection of the highest quality data with respect to the specifications demanded by the battery experts. Moreover, the Business Development Office, the service responsible for the industrial programme at the ESRF, also member of the Experiments Division will support the actions in support of innovation and the exploitation and valorisation of the outcome of the proposal.

CV or description of profile of key staff

- **Dr. Harald Reichert (M)**
  - PhD
  - Director of Research; at the ESRF since 2009
  - Before coming at the ESRF Harald was at the Max Planck Institute for Metal Research in Stuttgart (Germany) where he spent 11 years developing methods for the study of deeply buried interfaces. In the past 15 years he has become one of the leading experts for the exploitation of high energy X-rays for materials science including the development of dedicated instrumentation. In 2002, he received the Walter-Schottky-Award for Solid State Physics from the German Physical Society.
- **Dr. Ennio Capria (M)**
  - PhD
  - Deputy Head of Business Development; at the ESRF since 2013
  - Before coming at the ESRF Ennio worked on the development of nanobiosensors and on nanocomposites. In 2011 he joined Elettra where he worked on manufacturing of optoelectronic devices and particularly their characterisation with synchrotron light.

Relevant publications and/or products and/or services

- Fehse, Marcus; Sahle, Christoph J.; Hogan, Matteo P.; et al. Bulk-Sensitive Soft X-ray Edge Probing for Elucidation of Charge Compensation in Battery Electrodes. JOURNAL OF PHYSICAL CHEMISTRY C Volume: 123 Issue: 40 Pages: 24396-24403 Published: OCT 10 2019
- Vanpeene, Victor; Villanova, Julie; King, Andrew; et al. Dynamics of the Morphological Degradation of Si-Based Anodes for Li-Ion Batteries Characterized by In Situ Synchrotron X-Ray Tomography. *Advanced Energy Maerials* Volume: 9 Issue: 18 Article Number: 1803947 Published: MAY 9 2019
- Finegan, Donal P.; Darst, John; Walker, William; et al. Modelling and experiments to identify high-risk failure scenarios for testing the safety of lithium-ion cells. *Journal Of Power Sources* Volume: 417 Pages: 29-41 Published: MAR 31 2019
- Sottmann, Jonas; Di Michiel, Marco; Fjellvag, Helmer; et al. Chemical Structures of Specific Sodium Ion Battery Components Determined by Operando Pair Distribution Function and X-ray Diffraction Computed Tomography. *Angewandte Chemie-International Edition* Volume: 56 Issue: 38 Pages: 11385-11389 Published: SEP 11 2017
- Tonin, Guillaume; Vaughan, Gavin; Bouchet, Renaud; et al. Multiscale characterization of a lithium/sulfur battery by coupling operando X-ray tomography and spatially-resolved diffraction. Scientific Reports Volume: 7 Article Number: 2755 Published: JUN 5 2017

Relevant previous project of activities connected to subject of proposal

- TEESMAT: it is the Open Innovation Test Bed on battery, a flagship initiative at EU level on batteries; TEESMAT is a platform designed to serve industry, which is offering most of the techniques which could be

interesting for BIG-MAP and is working on a data repository infrastructure which would definitely overlap with what is developed in BIG-MAP.

- NFFA: it is a distributed research infrastructure on nanoscience offering free transnational access to excellent scientific experiments. The selection of the projects is done by peer- review. NFFA has an extensive activity in material characterisation, and occasionally supports the battery community. Also NFFA is developing a FAIR data policy implemented via an ad-hoc developed repository.
- PAC-G (Platform for Advanced Characterisation): it is a regional project offering access to neutrons and synchrotrons for the industry of microelectronics; it run some projects in the domain on micro-batteries.
- CALIPSO+: it is the project that support transnational access to the main synchrotron light sources in Europe.
- INNOVA XN: it is a co-fund initiative financed via H2020 that support 40 PhD students at the ESRF and the ILL to work on research project developed in collaboration with industry; a subset of the projects are in the domain of batteries.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

All the beamlines of the ESRF will be available for the BIG-MAP consortium. Nonetheless, if we consider the main advantages offered by the ESRF, being a 6GeV source, for sure the techniques that exploit high energy photons are privileged. Moreover, with the new EBS source, the increase in brilliance of the source would definitely results in an increase of the coherence, the flux and the focalisation of the X-ray beam. This will allow to improve the resolution of some imaging techniques, and in general the data quality and the acquisition speed.

With respect to the beamlines, some instrument developed during the first phase of "Upgrade" at the ESRF can offer a unique insight in battery investigations. Some examples are reported below:

+ X-ray Raman: it is an inelastic spectroscopy technique which offers the possibility to have electronic structure information in real conditions, in-situ and in depth; this is not possible with the most established photo-emission techniques.

+ XRD tomography associated with PDF: it would give unique structural information and a comprehensive understanding on full battery devices, in-situ and in operando, both on the crystalline phases and on the amorphous ones.

μ-XRD-CT
z (mm)
Ni Precursor
Support

4.1.22 INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL)

NEUTRONS FOR SOCIETY	**Name:** INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL)	**Partner no:22**	**Country: France**
	Type: RTO	**Number of R&D personnel: 170** **Number of employees: 516**	**Turnover: 103 M€**

Interest in the project

The Institut Laue Langevin (ILL), the European Neutron Source, is the leading global player in the provision of neutrons for science. In particular, we are committed to confronting the societal challenge of developing sustainable energy sources, and in the case of batteries ILL's high neutron flux provides the consortium with a unique tool for visualizing real-time chemical changes in operational cells from angstrom to cm scales.

Previous experience vs. main tasks in the project

WP5: the ILL has a proven track record in cutting-edge battery research. Our instrument suite is continuously upgraded, addressing technological barriers with state-of-the-art solutions in the domains of neutron diffraction (ND), small angle neutron scattering (SANS), reflectometry (NR), inelastic scattering (INS) and imaging (NI). Detector innovations and recently developed custom electrochemical cells (including in-house preparation laboratory) permit access to unprecedented temporal and spatial resolutions at relatively high throughputs, whilst new multimodal capabilities provide exciting insights combining x-ray and neutron datasets.

The ILL currently chairs the League of advanced European Neutron Sources (LENS https://www.lens-initiative.org/) and as such is ideally positioned to propose multilateral solutions for beamtime access and standardized experimental protocols, including data treatment (AI) and sharing.

WP8: ILL's track-record of constant re-evaluation and improvement in support and services to European users (e.g. through our Millennium and Endurance upgrades) speaks for itself. The ILL has been at the forefront in defining standards in open data policies, which can be demonstrated through our major role in the Photon and Neutron Open Science Cloud (PaNOSC https://www.panosc.eu/).

Description of legal entity and main tasks

The ILL is an international research centre at the leading edge of neutron science and technology. The Institute operates the most intense reactor source in the world, supplying neutrons to a suite of 40 high-performance instruments that are constantly upgraded. The ILL is funded and managed by France, Germany and the United Kingdom, in partnership with 11 other European countries and India.
Some 1500 researchers from over 40 countries visit the ILL each year. Over 800 experiments, producing about 600 published papers, focus primarily on fundamental science in a variety of fields such as condensed matter physics, chemistry, biology, materials science and nuclear physics. We can estimate that around 10% of our beamtime is dedicated to research in sustainable energy sources
ILL staff have expertise and experience in neutron production (reactor physics, reactor design and operation, cold and hot source design and operation), neutron beam delivery (beam-tubes, neutron guides including supermirror guides), neutron optics (collimators, monochromators, neutron velocity selectors and choppers), neutron detection, massive data collection/treatment and the complete range of neutron instruments for scientific research and its sample environment.

The ILL is located in France but has 32% non-French scientists, engineers, and technical and administrative personnel. The ILL supports some 45 PhD students, registered at Universities across Europe.

CV or description of profile of key staff

- **Prof. Mark Johnson (M):** Science Director at ILL since 2016. He has 17 years experience as head of the Computing for Science group at ILL and is therefore fully versed in the role of data treatment at large scale facilities in delivering scientific results in the way that is envisaged in the BIG-MAP project. He has led major EU projects for the neutron community like NMI3 (https://nmi3.eu/) and SINE2020 (https://www.sine2020.eu/) and played a leading role in the successful application for and implementation of projects like FILL2030 (http://www.fill2030.eu/) and InnovaXN (https://www.innovaxn.eu/), the latter being a co-funded PhD program with industry.
- **Duncan Atkins (M):** Industrial Liaison Engineer in Division Science ILL (since 2013), previously Head of Reactor Operations Group ILL (since 1990). Initiator and ILL project supervisor of new bimodal imaging instrument D50, widely used in Li-ion battery research. Founding member of Battery Innovation @ GIANT (https://www.giant-grenoble.org/en/workshop-on-batteries-2/), joint ILL/CEA/ESRF synergy initiative. Research including hydrogen fuel cells and batteries (supervisor on joint ILL/CEA/ESRF battery related PhD).
- **Dr.-Ing. Lukas Helfen (M):** received his physics diploma at the Saarland University (Germany) in 1998. Until 2004 he worked for the Fraunhofer Institute for Non-Destructive Testing (Saarbrücken and Dresden, Germany), submitting at the Saarland University in 2003 his Ph.D. thesis on investigation of porous materials by synchrotron radiation imaging. From 2004 onwards he worked for the Karlsruhe Institute of Technology (Germany) to develop and apply advanced X-ray imaging methods, principally at the microtomography beamline ID19 of the European Synchrotron ESRF. He joined the Institute Laue-Langevin in June 2019 to develop advanced imaging methods there and to prepare an instrument dedicated to correlative neutron and x-ray imaging for ILL's user community.

Relevant publications and/or products and/or services

1. Bianchini, M., Suard, E., Croguennec, L., Masquelier, C., "Li-Rich Li1+xMn2–xO4 Spinel Electrode Materials: An Operando Neutron Diffraction Study during Li+ Extraction/Insertion" ***J. Phys. Chem. C,*** 118 (45): 25947-25955. (2014)
2. Freire M., Diaz-Lopez M., Bordet P., Colin C.V., Lebedev O.I., Kosova N.V., Jordy C., Chateigner D., Chuvilin A.L., Maignan A., Pralong V., "Investigation of the exceptional charge performance of the $0.93Li_{4-x}Mn_2O_5$-$0.07Li_2O$ composite cathode for Li-ion batteries" ***J. Mater. Chem. A,*** 6: 5156-5165. (2018)
3. Perez, A.J., Rousse, G., Tarascon, J.M., "Structural instability driven by Li/Na competition in $Na(Li_{1/3}Ir_{2/3})O_2$ cathode material for Li-ion and Na-ion Batteries" ***Inorg. Chem.***, 58: 15644-15651. (2019)
4. Seidlhofer, B., Jerliu, B., Trapp, M., Hûger, E., Risse, S., Cubitt, R., Schmitt, H., Steitz, R., Ballauff, M., "Lithiation of Crystalline Silicon As Analyzed by Operando Neutron Reflectivity" ***ACS Nano,*** 10 (8): 7458-7466. (2016)
5. Ziesche, R., Arlt, T., Finegan, D., Heenan, T., Tengattini, A., Baum, D., Kardjilov, N., Markötter, H., Manke, I., Kockelmann, W., Brett, D., Shearing, P. "4D imaging of Li-batteries using correlative neutron and X-ray tomography with a virtual unrolling technique" ***Nat. Commun.*** (pending publishing 2020)

Relevant previous project of activities connected to subject of proposal

Current project:

1. MSCA: InnovaXN (Cofund) partner organisation (2019-2024)
2. ILL coordination: FILL2030 (mono-beneficiary) H2020

3. ILL participation: ATTRACT, PANOSC (H2020)SAFTOREvER (EURATOM)

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

The ILL, sharing the EPN campus in Grenoble (France) with the ESRF, provides the European scientific community with the brightest beams of neutrons possible, serving around 40 complementary state-of-the-art instruments. Battery interface research benefits from various experimental neutron techniques, and the ILL offers flagship instruments in each domain, many of which having benefited from recent upgrades:

D20 (ND) is very high intensity 2-axis diffractometer equipped with a large microstrip detector. Due to the extremely high neutron flux, it opens up new possibilities for real-time experiments on very small samples. The complete diffraction pattern at 1536 positions, covering a scattering range of 153.6°, can be obtained in a matter of seconds, and followed as a function of temperature, pressure or other parameter. The variable monochromator take-off angle, up to 120°, increases the flexibility of the instrument, providing high resolution over the complete diffraction pattern at the highest take-off angle with a neutron flux of up to $10^7 ns^{-1}cm^{-2}$ or a high flux of up to 108ns-1cm^{-2} at medium resolution at lower take-off angle.

D22 (SANS), Small-angle neutron scattering (SANS) is a technique that measures the deviation at small angles (much less than one degree to several degrees) of a neutron beam due to structures of small size in the sample. "Small" means dimensions of a few tenths to about 100 nanometres, such as clusters in alloys, polymers, or biological macromolecules. In general, these structures are disordered. The high neutron flux and the flexibility of its setup make D22 an instrument that is particularly suited for real-time experiments and weakly scattering samples. The recent addition of a small angle x-ray scattering (SAXS) set-up enables D22 to perform simultaneous SANS/SAXS.

D17 (NR) is a neutron reflectometer with horizontal scattering geometry (vertical surfaces) designed to be as flexible as possible in resolution and modes of operation. It is suitable for the study of surface structures in solids and solid/liquid interfaces over a wide range of length scales. ILL has developed the recent RAINBOWS method which promises a gain of 19x in the instrument's performance.

IN16B (INS) is a sub-microeV energy resolution backscattering spectrometer with a very high count rate and wide dynamic range. Recent upgrades have enabled a 2x increase in the energy transfer range at sub-microeV energy resolutions and a new in-house multi-tube detector nearly doubles the count range at large scattering angles.

D50-NeXT is a recent addition to ILL's instrument park, enabling bimodal neutron and x-ray imaging (2 & 3D) at world leading spatial and temporal resolutions. This instrument will undergo a major upgrade in the near future, providing researchers with a full range of up-to-date imaging techniques.

4.1.23 SYNCHROTRON SOLEIL SOCIETE CIVILE (SOLEIL)

	Name: SYNCHROTRON SOLEIL SOCIETE CIVILE (SOLEIL)	**Partner no:** 23	**Country:** France
	Type: RTO	**Number of R&D personnel:** 250 **Number of employees:** 450	**Turnover:** 60 M€

Interest in the project

As a large scale facility Synchrotron SOLEIL is deeply involved in battery research, in particular via a close collaboration with the French research network on electrochemical energy storage (RS2E, https://www.energie-rs2e.com/en). This project represents a way to develop activity and strengthen our position in the field.

Even more importantly, BIG-MAP project is developing a new scheme putting data at the center of the approach and fully exploiting the potential of AI for reverse engineering. Such an approach has the potential to revolutionize methods in materials science, and it is critical for a facility like Synchrotron SOLEIL to participate in order to learn how to contribute to such an integrated project. BIG-MAP project will be a real-size test to adapt our methods and will offer us the opportunity to maximize our impact in battery research and beyond in materials science in the future.

Previous experience vs. main tasks in the project

Synchrotron SOLEIL is already deeply involved in the Competence Pillar "Characterization" and in the Cross-Cutting Initiatives "Battery interface ontology", "Standardization & protocols", "Infrastructure and Interoperability".

Synchrotron SOLEIL offers a combination of advanced facilities and a very high level of expert advice/support for users. Since 2008 to 2017, Synchrotron SOLEIL has welcomed more than 9000 users coming from 2000 laboratories (French, Europeans and overseas). Many beamlines are involved in battery research and provide access to the analyses of complex materials over all regions of the electromagnetic spectrum (infrared, UV/visible, soft X-rays, hard X-rays) and advanced structural characterization (X-ray diffraction, small-angle X-ray scattering, XAS, …) at different scales (from mm to nano) with more than 20 projects per year (22 projects in 2019).

Several beamlines are or will be soon involved in battery research: ROCK (operando spectroscopy), LUCIA (tender x-ray spectroscopy), GALAXIES (Inelastic and Raman X-ray scattering), HERMES (Scanning X-ray Transmission Spectroscopy), CRISTAL (powder diffraction and coherent scattering), SIXS (coherent scattering) PSICHE (X-ray tomography), ANATOMIX (X-ray nanotomography), AILES (Infrared spectroscopy), SWING (small-angle X-ray scattering). We are presently developing more specific methods for interface characterization in batteries, in particular at the GALAXIES and HERMES beamlines.

Synchrotron SOLEIL also has a strong experience in developing analysis software which could be very useful in the project, e.g. for data reduction and chemiometric analysis. We are used to the management of large data sets using standardized data formats.

Synchrotron SOLEIL is involved in many current H2020 INFRA projects among which can be mentioned:

- CALIPSOPlus (http://www.calipsoplus.eu/) [grant 730872]
- NFFA-Europe (https://www.nffa.eu/) [grant 654360]. This project has certain similar objectives to BIG-MAP, particularly involving sample environment - Rachid BELKHOU is the main actor.
- IPERION-CH (http://www.iperionch.eu/) [grant 654028] and IPERION-HS [grant 871034]
- I-NEXT (http://www.inext-eu.org/) [grant 730872] and I-NEXT DISCOVERY [grant 871037]

Such projects give to SOLEIL the opportunity to offer Trans National Access (TNA) to several communities of users in Europe, and to be involved in many Joint Research Activities (JRA) and Networking Activities (NA).

Description of legal entity and main tasks

SOLEIL is the French synchrotron facility, located on the Saclay Plateau near Paris. It is a multi-disciplinary instrument and a research laboratory, whose mission is to run research programs using synchrotron radiation, to develop state-of-the-art instrumentation on the beamlines, and to make those available to the scientific community. SOLEIL offers a unique panorama of experiments with 29 beamlines in operation, covering the far IR to the hard X-ray range, and is open to a large scientific and industrial community in a very broad range of fields from life-sciences to material science including surface, solid states and gas phase physics and chemistry. The facility is a public non-profit company employing about 450 people, whose shareholders are CNRS and CEA. Users are hosted on the various beamlines by a local contact (one of the beamline scientists), who will assist users in conducting the experiment at various levels: preparation of the experiment, data acquisition and data treatment.

CV or description of profile of key staff

- **Andrew Thompson** (M) is the Life Science Director at Synchrotron SOLEIL. He was part of BioXHIT project (FP6, I3, BiocrystallographyX on a highly integrated technology platform), and has considerable experience in the provision of integrated workflows linking science and synchrotron related activities). In particular he was group leader, at EMBL Grenoble, for the team that developed the sample delivery "SPINE standard" for MX, that led the way in Europe for automated sample changing and adapted goniometry.
- **Stéphanie Belin** (F) is Beamline Scientist of ROCK and has been involved for many years in research on the electrochemical storage of energy (batteries and supercapacitors). She is strongly involved in RS2E network.
- **Jean-Pascal Rueff** (M) is the Beamline Head of GALAXIES dedicated to Inelastic X-ray scattering and hard-X photoemission spectroscopy.

Relevant publications and/or products and/or services

1. Assat, G., Iadecola, A., Foix, D., Dedryvère, R., Tarascon, J.M. "Direct Quantification of Anionic Redox over Long Cycling of Li-Rich NMC via Hard X-ray Photoemission Spectroscopy" ***ACS Energy Letters.***, 3(11): 2721–2728. (2018)
2. Jacquet, Q., Iadecola, A., Saubanère, M., Lemarquis, L., Berg, E.J., Alves Dalla Corte, D., Rousse, G., Doublet, M.L., Tarascon, J.M. "Competition between metal dissolution and gas release in Li-rich Li3RuyIr1-yO4 model compounds showing anionic redox" ***Chemistry of Materials***, 30(21): 7682-7690. (2018)
3. Leriche, J.B., Hamelet, S., Shu, J., Morcrette, M., Masquelier, C., Ouvrard, G., Zerrouki, M., Soudan, P., Belin, S., Elkaïm, E., Baudelet, F. "An Electrochemical Cell for Operando Study of Lithium Batteries Using Synchrotron Radiation" ***Journal of the Electrochemical Society***, 157(5): A606-A610. (2010)
4. Perticarari, S., Doizy, T., Soudan, P., Ewels, C., Latouche, C., Guyomard, D., Odobel, F., Poizot, P., Gaubicher, J. "Intermixed Cation–Anion Aqueous Battery Based on an Extremely Fast and Long-Cycling Di-Block Bipyridinium–Naphthalene Diimide Oligomer" ***Advanced Energy Materials***., 9(25): art.n° 1803688. (2019)
5. Dalla Bernardina, S., Brubach, J.B., Berrod, Q., Guillermo, A., Judeinstein, P., Roy, P., Lyonnard, S. "Mechanism of Ionization, Hydration, and Intermolecular H-Bonding in Proton Conducting Nanostructured Ionomers" Journal of Physical Chemistry C, 118(44): 25468−25479 (2014)

Relevant previous project of activities connected to subject of proposal

1. RS2E: French Research Network on Energy Storage (https://www.energie-rs2e.com/en). SOLEIL is partner of the consortium.
2. ROCK EQUIPEX : The purpose of this EQUIPEX project (French National Funding by ANR https://anr.fr/en/investments-for-the-future/investments-for-the-future/) is to build within the existing SOLEIL synchrotron facility and to operate for the benefit of academic and private research projects a new time-resolved X-ray absorption spectroscopy (XAS) beamline based on the quick-scanning energy principle, the so called QuEXAFS. Synchrotron SOLEIL was coordinator of the project.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Picture of Synchrotron SOLEIL

AILES (Advanced Infrared Line Exploited for Spectroscopy): AILES beamline is conceived for absorption spectroscopy, applied to the study of molecular orsolid state systems. It covers the electromagnetic spectrum region ranging from the mid- to far infrared (IR) or THz range (4000 to 5 cm-1). The two experimental workstations are complemented by various sampling devices, enabling the different studies of matter in gaseous, liquid and solid phases. Research projects on AILES concern different applications in physics, chemistry and biology. The aim of the beamline is to answer the needs of scientific projects for which bridging the spectral gap between conventionel IR and microwave radiation is particularly important, and combining high flux and stability over a broad band source.

ANATOMIX (Advanced Nanotomography and Imaging with coherent X rays): ANATOMIX beamline works at photon energies between 5 and 50 keV. It is dedicated to full-field radiography and tomography in absorption and phase contrast, with pixel sizes from 30 nm to 10 µm. ANATOMIX allows its users to obtain two- and three-dimensional radiographic images of bulk volume samples of macroscopic size (up to several cm thickness). For smaller samples, a spatial resolution down to 100 nm (30 nm pixel size) will be available. Real-time studies will be possible at speeds of up to at least one microtomography scan per second. The sample interface has been designed to be as flexible as possible, to enable in situ and/or operando studies under conditions similar to the natural or working environment of the samples (temperature, humidity, mechanical load, transport processes). Biological samples can be measured without dehydration and, in many cases, without chemical fixation.

CRISTAL (Cristallography and structure of condensed matter): CRISTAL beamline is a diffraction beamline dedicated to the study of single crystals and powders. CRISTAL is an undulator-based multi-technique diffraction beamline, dedicated to studies of the structural properties of condensed matter, on different length and time scales, possibly in non-ambient conditions. All the standard techniques for structural analysis on single crystals and

powders are proposed, as well as more advances techniques like coherent diffraction imaging and time-resolved diffraction in a pump-probe scheme.

GALAXIES (Great beAmLine for Advanced X-ray Inelastic scattering and Electron Spectroscopy): GALAXIES beamline is dedicated to inelastic X-rays scattering (RIXS) and hard X-ray photoemission spectroscopy (HAXPES) in the tender up to hard x-ray ranges. These spectroscopic techniques are powerful probes of the local electronic properties of materials and matter.

HERMES (High Efficiency and Resolution beamline for x-ray Microscopy and Electron Spectromicroscopy): HERMES beamline is dedicated to X-Ray microscopy. It is made up of two branches, each one having a microscope available: STXM (Scanning Transmission X-ray Microscopy) and X-PEEM (X-ray PhotoEmitted Electron Microscopy). Both microscope are complem**PSICHE (Pressure structure imaging using high energy contrast):** PSICHE is a beamline dedicated to x-ray diffraction under extreme conditions (pressure-temperature) and to high-energy absorption contrast tomography (20-50 keV).

ROCK (Rocking Optics for Chemical Kinetics): ROCK beamline is devoted to the study of fast kinetic processes in nanomaterials used in catalysis and batteries. The objective is to contribute to the development of more efficient catalysts and batteries which should find successful industrial applications in the field of energy generation and storage in compliance with the protection of public health and environment. The better knowledge at the atomic scale of nanomaterials involved in catalysis or energy storage provided by time-resolved XAS is recognized by the concerned communities as mandatory for establishing synthesis strategies leading to important breakthroughs in the production of energy from renewable sources and in the development of advanced energy storage devices.

SIXS (Surface Interface X-ray Scattering): SIXS is a wide-energy range beamline dedicated to the structural characterization of surfaces, interfaces (solid/solid or solid/liquid), as well as nano-objects in controlled environments using surface-sensitive x-ray scattering techniques. Grazing Incidence X-ray diffraction (GIXD), grazing Incidence small-angle X-ray scattering (GISAXS), Xray reflectivity (XRR), magnetic surface X-ray scattering.

SWING (Small and Wide angle x-ray scattering): By providing information on the structure of matter at scales varying between nanometer and micrometer, the beamline SWING will help answering the numerous questions related to soft condensed matter, conformation of macro-molecules in solution and composite materials in material sciences. Our experimental set up allows small-angle X-ray scattering (SAXS) and wide-angle X-ray scattering measurements (WAXS) to be performed simultaneously in the 5-16 keV energy range, as well as grazing incidence small angle scattering (GISAXS). Anomalous scattering experiments will be facilitated. Emphasis will be put on the variety of samples that can be studied, solutions, gels, amorphous solids, crystallised solids and the corresponding diversity of sample environments.

4.1.24 FUNDACION CIDETEC (CID)

cidetec energy storage	**Name:** FUNDACION CIDETEC (CID)	**Partner no:** 24	**Country:** Spain
	Type: RTO	**Number of R&D personnel: 152** **Number of employees:**180	**Turnover:** 13.1 M€

Interest in the project

CID benefits will be:

- Extend the multiphysics models to chemistry neutral
- Extend the multiphysics models to ageing multiphysics models (implementing the mechanical/electrochemical degradation equations)
- Combine experimental and phase-field models for in-depth understanding of the evolution of the interfaces (SEI, CEI)
- Extend the Big-data structure to the cloud
- Combine experimental and simulation data building hybrid-data-driven models.

Previous experience vs. main tasks in the project

CID has expertise on the following activities:

- Li ion Multiphysics models implementation (P2D, 3D, P4D, ROM – P4D) coupled to optimization algorithms for cell optimization purposes
- Phase field models for interface performance understanding implementation
- Post-mortem activities
- Model parametrization
- Building a Big-data baseline of cell manufacturing data
- Machine learning algorithm libraries usage for cell performance prediction
- Electrode manufacturing at pilot plant level and cell assembly
- Cell (large and small) ageing electrical/electrochemical testing

Role in the project:

- Extend the multiphysics models to chemistry neutral
- Extend the multiphysics models – P4D- to ageing multiphysics models (implementing the mechanical/electrochemical degradation equations)
- Combine experimental and phase-field models for in-depth understanding of the evolution of the interfaces (SEI, CEI)
- Extend the Big-data structure to the cloud
- Combine experimental and simulation data building hybrid-data-driven models.
- Electrode manufacturing
- Cell testing

Description of legal entity and main tasks

CID is a private organization for applied research founded in 1997. Located in the city of Donostia-San Sebastián, CIDETEC is comprised of three international technological reference institutes in Energy Storage, Surface engineering and Nanomedicine.

CID Energy Storage is specialised in creating new battery technologies according to specific challenges, and its ultimate transference to the industry. The institute has the capacity to develop complete products and processes

and offers material validation, pilot manufacture, pack engineering and battery testing services. CID overall workforce consists of 180 employees, 95 % of whom are university graduates and 45 % PhD holders. Its volume of activity came up to € 13.1M in 2018.

CID Energy Storage involves up to 60 specialized researchers distributed into two technological units: Materials for Energy –approx. 2/3 of the workforce with a background of chemistry, electrochemistry and materials- and Systems Engineering - mainly electrical and mechanical engineers. As a result of this approach, CID Energy Storage cooperates closely with the industry in the context of bilateral, direct contract research and product development projects, both at the National and International level.

CID Energy Storage is heavily involved in the European batteries community, including several EU level platforms and associations where energy storage and its applications is at the core. We are active member in several industrial and research associations and platforms like the ETIP Batteries Europe, the European Battery Alliance (EBA), EGVIA, EARPA, EMIRI or EERA. In particular, Dr Oscar Miguel, Director of CID Energy Storage, was appointed Chairman of Working Group #4 on Cell design and Manufacturing within the recently launched ETIP Batteries Europe.

CID Energy Storage is also regular participant in H2020 European funded projects, frequently from the coordination of international consortia –currently CID Energy Storage is coordinator of iModBatt, iHeCoBatt, and E-Magic projects, plus one more from the last CC-BAT-2019 calls-. We accumulate more than 15 participations in EU funded R+D battery projects under FP7 and H2020. Finally, CID Energy Storage is involved as well in the core team of BATTERY 2030+, the initiative for a long-term large-scale research program towards the European battery of the future.

CV or description of profile of key staff

- **Mrs Elixabete Ayerbe (F)** received her degree of Chemical Engineer at the Technical School of University of Zaragoza in 2002 and master's in industrial mathematics delivered by the Technical University of Madrid (UPM) in 2017. After several years working on the research centres such Ceit-Ik4 and CENER, in 2007 she started her current job, as Project Manager in the Materials for Energy Unit. At the moment, she is leading the modelling and post-mortem group of the unit that works on the development of multiphysic and optimization models for lithiumion and advanced li-ion batteries. She is currently coordinating H2020 DEFACTO project and coordinated in the past the FP7 SHEL project. Additionally, she represented and represents the multiphysic modelling activity of CID in H2020 SPICY, HIFI ELEMENTS, SPIDER and Battery 2030+ projects.
- **Dr Oscar Miguel (M)** holds a PhD in Chemistry by the University of the Basque Country (Spain). He joined CID back in 1999, and currently works as Director of the CID Energy Storage Institute. He has been involved in energy related industrial research activities for more than 15 years including technology generation, transference and product development. Today he and his team are fully devoted to advanced battery technologies, including Li ion and Post-Li ion technologies. The team that he represents currently covers all the value chain from materials to battery packs, including battery cell manufacturing at pilot scale. All this activity covers from knowledge generation to product development and transference in close cooperation with industry partners all through Europe.

  He is heavily involved in the European batteries community, representing CID Energy Storage in industrial and research associations like European Battery Alliance (EBA), European Green Vehicles Association (EGVIA), European Materials Industrial Research Initiative (EMIRI) and others.

  More recently, he has been appointed Chairman of Working Group #4 on Cell design and Manufacturing within the recently launched European Technology and Innovation Platform "ETIP Batteries Europe".
- **Mrs Idoia Urdampilleta (F)** is responsible of the Materials for Energy Unit at CID Energy Storage. She has more than 10 years of industrial experience in research and development of electrochemical storage systems such as lithium-ion batteries. She is author of more than 10 scientific papers. She has participated in several national

and international scientific and R&D projects related to the development of lithium, post lithium ion batteries, modeling and pilot plants.

- **Dr Francisco Alcaide Monterrubio (M)** is Doctor in Chemistry (Electrochemistry, University of Barcelona). Project Manager and PI in the Materials for Energy Unit at CID Energy Storage, he has 23 years of experience in R+D+I in electrochemical energy storage and conversion devices, particularly, in batteries and low temp. fuel cells. He is specialized in electrodics and electrocatalysis at electrochemical interfaces. Since 2003 at CID, he has led (PI) more than 20 R+D+I projects and contracts. He has been involved in several European projects: ZEOCELL, SUSHGEN, ARTEMIS, DEMSTACK, COBRA, SPIDER, HIFI-ELEMENTS, SPIDER, DEFACTO and Battery 2030+. He is co-author of > 40 SCI publications (h-index = 21), 8 book chapters, 70 contributions in conferences, one patent, and co-advisor of 2 PhDs and 1 MSc. Currently, he is responsible of advanced electrochemical parameterization techniques for the characterization of Li and post-Li ion batteries.

Relevant publications and/or products and/or services

1. M. Philippot, G. Álvarez, E. Ayerbe, J. Van Mierlo, M. Messagie. Eco-Efficiency of a Lithium-Ion Battery for Electric Vehicles: Influence of Manufacturing Country and Commodity Prices on GHG Emissions and Costs, Batteries 5 (2019) 23.B
2. S. Kosch, Y. Zhao, J. Sturm, J. Schuster, G. Mulder, E. Ayerbe, A. Jossen. A Computationally Efficient Multi-Scale Model for Lithium-Ion Cells, J. Electrochem. Soc. 165 (2018) A2374.
3. Iturrondobeitia, A. Kvasha, J.-M. López del Amo, J. F. Colin, D. Sotta, I. Urdampilleta, M. Casas-Cabanas. A Comparative Study of Aqueous and Organic Processed Li1.2Ni0.2Mn0.6O2 Li-Rich Cathode Materials for Advanced Lithium-Ion Batteries. Electrochim. Acta 247 (2017) 420.

Relevant previous project of activities connected to subject of proposal

1. **BATTERY 2030+,** "At the heart of a connected green society", H2020-FETPROACT-2019-01, Coordinator: UPPSALA UNIVERSITET (UU)
2. **E-MAGIC,** "European Magnesium Interactive Battery Community", H2020-FETPROACT-2018-01. Coordinador: CID
3. **DEFACTO,** "Battery DEsign and manuFACTuring Optimization through multiphysic modelling", H2020-LC-BAT-2019, Coordinator: CID
4. **SPIDER**, "Safe and Prelithiated hIgh energy DEnsity batteries based on sulphur Rocksalt and silicon chemistries", H2020-NMBP-ST-IND-2018, Coordinator: CEA
5. **SAFELIMOVE,** "advanced all Solid stAte saFE LIthium Metal technology tOwards Vehicle Electrification", H2020-LC-BAT-2019, Coordinador: CIC ENERGIGUNE

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

- Materials characterization equipment: XRD, SEM, FESEM, DSC, TGA, FTIR, UV-vis, Karl Fischer Titrator – Liquid samples and Oven method; Glove box (Ar, < 1ppm O2& H2O)
- Dry room (D.P. -60ºC) with tools and equipment for small pouch cell assembly.
- Research Battery Manufacturing Pilot Plant: Dedicated anode and cathode mixers for slurry fabrication: Planetary mixers, 5&15 litre slurry sizes, avoiding cross-contamination. Roll-2-Roll electrode coating line: flexible and modular 10 m length machine (Basecoater, Coatema) for self-metered (Knife, Commabar) and pre-metered (slot-die) technologies. R2R calendar (roll-press) for electrode post-processing (porosity adjustment). Lamination and stacking authomatic line for large pouch cell assembly –up to ca. 40Ah-
- Battery Testing Facility: 350 channels (5V/5A); 12 channels (5V/25A), 18 channels (5V/50A), 4 channels (6V/100A), 28 channels (6V/60A), 12 channels (6V/240A) with up to 1000A maximum current in parallel. 12 channels with impedance analysis capability. 750 channels for coin cell testing and cycling under controlled T.
- Adiabatic calorimeter (THT EV-ARC) for thermal characterization of cells

4.1.25 ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL (EMIRI)

	Name: ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL (EMIRI)	**Partner no:** 25	**Country:** Belgium
	Type: Association	**Number of R&D personnel:** 0 **Number of employees:** 0	

Interest in the project

Having a unique position bridging the academic and industrial research actors, EMIRI can act as a gateway to industry and help ensure that we are "educating the workforce" for the new tools to be developed in BIG-MAP/Battery 2030+.

Previous experience vs. main tasks in the project

EMIRI will contribute to PM2 (Education, Exploitation & Outreach), mainly by

(i) contributing to the elaboration of a communication, dissemination and exploitation plan
(ii) seeking opportunities to increase awareness of the project and disseminate the project results through its existing distribution channels
(iii) (co-)organising workshops to promote, disseminate and provide training in data-based discovery to different groups of stakeholders throughout the whole battery chain value.

EMIRI has a large network and experience in organising workshops (EMIRI Tech Talks and EU projects portfolio workshops)

Description of legal entity and main tasks

EMIRI represents more than 50 organizations (industry, research, associations) active in Advanced Materials Technologies for clean and sustainable energy & mobility. The association contributes to industrial leadership of developers, producers and key users of Advanced Materials by shaping an appropriate innovation, energy and industrial policy framework at European level. In frame of the R&D Framework Programmes, EMIRI collaborates with the European Commission to develop the Innovation Pillar on Advanced Materials for clean and sustainable energy & mobility technologies proposed in the EMERI Technology Roadmap. In frame of Integrated SET Plan, EMIRI contributed to various discussions and contributed more actively to Action 7 (batteries) in which EMIRI was in charge of implementation plan's aspects related to advanced materials. EMIRI is actively involved in different working groups of the ETIP BATTERIES EUROPE.

CV or description of profile of key staff

- **Philippe JACQUES (M)** is Managing Director of the Energy Materials Industrial Research Initiative (EMIRI) Association based in Brussels. He holds a Master in Chemical Engineering from the University of Louvain-la-Neuve in Belgium. Philippe joined Solvay, a global **advanced materials and specialty chemicals company,** in 1988 in Brussels, Belgium, and moved to various IP, R&D management and senior leadership roles. Qualified European Patent Attorney, he managed Solvay Patent Department before joining Corporate R&I Management Team in 2011. After a 5-year assignment in the management of Solvay biggest R&I Center in Lyon, France, he has been seconded to EMIRI since October 1st, 2018.

Relevant publications and/or products and/or services

1. EMIRI Technology Roadmap (September, 2019)
2. EMIRI Horizon 2020 roadmap (elements on technology synergies from advanced materials perspective)
3. Implementation Plan of SET Plan Action 7
4. EMIRI – A call for action in FP9 on advanced materials for clean energy & clean mobility
5. EMIRI – Europe needs a focus on "accelerating innovation & restoring EU competitiveness in clean energy & clean mobility technologies", enabled by advanced materials and other key enabling technologies

Relevant previous project of activities connected to subject of proposal

1. H2020-LC-SC3-2018-Joint-Actions-3 - CSA project SMARTSPEND (partner)
2. H2020-FETPROACT-2019-01 - CSA project BATTERY 2030+ (partner)
3. H2020-FETFLAG-2018-01 - CSA project SUNRISE (partner)
4. H2020-LC-BAT-2019 - CSA project LIPLANET (partner)
5. EMIRI Technology roadmap (elements on technology synergies from advanced materials perspective)
6. EMIRI Tech Talks and EU projects portfolio workshops

4.1.26 UMICORE (UMI)

umicore	**Name:** UMICORE (UMI)	**Partner no:**	**Country: Belgium**
	Type: IND	**Number of R&D personnel:** **Number of employees: 10 000**	**Turnover: 3.3 b€ (excluding metals, 2018)**

Interest in the project

Umicore (UMI) is a company specialized in the development and commercialization of advanced materials for various applications, rechargeable batteries being one of them. We use classical R&D methodology on a day to day basis and are interested to understand how the approach proposed in BIG-MAP could facilitate the development of new solutions for our customers.

Previous experience vs. main tasks in the project

As a materials technology group, we are used to and able to provide suitable materials so that the tasks described in the project can be carried out by the different partners. We will also be able to bring industrial expertise to the tools and methodology developed in the project.

Description of legal entity and main tasks

UMI is a global materials technology and recycling group. It focuses on application areas where its expertise in materials science, chemistry and metallurgy makes a real difference. Its activities are organized in three business groups: Catalysis, Energy & Surface Technologies and Recycling. Each business group is divided into market-focused business units offering materials and solutions that are at the cutting edge of new technological developments and essential to everyday life.

In BIG-MAP, we will bring our expertise in rechargeable batteries and NMC materials by providing suitable materials for the project.

CV or description of profile of key staff

- **Dr. Amada Montesdeoca, Open Innovation Manager (F)** received her Master degree in Chemical Engineering in 2007 and obtained her PhD in Materials Physics in 2012 from University of La Laguna (Spain). She has worked in research and development for silicon photovoltaics first as guest researcher in Fraunhofer ISE (Germany); and later as industrial resident at imec (Belgium) working for the private sector as R&D engineer and project leader in the area of silicon photovoltaic device manufacturing. Since 2018 she works for UMI Rechargeable Battery Materials R&T as Open Innovation Manager, in charge of global external collaboration research projects.

- **Mr. Dr. Pierre-Etienne Cabelguen, Technology Manager (M)** received his Master's in 2013 as a double-degree in engineering and chemistry from Ecole Centrale de Lille (France) and the University of Waterloo (Canada), where he did a Master with Thesis on lithium-sulfur batteries in collaboration with BASF. He obtained his PhD in Material Science for energy storage in December 2016 in the University of Grenoble (France) and the Commissariat à l'Energie Atomique (CEA, France). Since January 2017, he is working at UMI as a Technology Manager for the Rechargeable Battert Materials (RMB) Business Unit in Europe.

Relevant publications and/or products and/or services

1. WO2012136473 “Glass-coated cathode powders for rechargeable batteries” and related patent family;
2. WO2012163660 “Positive electrode material having a size dependent composition” and related patent family;
3. US6277521 & US6582852 & US6794085 “Metal oxide containing multiple dopants and method of preparing same” and related patent family;
4. US6361756 "Doped lithium manganese oxide compounds and methods of preparing same" and related patent family;
5. US6589499 & US6620400 & US7074382 “Method of producing layered lithium metal oxides free of localized cubic spinel-like structural phases” and related patent family;
6. US6878490 “Positive electrode active materials for secondary batteries and methods of preparing same” and related patent family

Relevant previous project of activities connected to subject of proposal

SIMBA	Scaling-up of ICP technology for continuous production of Metallic nanopowders for Battery Applications	FP7-NMP-2008-SMALL-2
SimDOME	Digital Ontology-based Modelling Environment for Simulation of materials	H2020-NMBP-TO-IND-2018
SOMABAT	Development of novel SOlid MAterials for high power Li polymer BATteries (SOMABAT). Recyclability of components.	FP7-2010-GC-ELECTROCHEMICAL-STORAGE
STALLION	Safety Testing Approaches for Large Lithium-Ion battery systems	FP7-ENERGY-2012-1-2STAGE
TEESMAT	OPEN INNOVATION TEST BED FOR ELECTROCHEMICAL ENERGY STORAGE MATERIALS	H2020-NMBP-TO-IND-2018

Partner for all.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Synthesis lab of NMC materials at different scale (up to tons/day).

4.1.27 SOLVAY SA (SOLB)

	Name: SOLVAY SA (SOLB)	**Partner no:27**	**Country:BE**
	Type: IND	**Number of R&D personnel:2100** **Number of employees: 24500**	**Turnover: 10,890 M€**

Interest in the project

Solvay (SOLB) interest in the project is the acceleration of the search for high-performance batteries by identifying additives, solvents and salts that could act synergistically with active materials in order to form desired interfaces. The interest is on computational and experimental identification of such ingredients and blends.

Previous experience vs. main tasks in the project

SOLB has a long history of battery testing, especially on liquid electrolyte, with the development of several compounds for high energy batteries. In addition, SOLB already has performed some machine learning based on those data and managed to build models to predict the lifecycle of different formulations as well as some other properties such as gas generation during battery storage.

Description of legal entity and main tasks

SOLB is a large multi-specialties chemical group working on the forefront of innovation in chemicals and materials. Headquartered is in Brussels, Belgium, SOLB operates in 61 countries around the globe, employing 25,000 people with a turnover of 10 billion € per year. Its roots are in Europe where 44% of its workforce is located.
SOLB produces materialsfor (anodes, cathodes, electrolytes, separators…) to enhance theperformance of batteries. These materials are therefore supplied to battery makers and/or electrolyte makers which sells electrolytes to the battery manufacturers.

CV or description of profile of key staff

- **Dr Antoine Emery, (M**), graduated with a Master of science in materials science and engineering in 2011 (EPFL, Lausanne, Switzerland) before completing his PhD in computational materials science in 2017 at Northwestern University, Chicago IL, USA (Thesis title: "Materials Discovery for Water Splitting Applications Using First-Principles Calculations and Machine Learning"). He joined SOLB in 2017 where he is a modeling research scientist in charge of modeling and artificial intelligence activities for battery related topic within the company. He has a background in first-principle modeling of inorganic materials, thermodynamics properties and ab initio molecular dynamics and is experienced in machine learning, particularly on battery topics (formulations, cycle life, side reactions) based on data coming from SOLB.

- **Dr. Marc-David Braida (M),** graduated as a chemical engineer in 2007 and finished his PhD work in 2010 in the field of high temperature ceramic materials for fuel cell application. He joined SOLB in 2011 in the Advanced Lab for Inorganic Materials. He is in charge of new projects around synthesis and characterization of new materials for energy applications particularly secondary batteries (Li-ion, Na-Ion, Li-S, gel electrolyte and solid state batteries). He was recently involved in the FP7 MAT4BAT and H2020 NAIADES (as WP leader). Recent patent in the field of liquid electrolytes WO2018087473A1

Relevant publications and/or products and/or services

Relevant publications related to new materials discovery using first-principle calculations and machine learning for energy related applications:

- *Emery, A. A., Saal, J. E., Kirklin, S., Hegde, V. I., & Wolverton, C. (2016). High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications. Chemistry of Materials, 28(16), 5621–5634. https://doi.org/10.1021/acs.chemmater.6b01182Phys. Rev. Materials 2, 043802*
- *Balachandran, P. V., Emery, A. A., Gubernatis, J. E., Lookman, T., Wolverton, C., & Zunger, A. (2018). Predictions of new ABO3 perovskite compounds by combining machine learning and density functional theory. Physical Review Materials, 2(4), 043802. https://doi.org/10.1103/PhysRevMaterials.2.043802*

Patents:

- WO2019042741 - 2019-03-07 Fluorinated liquid electrolyte for electrochemical cells having a lithium metal anode

Relevant previous project of activities connected to subject of proposal

1. AMELIE FP7 Develop high energy batteries based on fluorinated products
2. MAT4BAT FP7 Develop innovative hybrid electrolytes
3. NAIADES H2020 Electrolytes for Na-Ion batteries.
4. MODALIS2 H2020 MODelling of Advanced LI Storage Systems
5. SPIDER H2020 High energy DEnsity batteries based on sulphur Rocksalt and silicon chemistries

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

SOLB has licenses for several first-principle calculations software such as VASP, materials studio and Gaussian as well as version of open source software such as Quantum Espresso, Gromacs and LAMMPS. In terms of computational resources, SOLB owns a supercomputer, physically located in Lyon, with 1600 CPUs and 40 GPUs.

4.1.28 BASF SE (BASF)

	Name: BASF SE (BASF)	**Partner no:** 28	**Country:** Germany
	Type: IND	**Number of R&D personnel:** 4 434 **Number of employees:** 35 316	**Turnover:** 23.6 B€

Interest in the project

BASF is a leading supplier of cathode active materials for lithium-ion batteries for the automotive industry. Moreover, within the new corporate strategy, digitalization is becoming one of the central drivers for the future success of the company. For digitalization in R&D BASF seeks the potential to accelerate and strengthen innovation through data science, scientific modeling, lab automation and knowledge system. The combination of these areas to make innovations, faster for battery materials is the core of the BIG-MAP project.

Previous experience vs. main tasks in the project

BASF synthesize and provides battery materials, in particular so-called cathode active materials, to the consortium that are used for the experiments by different university partners.

Previous experience: (i) BASF is one of the leading suppliers of cathode active materials for the lithium-ion battery industry; (ii) BASF SE is carrying out extensive research on these materials for over a decade. Its R&D centers are capable to synthesize and optimize high quality cathode active materials from 10g to several kg scale that is required to supply the consortium with reliable and high-performance materials.

Description of legal entity and main tasks

At BASF, we create chemistry for a sustainable future. We combine economic success with environmental protection and social responsibility. The approximately 122,000 employees in the BASF Group work on contributing to the success of our customers in nearly all sectors and almost every country in the world. Our portfolio is organized into six segments: Chemicals, Materials, Industrial Solutions, Surface Technologies, Nutrition & Care and Agricultural Solutions. BASF generated sales of around €63 billion in 2018. Further information at www.basf.com.

The research unit RCN, headquartered in Ludwigshafen, Germany, is responsible for battery material R&D within BASF to support the global battery material business in BASF. Several teams in four R&D sites (Ludwigshafen (DE), Beachwood (US), Amagasaki (JP), Shanghai (CN)), work on the synthesis, optimization and characterization of cathode active materials and process technologies, especially for Ni-rich NCM and NCA.

CV or description of profile of key staff

- **Dr. Andreas Fischer** (M) has been active in the field of electrochemical energy storage and conversion for more than 20 years. In 1996, he finished his doctoral studies with a thesis on "Investigations on the Technology of Proton Exchange Membrane Fuel Cells" at the Technical University of Darmstadt / Germany. After that he joined BASF R&D in Ludwigshafen / Germany working on industrial electrochemistry. Early 2000 he spent three years in marketing at BASF and returned to R&D taking over the group leader position "Electrochemical Research", where he started to work on materials for lithium ion batteries. Since 2011 he is Vice President and executive expert in the field of "Batteries and Electrochemistry" at BASF.
- **Dr. Pascal Hartmann** (M) received his PhD in physical chemistry from the University of Giessen in 2015. After a short postdoc in Giessen he joined R&D in BASF SE working on materials for lithium-ion and solid-state batteries in 2015. In 2016 he joined the Battery and Electrochemistry Laboratory (BELLA), a postdoc center jointly operated by BASF and KIT, as laboratory manager BASF. Since 2019 Dr. Hartmann, as research manager, is responsible for Digitalization in Battery Materials and Inorganics R&D in BASF SE.
- **Dr. Robert Lee (M)** received a PhD in theoretical physics from the university of Cambridge in 2011. He then worked as a postdoctoral researcher at the Interdisciplinary Center for Scientific Computing at Heidelberg University, where his focus was on optimization of dynamical systems and nonlinear design of experiments. In 2013 he joined BASF, where he uses approaches from data science to accelerate and enable R&D of battery materials.

Relevant publications and/or products and/or services

1. Schweidler, S.; De Biasi, L.; Garcia, G.; Mazilkin, A.; **Hartmann, P**.; Brezesinski, T.; Janek, J. Investigation into Mechanical Degradation and Fatigue of High-Ni NCM Cathode Material: A Long-Term Cycling Study of Full Cells . 2019. ACS applied energy materials, 2 (10), 7375–7384
2. de Biasi, L.; Schiele, A.; Roca-Ayats, M.; Garcia, G.; Brezesinski, T.; **Hartmann, P**.; Janek, J. Phase Transformation Behavior and Stability of LiNiO2 Cathode Material for Li-Ion Batteries Obtained from In Situ Gas Analysis and Operando X-Ray Diffraction. 2019. ChemSusChem, 12 (10), 2240–2250
3. Neudeck, S.; Mazilkin, A.; Reitz, C.; **Hartmann, P.;** Janek, J.; Brezesinski, T. Effect of Low-Temperature Al2O3 ALD Coating on Ni-Rich Layered Oxide Composite Cathode on the Long-Term Cycling Performance of Lithium-Ion Batteries. 2019. Scientific reports, 9 (1), 5328.
4. Neudeck, S.; Walther, F.; Bergfeldt, T.; Suchomski, C.; Rohnke, M.; **Hartmann, P.;** Janek, J.; Brezesinski, T. Molecular Surface Modification of NCM622 Cathode Material Using Organophosphates for Improved Li-Ion Battery Full-Cells. 2018. ACS applied materials & interfaces, 10 (24), 20487–20498

Relevant previous project of activities connected to subject of proposal

BASF participated in several cooperation projects from the EU and national R&D programs of Germany

1. Bundesministerium für Bildung und Forschung (BMBF) Project SafeBatt: Active and passive measures for intrinsically safe lithium-ion batteries. BASF is a partner in the consortium.
2. Bundesministerium für Bildung und Forschung (BMBF) Project FELIZIA: Solid electrolytes as enablers for lithium cells in automotive applications. BASF is a partner in the consortium.
3. Bundesministerium für Wirtschaft und Energie (BMWi) Project LIB.DE: Lithium-Ions-Batteries – made in Germany. The project deals with the development of high capacity anode and cathode materials for use in High-Energy-Lithium-Ion battery cells. BASF is a partner in the consortium.
4. Bundesministerium für Wirtschaft und Energie (BMWi) Project GO3: High-Energy-Lithium-Ion Battery for automotive and stationary applications. BASF is a partner in the consortium.
5. EU-funded EIT-Raw Materials Project ReLieVe: Recycling Li-ion batteries for electric Vehicles. BASF is a partner in the consortium.

4.1.29 NORTHVOLT AB (NVOLT)

northvolt	**Name:** NORTHVOLT AB (NVOLT)	**Partner no:** 29	**Country:** Sweden
	Type: IND	**Number of R&D personnel:** 150 **Number of employees:** 500	**Turnover:** 10 M€

Interest in the project

The Norhtvolt (NVOLT) interest in the BIG-MAP project is to be part of the European battery academia and industry collaboration. The huge potential in a data-driven approach when it comes to development and understanding the next generations of battery cells is a top priority to be part of. NVOLT believes that the magnitude of data that will be generated from its giga-scale manufacturing plants will be a main contributor the success of this project.

Previous experience vs. main tasks in the project

NVOLT as a company was founded in 2017 and is currently operating its first R&D facility and constructing its manufacturing facilities. However, it has a vast amount of experience and know-how when it comes to cell design and industrialization within its team.

Expected main value creation in the project:

(i) Construction of greenfield li-ion manufacturing plants with a state-of-the-art level of traceability and quality control will generate data that can be used to the project.
(ii) Stakeholder in development of automated and efficient material screening methodologies and equipments.

Description of legal entity and main tasks

Development of li-ion cells and manufacturing of li-ion cell. Producing the world greenest battery with the lowest CO_2 footprint.

CV or description of profile of key staff

- **Peter Olofsson (M)**

Diplomas: Master of science – Engineering Physics
Title/position: Technical Account Manager
Experience: 6 years within power system industry and 2.5 years within battery industry. Worked at NV since 2017.

Relevant previous project of activities connected to subject of proposal

1. European Battery Alliance – NVOLT has since the introduction of European Battery Alliance been a key stakeholder and has cooperated with the European Commission in forming the Alliance and supporting the goal of a European value chain for batteries. NVOLT is participating in EBA activities and is one of the industrial partners supporting the aim of EBA.
2. BatteRIes Europe – NVOLT is represented in the Governing board of the ETIP BatteRIes Europe. This means NVOLT will have a central role in forming the European research and innovation agenda for batteries in the upcoming Horizon2020. NVOLT is also represented in Batteries Europe workings groups for cell manufacturing- and design and raw materials & battery recycling.
3. Batteries2030+ - NVOLT is supporting the Europen research program for future battery technologies, Batteries2030+. NVOLT is involved as a stakeholder and has been involved in project activities such as workshops, meetings and strategic discussions.

4. SweBAL (Centre for Swedish Batteries) – NVOLT is one of the partners in the Centre for Swedish Batteries. The project aims to develop new types of lightweight, inexpensive, environmentally friendly, and safe ultra-high-energy storage batteries.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

NVOLT is currently expanding heavily in Research and Development facilities such as: Material Screening, Cell assembly line, Pilot Cathode Production, process innovation, Quality control development - to support the manufacturing and industrialization. Access to these R&D facilities and possibility to test different analysis methodologies developed within the BIG-MAP project will contribute to the success of the project.

4.1.30 UNIVERSITAT BASEL (UBAS)

University of Basel	**Name:** UNIVERSITAT BASEL (UBAS)	**Partner no: 30**	**Country: CH**
	Type: UNI	**Number of R&D personnel: 4500** **Number of employees: 6200**	**Turnover: 1'120000**

Interest in the project

The research group of Anatole von Lilienfeld develops and provides quantum machine learning models of quantum properties which can be trained and applied throughout materials compound space. Our interest in the project lies in the extension and application of such models to relevant battery properties and materials classes. If successful, these models can subsequently used throughout BIG-MAP in order to discover and identify promising new materials for subsequent in-depth investigation and possibly synthesis and characterization.

Previous experience vs. main tasks in the project

Anatole von Lilienfeld has been developing first principles based approaches for the exploration and navigation of materials compound space for more than 14 years. Apart from the PI the lab currently consists of one senior researcher, eight postdoctoral students, and ten PhD students. The lab is actively involved in an ERC Consolidator project, ``QML: Chemical Reactions with Unprecedented Speed and Accuracy'' (2018-2023), as well as various smaller projects funded by the Swiss National Science foundation. The lab's experience and expertise when it comes to the development of quantum machine learning models of electronic structure properties applicable throughout materials compound space is at the forefront of the field. Thanks to rigorous roots in quantum mechanics and statistical mechanics, and given the lab's expertise and infrastructure, extending current quantum machine learning models towards battery relevant system classes and properties. while challenging, seems feasible.

Description of legal entity and main tasks

The University of Basel (UBAS, www.unibas.ch) has an international reputation of outstanding achievements in research and teaching and is ranked as one of the world's 100 best universities. A research university with a high output of academic publications and a wealth of strong partnerships, the University of Basel is also an experienced participate and co-ordinator of EU framework programmes having participated in more than 110 Horizon 2020 projects. The department of chemistry at the University will provide office space as well as space for the compute nodes used in the group.

CV or description of profile of key staff

- **Anatole von Lilienfeld (M)**
  2001 Diploma Chemistry, ETHZ, CH
  2005 PhD Computational Chemistry, EPFL, CH
  2005-2006 Postdoctoral Fellow, New York University, USA
  2006-2010 Truman Fellow, Sandia National Laboratories, USA
  2010-2011 Scientific Staff, Sandia National Laboratories, USA
  2011-2013 Scientific Staff, Argonne National Laboratory, USA
  2013-2015 Foerder Prof University of Basel, CH
  2016 Associate Prof Free University of Brussels, BE
  2016 - 2019 Assistant Prof University of Basel, CH
  2019 - now Associate Prof University of Basel, CH
  2019 - now Editor in Chief of new IOP journal: Machine Learning: Science and Technology

2019 - now Associate Editor of AAAS journal: Science Advances
2018 Feynman Prize Nanotechnology Theory, Foresight Institute, USA
2017 ERC Consolidator Grant
2014-2019 Editorial Board member of Nature journal: Scientific Data
2013 Thomas Kuhn Paradigm Shift Award, ACS, USA

Relevant publications and/or products and/or services

1. "Fast and accurate modeling of molecular atomization energies with machine learning", M. Rupp, A. Tkatchenko, K.-R. Mueller, O. A. von Lilienfeld, Phys. Rev. Lett. 108 058301 (2012)
2. "Boosting quantum machine learning models with multi-level combination technique: Pople diagrams revisited" P. Zaspel, B. Huang, H. Harbrecht, O. A. von Lilienfeld, J. Chem. Theory Comput. 15 3,1546 (2019)
3. "Alchemical and structural distribution based representation for improved QML", F. A. Faber, A. S. Christensen, B. Huang, O. A. von Lilienfeld, J Chem Phys 148 241717 (2018),
4. "Quantum chemistry structures and properties of 134 kilo molecules", R. Ramakrishnan, P. O. Dral, M. Rupp, O. A. von Lilienfeld, Scientific Data 1 140022 (2014).
5. "Quantum machine learning in chemical compound space", O. A. von Lilienfeld, Angew. Chem. Int. Ed. 57 4164 (2017).

Relevant previous project of activities connected to subject of proposal

1. 2018-2023 2 M€ PI on ERC Consolidator QML: "Quantum Machine Learning: Chemical Reactions with Unprecedented Speed and Accuracy". This project deals with the development of advanced machine learning models of reaction energy profiles applicable throughout chemical compound space.
2. 2017-2021 0.6M CHF PI on project funded by Swiss National Science Foundation: "Sampling chemical space with alchemical perturbation theory". This project deals with the development of perturbation theory based methods applicable to the prediction of properties throughout chemical compound space.
3. 2014-2018 0.8M CHF co-PI in project funded by NCCR MARVEL, Swiss National Science Foundation: "Computational Design and Discovery of Materials". This project dealt with the development of advanced machine learning models for the computational design of materials.
4. 2013-2016 1.5M CHF Foerderprofessor grant: "From atomistic exploration of chemical compound space towards bio-molecular design". This project dealt with the development of perturbation theory and machine learning based models for the accelerated exploration of chemical compound space.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

The lab is the main developer of the open source QML code in which all of the most recent quantum machine learning methods have been implemented: https://github.com/qmlcode/qml

In terms of hardware, the PI's lab has access to considerable CPU resources at University of Basel in order to support and augment necessary training and reference calculations for this project. More specifically, sciCORE (https://scicore.unibas.ch/) the university's center for scientific computing hosts and maintains a small cluster with currently 300 modern compute nodes (nearly 8000 cores, incl. 64 GPUs, 50 TB of Ram, and Infiniband). The PI's lab, being the dominant user at UB, consumes on average more than 30% of sciCORE's yearly CPU time. The PI's lab also maintains its own compute cluster (ALCHEMY) located in a rack in an air-conditioned room in the basement of its building. Apart from a large server with back-up, ALCHEMY consists of more than 40 nodes without fast switch (typically each node corresponds to 2 Intel Xeon E5-2680v3 12-core-processors (2.5 GHz) with 128 GB Ram, or similar) with more than 1000 cores. Multiple powerful workstations (with up to 48 cores or up to 2 TB memory) are also available in the group's offices. The PI's yearly budget for hardware upgrades and new acquisitions averaged at 50'000 Euro since his lab was established in 2013. A R'Equip proposal to the tune of 600'000 CHF for purchasing and adding a substantially larger cluster at 600'000 CHF in 2020 was submitted to the Swiss National Science Foundation in summer 2019.

4.1.31 IT-UNIVERSITETET I KOBENHAVN (ITU)

IT UNIVERSITY OF CPH	**Name:** IT-UNIVERSITETET I KOBENHAVN (ITU)	**Partner no:** 31	**Country:** Denmark
	Type: UNI	**Number of R&D personnel:** 150 **Number of employees:** 351	**Turnover:** 40 M€

Interest in the project

One of the strands of research we are investigating in previous E.U. research projects (EVOBLISS) and startups (Flow Robotics A/S) is the synergy between robotics, artificial intelligence and lab automation. These topics are part of the core component of the proposed project and, hence, the proposed project will develop our capacity further in this area.

Previous experience vs. main tasks in the project

We will participate in the work package related to "Modular Synthesis Robotics" for lab automation. We have been conducting research in modular robotics the last twenty years with numerous publications. A highlight is the MIT Press book on "Self-Reconfigurable Robots" a type of modular robots. We have further developed lab automation in the EC Future and Emergent Technologies funded project EVOBLISS where we developed an open-source lab automation platform. Finally, we are currently engaged with a startup in lab automation building pipetting robots.

We will also participate in the work package related to "AI Accelerated Materials Discovery" . We have been active in artificial intelligence research for two decades with a large research output. However, again the EVOBLISS project is a key point of departure as we there you used artificial intelligence to optimize chemical composition of artificial chemical life systems, which from an A.I. perspective is close to the aim of this work package.

Description of legal entity and main tasks

The IT University of Copenhagen (ITU) is a nonprofit publicly funded university. ITU performs research across a wide range of ICT related topics including but not limited to technology in practice, computer games, interaction design, software engineering, and robotics. The faculty is internationally oriented, comprising internationally respected researchers and is therefore able to provide academic support at a high international level. ITU has a policy that women and men must be treated equally at all levels of the organization and despite the subject areas taught are typically male dominated the current student body consist of 29% women.

CV or description of profile of key staff

- **Professor Kasper Stoy (M)**, Ph.D. (Principal Investigator), is a robotics and embodied artificial intelligence researcher holding a full professor position in the Department of Computer Science at the IT University of Copenhagen, Denmark. Kasper is an internationally recognized researcher in modular robotics and multi-robot systems. He has published more than seventy papers in international conference proceedings or journals. He holds a M.Sc. degree in computer science and physics from the University of Aarhus, Denmark (1999) as well as a Ph.D. degree in computer system engineering from the University of Southern Denmark (2003) where he also worked as assistant professor (2003-2006) and associate professor (2006-2013).
- **Andres Faiña (M)** is an Assistant Professor and mechatronics researcher at the IT University of Copenhagen. He received a diploma in Mechanics and Electronic Engineering from the Universidade da Coruna, Spain, in 2007 and received a PhD from the same University in 2011. He joined the IT University of Copenhagen in 2014 as postdoctoral researcher and he got an Assistant professorship in 2017. He has developed more than seven robotics systems (modular, underwater, educational or liquid handling robots) and he is the inventor of 4 patents.

Relevant publications and/or products and/or services

1. F. Nejatimoharrami, A. Faina, K. Støy, "A Low-Cost Open-Source Cloud-based Liquid Handling Robotic Platform for Performing Remote Real-Time Collaborative Experiments", SLAS2018, San Diego, USA.
2. F. Nejatimoharrami, A. Faina, K. Stoy, "New Capabilities of EvoBot: A Modular, Open-Source Liquid-Handling Robot", SLAS TECHNOLOGY: Translating Life Sciences Innovation 22 (5), 500-506, 2017.
3. P. Theodosiou, A. Faina, F. Nejatimoharrami, K. Stoy, J. Greenman, C. Melhuish, I. Ieropoulos, "EvoBot: towards a robot-chemostat for culturing and maintaining microbial fuel cells (MFCs)", Conference on Biomimetic and Biohybrid Systems, pages 453-464, 2017
4. K Stoy, M Hanczyc, J Cejkova, A Faíña, F Nejatimoharrami, "Robotic automation to augment quality of artificial chemical life experiments", Proceedings of the Artificial Life Conference 2016, 13, 634-635
5. K Stoy, D Brandt, DJ Christensen, "Self-reconfigurable robots: an introduction", MIT Press, 2010.

Relevant previous project of activities connected to subject of proposal

1. Coordinator and PI for the IT University of Copenhagen for the FET funded project EVOBLISS where we are developing mechatronics for a reactive liquid handling robot. (2014-2018).
2. PI for IT University of Copenhagen for the FET funded project Flora-Robotica responsible for developing robotic hardware (2014-2019).
3. PI for University of Southern Denmark for the FET funded project Locomorph where our main responsibility was mechatronic development of a modular robot construction kit (2009-2013).
4. Project participant for University of Southern Denmark in the FET funded project HYDRA where we developed distributed control algorithms and the ATRON self-reconfigurable robot (2002-2006)
5. Co-founder of Universal Robots A/S producing a light, user-friendly robot arm. Universal Robots currently has 700 employees selling in more than 55 countries (2018)

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

The IT University has staffed workshops with rapid prototyping machines relevant for mechanical prototyping (laser-cutter, cnc machines, and ten 3D-printers) and electronics development facilities from which this project can benefit.

4.1.32 DASSAULT SYSTEMES DEUTSCHLAND GMBH (3DS)

	Name: DASSAULT SYSTEMES DEUTSCHLAND GMBH (3DS)	**Partner no:** 32	**Country:** France
	Type: IND	**Number of R&D personnel:** 6 600 **Number of employees:** 16 000	**Turnover:** 3.4 B€

Interest in the project

Dassault Systèmes (3DS) is building an integrated solution for modelling batteries across all relevant length and time scales. An important role in this process is the combination of virtual and real experiments with data driven methods. The plan of the Big-Map project is exactly aligned with the plan of 3DS for establishing this multiscale solution. The explicit interests:

1. Standards for the interfaces and data exchange between tools.
2. The scientific workflows for automated property calculations.
3. Access to the experimental data bases as reference and parameterization of the system level models.
4. Building an atomistic model of the SEI.
5. Improved potentials for Molecular Dynamics.
6. We are also interested in the machine learning methods and the combination of experimental and simulations data to derive the models.

Previous experience vs. main tasks in the project

3DS have experience and tools on the three levels of atomistic, continuum and system level simulations and in addition data management and data driven methods. These tools are industry proven by our customers ranging from material suppliers via cell manufacturers to car companies. Within the Big-Map project 3DS plan to give contributions to the following Competence pillars and cross-cutting activities:

WP2 Accelerated atomistic simulations

WP 9 Infrastructure and Interoperability

WP 11 Battery Interface Genome

Description of legal entity and main tasks

Dassaults Systèmes Deutschland GmbH is the German, whole owned subsidiary of Dassaults Systèmes SE (3DS), with the head quarter in Stuttgart, Germany, where the project will be performed. The head quarter of the parent company Dassault Systèmes SE is located in Paris, France. 3DS, the 3DEXPERIENCE Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes' collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 220, 000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit www.3ds.com.

The BIOVIA R&D within 3DS develops scientific software solutions for the 3DEXPERIENCE Platform.

CV or description of profile of key staff

- **Dr. Johan M. Carlsson** (M) Senior Solution Scientist and Fellow of the BIOVIA Science Council, received his PhD in Physics from the University of Gothenburg in Sweden. He subsequently headed the Nanoporous Carbon group at the Theory Department of Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin for six years. In 2008, Dr. Carlsson joined the Contract Research group at the BIOVIA brand of DASSAULT SYSTEMES (3DS) and moved to the presales group in 2011, which is part of the BIOVIA Center of Excellence. In his role as Senior Solution Scientist, he helps customers to solve their scientific problems virtually by modelling and simulation techniques and practically by lab informatics using the BIOVIA and the greater 3DS Software Solution portfolio. As Fellow of the BIOVIA Science Council he is giving scientific guidance to the BIOVIA Brand and he is also part of the core team coordinating the multiscale battery simulations initiative at 3DS.
- **Dr. Felix Hanke** (M) completed his doctorate in statistical mechanics at Dalhousie University (Halifax, Canada), which was followed by postdoctoral research at the Fritz-Haber-Institute (Berlin, Germany) working on DFT method and code development and application research into carbon materials. A second postdoc at the University of Liverpool (UK) focused on surface science applications of DFT, particularly molecular assemblies and molecular switches. In 2012, Felix joined Accelrys (acquired by 3DS in 2014) where he has worked on DFT codes and on multiscale applications, most recently by leading the atomistic development of the 3DS battery solution

Relevant publications and/or products and/or services

1. F. Hanke et al., Multi-Scale Electrolyte Transport Simulations for Lithium Ion Batteries, Journal of The Electrochemical Society, 167 013522 (2020).
2. In addition, our software packages have been used by our customers in over 200 articles related to batteries. Three examples are:
3. LG Chemicals is electrolyte supplier: Han et al., J. Power Sources 187, 581 (2009).
4. Samsung is one of the top suppliers of battery cells: Lee and Park, J. Phys. Chem. C 116, 25190 (2012).
5. Toyota is a major car manufacturer: Ikuhara et al., J. Mater. Chem. A 5, 9329 (2017).

Relevant previous project of activities connected to subject of proposal

Battery modelling is a major topic across the relevant DS brands. We were part of an application for the LC-BAT-6-2019 EU-funding call, but our application was unfortunately not granted. So to date, our software tools have been exclusively developed in-house.

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

3DS provides the 3DEXPERIENCE Platform for data exchange, analysis and machine learning, collaboration and simulations tools on the three levels of atomistic, continuums level and system simulations.

4.1.33 FORSCHUNGSZENTRUM JULICH GMBH (FZJ)

	Name: FORSCHUNGSZENTRUM JULICH GMBH (FZJ)	**Partner no:** 33	**Country:** Germany
	Type: RTO	**Number of R&D personnel:** 2 296 **Number of employees:** 6 115	**Turnover:** 705 M€

Interest in the project

Research on electrolytes and their interfaces and interphases in battery cells, central to the scope of the BIG-MAP, has a well-established and long-lasting tradition in the experimental and theoretical work at FZJ/HI MS. More specifically, the build-up of a fully operational high-throughput screening (HTS) facility as well as the recent development of machine learning based algorithms for the formulation of accurate atomistic models contributes very well to the main goals of BIG-MAP.

Previous experience vs. main tasks in the project

The effectiveness for systematic screening of multicomponent liquid electrolyte formulations via the HTS system, including the appropriate data handling via the custom-developed laboratory information management system (LIMS), has been already demonstrated. From the theory side, a broad range of ab initio and atomistic modeling projects in corporation with the experiment have proven the efficiency of the interplay between both approaches for the development of advanced electrolyte formulations for targeted applications in different cell chemistries. Specific emphasis is set on building the machine learning (ML)-based force fields to study chemical systems at ab initio accuracies, so far used for the modelling of amorphous and simple liquids. Within the BIG-MAP project, we plan to build ML-based models for electrolytes and their interfaces which, among others, could be directly used for preselection of lead electrolyte candidates for given cell chemistries and would enable the bridging of ab initio and atomistic scales. Furthermore, ML-based methods shall be implemented for advanced interpretation of the large data pools, resulting from HTS experiments.

Description of legal entity and main tasks

Helmholtz Institute Münster (HI MS, IEK-12) is part of the Institute of Energy and Climate Research (IEK) of the Forschungszentrum Jülich (FZJ) with branch divisions in Aachen, Jülich and Münster. The major research areas of HI MS comprise battery cell using liquid, polymer, solid (anionic and cationic) electrolytes and hybrid electrolytes, thereby enabling new cell chemistries as well as new cell designs, developed in a systemic and holistic manner, covering not only synthesis and processing of advanced materials but also electrochemical processes occurring at electrolyte/electrode interfaces. The expertise and infrastructure of HI MS embrace a wide spectrum of the theory, chemistry, and technology of electrolytes and batteries in the whole field, ranging from basic research to application as well as technology transfer, hence facilitating a comprehensive gain in knowledge through interdisciplinary scientific cooperation from combined R&D activities along the battery value chain.

CV or description of profile of key staff

- **Prof. Prof. h.c. mult. Dr. Martin Winter (M)** is Director of the Helmholtz-Institute Muenster (FZJ-IEK 12) and MEET Battery Research Center of WWU Münster, Member of the National Academy of Science and Engineering, Member of the National Platform E-Mobility (NPE9), Chairman of the Advisory Board of German Battery Research by the Federal Ministry of Education and Research (BMBF), President of the International Meeting on Lithium Batteries (IMLB), Chairman of the International Battery Materials Association (IBA). He received more than 50 awards and recognitions, among them: Fellow of the International Society of Electrochemistry (ISE) and of the Electrochemical Society (ECS) and German Federal Cross of Merit-1st Class. He has been involved in the field of energy electrochemical energy storage and conversion for almost 30 years, with a focus on materials, components and cell design for Li-ion batteries and Li metal batteries, >600 articles, h=82 (Google), 'Highly cited researcher' 2008-2017 (Web of Science). Martin Winter holds a professorship for "Materials Science, Energy and Electrochemistry" at the Institute of Physical Chemistry at the University of Münster.

- **Dr. Isidora Cekic-Laskovic (F)** obtained her PhD in Physical Organic Chemistry at the Faculty of Physical Chemistry, University of Belgrade. In June 2012, she became a research scientist at MEET Battery Research Center and took over the leading responsibility of the research group Electrolyte. In the framework of the Electrolyte Lab project (German Federal Ministry of Education and Research – BMBF, 01.07.2013-31.12.2017), under her responsibility, a high throughput screening system was designed, developed and brought into operation. Since September 2016 she is a research group leader (Electrolyte & Interfaces) at the FZJ. The main scope of research is related to development of advanced functional electrolytes for lithium-based battery application from synthesis of novel electrolyte components all the way to interfacial electrochemistry and processes.

- **Dr. Diddo Diddens (M)** obtained his PhD in chemistry from the University of Münster in 2012. He has more than ten years of experience with various molecular simulation techniques such as Molecular Dynamics and Monte Carlo simulations, as well as quantum chemistry (more than 20 journal publications). After a postdoctoral stay at CNRS Institut Charles Sadron for polymer research in Strasbourg he moved to FZJ in August 2016. His research mainly focuses on two areas: i). Theoretical understanding of polymer and ion dynamics in various materials, and ii) modelling of electrochemical reaction and diffusion processes at interfaces.

Relevant publications and/or products and/or services

1. N. von Aspern, G.V. Röschenthaler, M. Winter, I. Cekic-Laskovic, *Fluorine and Lithium: Ideal Partners for High Performance Rechargeable Battery Electrolytes*, Angewandte Chemie, International Edition 58 (45) 2019 15978-16000
2. G. Bieker, D. Diddens, M. Kolek, O. Borodin, M. Winter, P. Bieker, K. Jalkanen, *The Cation-Dependent Electrochemistry of Polysulfides in Lithium and Magnesium Electrolyte Solutions*, Journal of Physical Chemistry C 2018, 122(38), 21770-21783
3. A. N. Kirshnamoorthy, K. Oldiges, M. Winter, A. Heuer, I. Cekic-Laskovic, C. Holm, J. Smiatek, Electrolyte solvents for high voltage lithium ion batteries: ion correlation and specific anion effects in adiponitrile, Physical Chemistry, Chemical Physics, 2018, 20, 25701-25715
4. N. von Aspern, D. Diddens, T. Kobayashi, M. Börner, O. Stubbmann-Kazakova, V. Kozel, G.-V. Röschenthaler, J. Smiatek, M. Winter, I. Cekic-Laskovic, *Fluorinated Cyclic Phosphorus(III)-based Electrolyte Additives for High Voltage Application in Lithium Ion Batteries: Impact of Structure-Reactivity Relationships on CEI Formation and Cell Performance*, ACS Applied Materials & Interfaces, 11 **2019** 16605-16618
5. K. Oldiges, D. Diddens, M. Ebrahiminia, J.B. Hooper, I. Cekic-Laskovic, A. Heuer, D. Bedrov, M. Winter, G. Brunklaus, *Understanding transport mechanisms in ionic liquid/carbonate solvent electrolyte blends*, Physical Chemistry, Chemical Physics 20(24) 2018 16579-16591

Relevant previous project of activities connected to subject of proposal

1. **SPIDER** (H2020-NMPB-ST-IND-2018-2020; partner), Topic: safe and prelithiated high energy density batteries based on sulpur rock salt and silicon chemistries
2. **LILLINT** (German Federal Ministry of Education and Research (BMBF); partner), Topic: interfaces and interphases in rechargeable Li metal-based batteries - thermodynamic and kinetic study of the lithium-liquid electrolyte
3. **ZeDaBase-Batteriezelldatenbank** (BASF-Helmholtz Cooperation, coordinator); Topic: detailed database creation for commercially available and prototype battery cells as a basis for the development of new materials and cell types
4. **GrEEN** (Ministry of Economy, Innovation, Digitization and Energy of North Rhine-Westphalia; partner); Topic: development of green electrochemical energy storage systems – tailored synthesis and comprehensive characterization of biogenic electrolytes and electrolyte components
5. **SeNSE** (H2020-LC_BAT_2019-2020/H2020-LC-BAT-2019, grant agreement number: 875548; partner) Topic: lithium-ion battery with silicon anode, nickel-rich cathode and in-cell sensor for electric vehicles

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Automated high throughput screening (HTS) approach for the effective optimization in liquid electrolyte formulation, enabling preselection of lead electrolyte candidates for targeted cell chemistry application comprising: fully automated formulation of up to 100 different liquid electrolytes per day; fully automated assembly of up to 100 cells per day with different chemistries in a two and three setup; Selected physicochemical and electrochemical measurements comprising linear sweep voltammetry and cyclic voltammetry, electrochemical impedance spectroscopy as well as constant current cycling tests serve as filtration effect (simultaneous measurements of 96 cells) and data storage and processing *via* laboratory information management system (LIMS) and additional, in house developed software. Additionally, all other standard equipment for tailored synthesis of electrolyte components (hoods, rotary evaporators etc.) and comprehensive physicochemical, electrochemical, analytical as well as structural characterization on electrolyte and cell level.

Three large High-Performance Computer (HPC) clusters are directly accessible to the FZJ/HI MS. (1) Supercomputer Cluster Jülich (in particular JUWELS, presently ranked number 30 in the worldwide TOP 500 computer list). (2) HPC cluster of the WWU, also accessible to FZJ/HI MS (also on the TOP 500 list after installation in 2018). (3) HPC cluster of the simulation group at FZJ/HI MS with more than 100 nodes.

4.1.34 SAFT (SAFT)

	Name: SAFT (SAFT)	**Partner no: 34**	**Country: France**
	Type: IND	**Number of R&D personnel: 50** **Number of employees: 4500**	**Turnover: €788 m**

Interest in the project

Saft (SAFT) is participating in this project in order to be a stakeholder of the development of European battery skills, especially in terms of standardization, modelling activity and fast development of advanced components. The database and all modelling tools developed in the frame of this project will be highly useful for Saft understanding of interfaces composition and ageing and fast development of advanced solutions for high performance batteries with significantly improved performances and life duration.

Previous experience vs. main tasks in the project

Saft will be part of WP5 and WP6. Saft will participate to the definition of a standardized methodology for materials and battery characterization. Saft will assemble cells with configurations close to commercial ones (cylindrical cells or pouch cells), make electrochemical tests, and open the cells after ageing for sample preparation to be delivered for analysis of degradation products. As battery manufacturer, Saft has all the know-how and long-term experience to carry out this task.

In addition, Saft will participate as industrial board member to WP2 and WP3.

Description of legal entity and main tasks

For nearly 100 years, Saft produces longer-lasting batteries and systems which have provided critical safety applications, back-up power and propulsion for our customers. Saft innovative, safe and reliable technology delivers high performance in space, at sea, in the air and on land. Saft is a fully owned subsidiary of Total. With 788 M€ of sales in 2018 and more than 3000 customers, Saft employs 4300 people from 49 countries. Saft invests 9.7% of its turnover in R&D and has some of the brightest minds working on developing and producing batteries; around 1.5 percent of Saft employees have PhDs.

Saft research and developments teams have developed new lithium-ion electrochemistries since beginning of 90's. Saft research department employs 50 people working on development of new materials, electrochemical concepts, electrode and cell design, processes for electrode preparation, modelling and battery management system.

Saft Research department will contribute to the realization of tasks in WP5 and WP6 and to the participation at industrial board meeting in WP2 and WP3. Research department is fully equipped for the assembly of prototype cells.

CV or description of profile of key staff

- **Cécile Tessier** (F)
  - Holds a diploma of the Graduate School of Chemistry of Strasbourg and a PhD in Solid State Chemistry and Materials Science from University of Bordeaux (with Dr. Claude Delmas).
  - In Saft since 2000, first as Research scientist on alkaline batteries, then on Li-ion batteries. Li-ion Research Group Manager at Saft since 2008. Skills in chemistry and electrochemistry covering all the components of Li-ion cells: active materials, electrolyte and separator and also electrodes formulation and process/process modelling
  - Cells assembly/testing and post-mortem analysis is a day to day activity at Saft and constituted the contribution of Saft in many different projects.

- **Lucille Gal** (F)

Research scientist at SAFT since 2010, main topics: Cathode materials for Li-ion batteries and ageing phenomena

Diplomas:

- 2007-2010: PhD in material science, topic: Nickel metal hydrides synthesis and characterization, PARIS EST UNIVERSITY, PARIS, FRANCE
- 2004-2007: Engineer diploma (specialty materials) ENSCBP, BORDEAUX, FRANCE
- 2007: Research Master, BORDEAUX UNIVERSITY, BORDEAUX, FRANCE

- **Julien Demeaux** (M)

- PhD in Materials Chemistry (2013), MSc. In Materials Chemistry (2010), BSc. In Chemistry (2008) at the University of Tours, France
- Electrolyte Research Scientist (2016 to present): Electrolyte development for SAFT's lithium-ion cell chemistries
- Electrolyte Scientist, 24M Technologies, Boston, MA, USA (2016)
- Postodoctoral Research Fellow, The University of Rhode Island, Kingston, RI, USA (2013-2016)
- PhD Candidate, French Alternative Energies and Atomic Energy Commission (CEA), Le Ripault, France (2010-2013)

- Probing the in-depth distribution of organic/inorganic molecular species within the SEI of LTO/NCM and LTO/LMO batteries: a complementary ToF-SIMS and XPS study, Applied Surface Science (2020)
- The impact of CO2 evolved from VC and FEC during formation of graphite anodes in lithium-ion batteries, Journal of the Electrochemical Society (2019)
- Development of novel lithium borate additives for designed surface modification of high voltage LNMO cathodes, Energy and Environmental Science (2016)
- Nonaqueous electrolytes for lithium-ion batteries comprising asymmetric borates, EU WO2017102550 A1
- Pyridine sulfur trioxide complexes as electrolyte component for high voltage batteries, US20190326642 A1

Relevant publications and/or products and/or services

1. Probing the in-depth distribution of organic/inorganic molecular species within the SEI of LTO/NMC and LTO/LMO batteries: A complementary ToF-SIMS and XPS study, N. Gauthier, C. Courrèges, J. Demeaux, C. Tessier, H. Martinez, *Applied Surface Science* **2020**, *501,* 144266
2. Lithium-Ion Batteries Working at 85°C: Aging Phenomena and Electrode/Electrolyte Interfaces Studied by XPS, L. Bodenes, R. Dedryvère, H. Martinez, F. Fischer, C. Tessier, J.-P. Pérès, *Journal of The Electrochemical Society* **2012,** *159* (10), A1739-A1746
3. Aging Mechanisms of LiFePO4 // Graphite Cells Studied by XPS: Redox Reaction and Electrode/Electrolyte Interfaces, L. Castro, R. Dedryvère, J.-B. Ledeuil, J.-B, J. Bréger, C. Tessier, D. Gonbeau, *Journal of The Electrochemical Society* **2012,** *159* (4), A357-A363
4. Lithium secondary batteries working at very high temperature: Capacity fade and understanding of aging mechanisms, L. Bodenes, R. Naturel, H. Martinez, R. Dedryvère, M. Menetrier, L. Croguennec, J.-P., C. Tessier, F. Fischer, *Journal of Power Sources* **2013**, *236,* 265-275
5. HRSTEM and EELS study of NMC aging mechanisms for renewable energy application, C. Davoisne, M. Ben Hassine, C. Tessier, G. Drazic,, L. Dupont, *European Microscopy Congress* **2016**: Proceedings

Relevant previous project of activities connected to subject of proposal

No participation in projects with modelling at atomic scale

Description of any significant infrastructure and/or any major items of technical equipment relevant to the proposed work

Saft research centre located in Bordeaux is well equipped to characterize material (XRD, SAXS, SEM, Ar beam cross polisher, XRF, ICP, DLS, Laser particle size distribution measurement , BET, DSC, TGA, contact angle measurement, GC-MS, rheometer, low and high current potentiostat -galvanostat, impedance spectroscopy, climatic chambers (low & high temperature), ..). The R&T department is also equipped with various mixers, calendering machine, welding and laser cutting machines, equipment to manufacture many sizes of cells (coin, 18650 and pouch cells). The process which requires any moisture traces are done in a large dry room.

4.2 Third parties involved in the project (including use of third party resources)

4.2.1 DANMARKS TEKNISKE UNIVERSITET (DTU)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	Y
Third Party (TP) funding of 350k€ for Stakeholder Initiated Initiatives (SII) will be supported by the coordinator DTU, in order to engage non-BIG-MAP partners in the project activities as discussed under Section 2.3.1.2.	

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.2 UPPSALA UNIVERSITET (UU)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.3 KARLSRUHER INSTITUT FUER TECHNOLOGIE (KIT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.4 CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	**Y**
Universite De Picardie Jules Verne (UPJV) will act as linked third parties (LTP) for CNRS and be responsible for performing the multiscale modelling activities in WP3. A total personnel cost of 35.000€ has been allocated to UPJV from the CNRS budget.	

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.5 WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER (WWU)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.6 COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES (CEA)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.7 KEMIJSKI INSTITUT (NIC)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.8 SINTEF AS (SINTEF)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.9 POLITECNICO DI TORINO (PDT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.10 FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V. (FRAUNHOFER)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.11 CHALMERS TEKNISKA HOEGSKOLA AB (CTH)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.12 POLITECHNIKA WARSZAWSKA (WUT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.13 AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS (CSIC)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.14 TECHNISCHE UNIVERSITEIT DELFT (TUD)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.15 CONSIGLIO NAZIONALE DELLE RICERCHE (CNR)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.16 ECOLE ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.17 THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE (UCAM)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.18 THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD (OXFORD)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.19 TARTU ULIKOOL (UT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.20 THE UNIVERSITY OF LIVERPOOL (ULIV)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.21 EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.22 INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.23 SYNCHROTRON SOLEIL SOCIETE CIVILE (SOLEIL)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.24 FUNDACION CIDETEC (CID)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.25 ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL (EMIRI)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.26 UMICORE (UMI)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.27 SOLVAY SA (SOLB)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.28 BASF SE (BASF)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.29 NORTHVOLT AB (NVOLT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.30 UNIVERSITAT BASEL (UBAS)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.31 IT-UNIVERSITETET I KOBENHAVN (ITU)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.32 DASSAULT SYSTEMES DEUTSCHLAND GMBH (3DS)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.33 FORSCHUNGSZENTRUM JULICH GMBH (FZJ)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

4.2.34 SAFT (SAFT)

Third parties involved in the project (including use of third party resources)

Does the participant plan to subcontract certain tasks (please note that core tasks of the project should not be sub-contracted)	N

Does the participant envisage that part of its work is performed by linked third parties	N

Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N

5 Ethics and Security

5.1 Ethics

BIG-MAP has no ethical issue.

5.2 Security

BIG-MAP will not involve:

- Activities or results rising security issues
- 'EU classified information' as background or results

6 Letters of Intent

6.1.1 DIFFER

DIFFER
Dutch Institute for
Fundamental Energy Research
De Zaale 20, 5612 AJ, Eindhoven NL
PO Box 6336, 5600 HH, Eindhoven NL
T +31 (0)40 3334 999 | www.differ.nl

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+

Date: January 3rd, 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of **DIFFER**, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. DIFFER have special competences in developing and using multi-scale high-throughput computational screening and artificial intelligence methods to accelerate the accurate prediction of candidate functional materials for energy conversion and storage. Our long-term vision is to develop a fully autonomous, active-learning based energy materials design methodology to open a new path in energy materials discovery.

As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Dr. Süleyman Er
Research Group Leader
Autonomous Energy Materials Discovery [AMD]
DIFFER – Dutch Institute for Fundamental Energy Research
De Zaale 20, 5612 AJ, Eindhoven, the Netherlands
Tel: +31 40 3334936 | Email: s.er@differ.nl
https://www.differ.nl/research/amd | https://www.amdlab.nl

IBAN: NL78 ABNA 06 42 38 35 96 | BIC: ABNA NL 2A
CoC: 411 500 68 | VAT: NL 002 88 2243 B01

DIFFER is part of the Netherlands Organisation for Scientific Research (NWO)

6.1.2 European Spallation Source

EUROPEAN SPALLATION SOURCE

18th December, 2019

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Letter of Intent - Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of the European Spallation Source ERIC (ESS), we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. ESS will be the world's brightest neutron source beginning operation 2022. Neutron scattering and imaging is already and will continue to provide key information for the advancement of battery technologies. The Data Management and Software Center (DMSC) of ESS is our competence center for scientific computing and software. As a BIG-MAP Priority Stakeholder, ESS via its DMSC:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP resources to assist in developing Apps for the BIG-MAP App Store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

John Womersley
Director General

European Spallation Source ERIC
Visiting address: ESS, Odarslövsvägen 113
P.O. Box 176
SE-221 00 Lund
SWEDEN
www.esss.se

6.1.3 CIC energiGUNE

DTU Energy

DTU

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Vitoria-Gasteiz (Spain), 17th December, 2019

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of CIC energiGUNE, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. CIC Energigune has special competences in: (i) Computational data generation to feed models/modules (e.g. DFT-level calculations of crystalline solid electrodes and electrolytes, FF-based molecular dynamics simulations of ionic transport on solid ionic conductors and solid-polymer interfaces, and coarse-grain-level calculations for quick screening of large existing); (ii) Experimental validation and high-throughput data analysis of operando experiments (e.g. Synchrotron XRD, XAS, etc.); and (iii) Data sharing related to bulk and interface characterization, contributing to novel standardized data streams generated in BIG-MAP (e.g. developing fingerprint catalogues of electrode materials and interfaces).

As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.

Technical University of Denmark
DTU Energy
Fysikvej, Building 309
DK-2800 Kgs. Lyngby
Denmark
Tel +45 45 25 25 25
Dir. +45 54 64 17 87
teve@dtu.dk
www.ecs.dtu.dk

DTU

- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We a please to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

CIC energi GUNE energy cooperative research centre C.I.F. G01241876

Dr. Raquel Ferret
Technology Coordinator of the Electrochemical Energy Storage Area
Business Development Manager

6.1.4 ICAMCyl

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

17th December, 2019

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of **ICAMCyL**, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. ICAMCyL has special competences in Materials Discovery and Multiscale Modelling, with special interest in the development of advanced materials for energy. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We a please to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Santiago Cuesta-Lopez

Fundación ICAMCyL Parque Tecnológico de León
Edificio de Usos Múltiples
C/ Julia Morros s/n Primera Planta,
Oficinas 106-108
24009 Armunia (León)
España
Tel +34 987 440 481 director.general@icamcyl.com

6.1.5 IFP Energies Nouvelles

Gaëtan Monnier
Director
Institut Carnot Transports Energie
Transport Business Unit
gaetan.monnier@ifpen.fr

To whom it may concern:

Prof. Tejs Vegge

DTU Energy
Technical University of Denmark

Fysikvej, Building 309
2800 Kgs Lyngby
Denmark

Rueil-Malmaison, le 19/12/2019

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our interest and support for your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of IFP Energies nouvelles, we would welcome the proposal being accepted by the European Commission since we believe that its goals align with our mission, and we express our interest in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder, and then support and build together future initiatives in the framework of the European Research. IFP Energies nouvelles has special competences in new methodology of modelling and digital characterization.

As a BIG-MAP Priority Stakeholders, we agree to:

- Participate in BIG-MAP training events and workshops.
- Obtain early access to select software packages and models developed in BIG-MAP.
- Apply for BIG-MAP resources to support the project when considered in close interaction with IFPEN internal development in batteries.
- Follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

Sincerely

Gaëtan Monnier
Director

IFP Energies nouvelles
EPIC – RCS 775 729 155 Nanterre – APE : 7219Z
1 et 4 avenue de Bois-Préau - 92852 Rueil-Malmaison Cedex - France
Tél. +33 1 47 52 60 00 – Fax. +33 1 47 52 70 00

www.ifpenergiesnouvelles.fr

6.1.6 Virtual Vehicule Research GmbH

DTU Energy

DTU

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

18th December, 2019

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of Virtual Vehicle Research GmbH (Virtual Vehicle), we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. Virtual Vehicle has special competences in design and execution of battery cell ageing experiments. Furthermore, Virtual Vehicle has developed a multi-level cell model and successfully validated a high-performance computing software package implementing this model. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

virtual vehicle

VIRTUAL VEHICLE Research GmbH
Inffeldgasse 21a ■ 8010 Graz
www.v2c2.at

Aldo Ofenheimer, ppa
Head of Organisation & Business Development

Dr. Gerhard Zrim, ppa
Head of Finance & Reporting

Technical University of Denmark
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Tel +45 45 25 25 25
Dir. +45 54 64 17 87
teve@dtu.dk
www.ecs.dtu.dk

6.1.7 ENEA

AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE,
L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE

Dipartimento Tecnologie Energetiche
Divisione DTE-ICT

Roma, 2 January 2020

To: Prof. Tejs Vegge
Battery Interface Genome – Materials
Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,
I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.
On behalf of DTE-ICT Division of ENEA, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. DTE-ICT Division has special competences in High Performance Computing (including materials modeling, data management and workflows) and is actively involved in the EoCoE Centre of Excellence (The Energy oriented Centre of Excellence). Moreover our institution ENEA has experimental laboratories fully covering the production line of innovative batteries, from materials design to the final testing and benchmark. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops;
- Can obtain early access to select software packages and models developed in BIG-MAP;
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software;
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis;
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Silvio Migliori
DTE-ICT Division Head

DTE-ICT Division
Centro Ricerche Casaccia
Via Anguillarese 301
00123 Santa Maria di Galeria (Roma)
Tel. +39-06-3627-2232
silvio.migliori@enea.it
Sede Legale - Lungotevere Thaon di Revel, 76 - 00196 Roma - Italia – Tel. +39-06-36271
Partita IVA 00985801000 - Codice Fiscale 01320740580 - www.enea.it

6.1.8 PAUL SCHERRER INSTITUTE

PAUL SCHERRER INSTITUT

Paul Scherrer Institut
5232 Villigen PSI
Switzerland

+41 56 310 21 11
www.psi.ch

Markus Strobl
Laboratory for Neutron Scattering and Imaging
WBBA/118
direct +41 76 223 8859
markus.strobl@psi.ch

Sigita Trabesinger
Laboratory of Electrochemistry
OFLB/U112
direct: +41 56 310 5775
sigita.trabesinger@psi.ch

Villigen PSI, 18 Dec. 2019

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Letter of Intent — Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

We are writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: *"Novel methodologies for autonomous discovery of advanced battery chemistries"*. Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries. On behalf of PSI, in particular the Laboratory for Neutron Scattering and Imaging — LNS, represented by Markus Strobl, and the Laboratory of Electrochemistry — LEC, represented by Sigita Trabesinger, we declare interest in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. PSI's relevant competences lie in battery materials synthesis, advanced electrochemical and ex-situ and operando battery materials characterization, utilizing the synergies of lab-scale investigations with our large-scale research infrastructure. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our

PAUL SCHERRER INSTITUT

Paul Scherrer Institut
5232 Villigen PSI
Switzerland

+41 56 310 21 11
www.psi.ch

Villigen PSI, 18 December 2019
page 2/2

experimental/computational software.

- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s)

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Yours sincerely,

Prof. Dr. Markus Strobl
Head of Neutron Imaging and Applied Materials Group
Paul Scherrer Institut

Dr. Sigita Trabesinger
Head of Battery Electrodes and Cells Group
Paul Scherrer Institut

6.1.9 HALDOR TOPSOE

HALDOR TOPSØE

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Haldor Topsoe A/S
Nymøllevej 55
2800 Kgs. Lyngby
Denmark

CVR nr. 41853816

Tlf +45 4527 2000
Fax +45 4527 2999
www.topsoe.com

January 8, 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of Haldor Topsoe A/S, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. Haldor Topsoe A/S has special experience in high voltage Li-ion cathode materials and low cost Na-ion cathode materials. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We a please to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Søren Dahl

Søren Dahl
R&D director Advanced Materials R&D
Haldor Topsoe A/S
sda@topsoe.dk, +45 4139 0316

6.1.10 SCM

SCM
Software for Chemistry & Materials

Software for Chemistry & Materials B.V.
De Boelelaan 1083
1081 HV Amsterdam
The Netherlands

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

13th January, 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of Software for Chemistry & Materials B.V. (SCM), we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. SCM is a scientific software company specializing in chemistry and materials modeling on the atomistic scale, with additional focus on machine learning and high-throughput workflows and software. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP resources to help develop interfaces between the BIG-MAP data infrastructure and our computational software.
- Have the opportunity to apply for BIG-MAP resources to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Dr. S.J.A. van Gisbergen
CEO of SCM

Software for Chemistry & Materials B.V .• +31 20 598 7625 • sales@scm.com • www.scm.com
VAT no. NL 8072 70 143 B01 • Chamber of Commerce no. 3330 1537

6.1.11 VTT

VTT

14th of January, 2020 1 (1)

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: *"Novel methodologies for autonomous discovery of advanced battery chemistries".* Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of VTT, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. VTT has special competences in advanced multi-scale materials modelling from atomic scale to composite and layered structures. VTT's materials modelling framework, battery laboratories and materials processing and manufacture facilities can be directly linked to the BIG-MAP consortium activities. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We a please to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded. VTT's point of contact is: Dr. Mikko Pihlatie, mikko.pihlatie@vtt.fi

Best regards,

Jukka Lehtomäki
Manager, Operations support
Smart Industry and energy systems, Transport and mobility
VTT Technical Research Centre of Finland Ltd

VTT TECHNICAL RESEARCH CENTRE OF FINLAND LTD
Vuorimiehentie 3, Espoo
P.O.Box 1000, FI-02044 VTT, FINLAND
Tel. +358 20 722 111
Fax +358 20 722 7000
name.surname@vtt.fi
www.vtt.fi
Business ID 2647375-4

6.1.12 Volvo Cars

DTU Energy

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

15th January, 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of Volvo Cars, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. Volvo Cars have special competences in the automotive industry, with electrified vehicles in serial production since 2013. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Hanna Bryngelsson

Technical University of Denmark
DTU Energy
Fysikvej, Building 309
DK-2800 Kgs. Lyngby
Denmark
Tel +45 45 25 25 25
Dir. +45 54 64 17 87
teve@dtu.dk
www.ecs.dtu.dk

6.1.13 Lithium Balance

DTU Energy

DTU

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

10th January, 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries*". Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of Lithium Balance A/S, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. Lithium Balance have special competences in battery management systems electric and hybrid machines, vehicles and energy storage systems, and we specialize in lithium-ion and new battery chemistries. As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP recourses to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give you and your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Lars Barkler
CEO, Lithium Balance A/S

Technical University of Denmark
DTU Energy

Fysikvej, Building 309
DK 2800 Kgs. Lyngby
Denmark

Tel +45 45 25 25 25
Dir +45 54 64 17 87

ieve@dtu.dk
www.ecs.dtu.dk

6.1.14 ChemOS Inc

DTU Energy

DTU

To: Prof. Tejs Vegge
Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)
Battery 2030+
Re: LC-BAT-12-2020

February , 2020

Letter of Intent – Priority Stakeholder in BIG-MAP for LC-BAT-12-2020

Dear Prof. Tejs Vegge,

I am writing this letter to express our strong interest and support of your proposed research project "Battery Interface Genome – Materials Acceleration Platform (BIG-MAP)", to be submitted for the LC-BAT-12-2020 call: "*Novel methodologies for autonomous discovery of advanced battery chemistries"***.** Your proposal addresses one of the key challenges in enabling accelerated discovery and development of future, ultra-high performance, fully sustainable and smart batteries.

On behalf of ChemOS Sárl with Headquarters in Lausanne and its parent company ChemOS Inc. based in Silicon Valley, we are very interested in collaborating closely with the BIG-MAP consortium as a BIG-MAP Priority Stakeholder. ChemOS Sárl and our team have special competences and expertise in artificial intelligence, machine learning, chemistry, physics, high-performance computing and economics. Before co-founding ChemOS, I had the privilege to co-author and co-lead the Clean Energy Materials Innovation Challenge of Mission Innovation and to serve as Executive Chair, along with our Academic Co-Chairs, Profs. Alán Aspuru-Guzik and Kristin Persson, of the 4-day workshop that led to the publication of our report titled Materials Acceleration Platform.[1]

ChemOS is an early-stage AI/ML software startup; the Chemical Operating System for Industry 4.0. Our technology orchestrates Materials Acceleration Platforms (MAPs) or self-driving laboratories that accelerate innovation. The ChemOS software platform makes process optimization and materials discovery smarter, faster, and cheaper by fully integrating AI, machine learning, high-performance computing and robotics with the natural sciences. ChemOS can operate with limited data, with or without robots, or in computer simulations. Current applications include materials discovery for flow batteries, organic solar cells, optimization of various chemical reactions. These pilot projects demonstrate an acceleration of up to 34X compared to state-of-the-art methodologies, such as High-throughput Experimentation (HTE) and Design of Experiment (DoE).

As a BIG-MAP Priority Stakeholders, we:

- Will receive invitations to participate in BIG-MAP training events and workshops.
- Can obtain early access to select software packages and models developed in BIG-MAP.
- Have the opportunity to apply for BIG-MAP resources to help develop interfaces between the BIG-MAP data infrastructure and our experimental/computational software.
- Have the opportunity to apply for BIG-MAP recourses to assist in developing Apps for the BIG-MAP App store, e.g. specialized modules for automated data analysis.
- Will follow the BIG-MAP data standards and protocols for acquisition and reporting of data to the BIG-MAP database(s).

We are pleased to give your proposal our strongest support, and sincerely hope that the proposal will be funded.

Best regards,

Hermann Tribukait, PhD
ChemOS Inc.
Co-Founder & CEO, Menlo Park, CA
ChemOS Sárl
Lausanne, Switzerland
M: +1-650-248-3679
e: ht@chemos.io
@: www.chemosio

CHEM OS
Accelerate Innovation

[1] Link to the MAPs Report: http://mission-innovation.net/wp-content/uploads/2018/01/Mission-Innovation-IC6-Report-Materials-Acceleration-Platform-Jan-2018.pdf

REG-no. DK 30 06 09 46

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Dir. +45 54 64 17 87
teve@dtu.dk
www.ecs.dtu.dk

ESTIMATED BUDGET FOR THE ACTION

	Estimated eligible[1] costs (per budget category)										EU contribution			Additional information		
	A. Direct personnel costs				B. Direct costs of subcontracting	*[C. Direct costs of fin. support]*	D. Other direct costs		E. Indirect costs[2]	Total costs	Reimbursement rate %	Maximum EU contribution[3]	Maximum grant amount[4]	Information for indirect costs	Information for auditors	Other information:
	A.1 Employees (or equivalent) A.2 Natural persons under direct contract A.3 Seconded persons *[A.6 Personnel for providing access to research infrastructure]*	A.4 SME owners without salary A.5 Beneficiaries that are natural persons without salary					D.1 Travel D.2 Equipment D.3 Other goods and services *[D.4 Costs of large research infrastructure]*	D.5 Costs of internally invoiced goods and services						Estimated costs of in-kind contributions not used on premises	Declaration of costs under Point D.4	Estimated costs of beneficiaries/ linked third parties not receiving funding/ international partners
Form of costs[6]	Actual	Unit[7]	Unit[8]		Actual	Actual	Actual	Unit[9]	Flat-rate[10] 25%							
	a	Total b	No hours	Total c	d	*[e]*	f	Total g	h = 0,25 x (a +b+c+f+g +*[i1]*[13]+*[i2]*[13]-n)	j = a+b+c+d +*[e]*+f+g+h +*[i1]*+*[i2]*	k	l	m	n	Yes/No	
1. DTU	1 299 880.00	0.00	0.00	0.00	350 000.00	0.00	584 114.00	0.00	470 998.50	2 704 992.50	100.00	2 704 992.50	2 704 992.50	0.00	No	n/a
2. UU	672 411.00	0.00	0.00	0.00	0.00	0.00	63 000.00	0.00	183 852.75	919 263.75	100.00	919 263.75	919 263.75	0.00	No	n/a
3. KIT	934 665.00	0.00	0.00	0.00	0.00	0.00	165 335.00	0.00	275 000.00	1 375 000.00	100.00	1 375 000.00	1 375 000.00	0.00	No	n/a
4. CNRS	567 228.00	0.00	0.00	0.00	0.00	0.00	237 000.00	0.00	201 057.00	1 005 285.00	100.00	1 005 285.00	1 005 285.00	0.00	No	n/a
- UPJV	35 000.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8 750.00	43 750.00	100.00	43 750.00	43 750.00	0.00	No	n/a
Total beneficiary	602 228.00	0.00			0.00	0.00	237 000.00	0.00	209 807.00	1 049 035.00		1 049 035.00	1 049 035.00	n/a	n/a	0.00
5. WWU	219 600.00	0.00	0.00	0.00	0.00	0.00	20 000.00	0.00	59 900.00	299 500.00	100.00	299 500.00	299 500.00	0.00	No	n/a
6. CEA	0.00	526 146.00	0.00	0.00	0.00	0.00	116 340.00	0.00	160 621.50	803 107.50	100.00	803 107.50	803 107.50	0.00	Yes	n/a
7. NIC	267 600.00	0.00	0.00	0.00	0.00	0.00	52 000.00	0.00	79 900.00	399 500.00	100.00	399 500.00	399 500.00	0.00	No	n/a
8. SINTEF	472 500.00	0.00	0.00	0.00	0.00	0.00	27 500.00	0.00	125 000.00	625 000.00	100.00	625 000.00	625 000.00	0.00	No	n/a
9. PDT	142 320.00	0.00	0.00	0.00	0.00	0.00	25 700.00	0.00	42 005.00	210 025.00	100.00	210 025.00	210 025.00	0.00	No	n/a
10. Fraunhofer	0.00	366 995.00	0.00	0.00	0.00	0.00	73 000.00	0.00	109 998.75	549 993.75	100.00	549 993.75	549 993.75	0.00	No	n/a
11. CTH	402 800.00	0.00	0.00	0.00	0.00	0.00	37 100.00	0.00	109 975.00	549 875.00	100.00	549 875.00	549 875.00	0.00	No	n/a
12. WUT	102 000.00	0.00	0.00	0.00	0.00	0.00	204 000.00	0.00	76 500.00	382 500.00	100.00	382 500.00	382 500.00	0.00	No	n/a
13. CSIC	253 767.00	0.00	0.00	0.00	0.00	0.00	54 120.00	0.00	76 971.75	384 858.75	100.00	384 858.75	384 858.75	0.00	No	n/a
14. TUD	0.00	232 848.00	0.00	0.00	0.00	0.00	46 500.00	0.00	69 837.00	349 185.00	100.00	349 185.00	349 185.00	0.00	No	n/a
15. CNR	162 758.00	0.00	0.00	0.00	0.00	0.00	29 242.00	0.00	48 000.00	240 000.00	100.00	240 000.00	240 000.00	0.00	No	n/a
16. EPFL	540 000.00	0.00	0.00	0.00	0.00	0.00	148 000.00	0.00	172 000.00	860 000.00	100.00	860 000.00	860 000.00	0.00	No	n/a
17. UCAM	523 613.00	0.00	0.00	0.00	0.00	0.00	247 800.00	0.00	192 853.25	964 266.25	100.00	964 266.25	964 266.25	0.00	No	n/a
18. UOXF	290 498.00	0.00	0.00	0.00	0.00	0.00	97 330.00	0.00	96 957.00	484 785.00	100.00	484 785.00	484 785.00	0.00	No	n/a
19. UT	156 500.00	0.00	0.00	0.00	0.00	0.00	43 000.00	0.00	49 875.00	249 375.00	100.00	249 375.00	249 375.00	0.00	No	n/a
20. ULIV	443 263.00	0.00	0.00	0.00	0.00	0.00	76 519.00	0.00	129 945.50	649 727.50	100.00	649 727.50	649 727.50	0.00	No	n/a
21. ESRF	336 000.00	0.00	0.00	0.00	0.00	0.00	23 000.00	0.00	89 750.00	448 750.00	100.00	448 750.00	448 750.00	0.00	No	n/a
22. ILL	289 800.00	0.00	0.00	0.00	0.00	0.00	23 000.00	0.00	78 200.00	391 000.00	100.00	391 000.00	391 000.00	0.00	No	n/a
23. SOLEIL	329 000.00	0.00	0.00	0.00	0.00	0.00	80 500.00	0.00	102 375.00	511 875.00	100.00	511 875.00	511 875.00	0.00	No	n/a
24. CID	380 700.00	0.00	0.00	0.00	0.00	0.00	38 700.00	0.00	104 850.00	524 250.00	100.00	524 250.00	524 250.00	0.00	No	n/a
25. EMIRI	188 000.00	0.00	0.00	0.00	0.00	0.00	40 000.00	0.00	57 000.00	285 000.00	100.00	285 000.00	285 000.00	0.00	No	n/a
26. UMI	154 826.00	0.00	0.00	0.00	0.00	0.00	12 000.00	0.00	41 706.50	208 532.50	100.00	208 532.50	208 532.50	0.00	No	n/a
27. SOLB	168 600.00	0.00	0.00	0.00	0.00	0.00	16 000.00	0.00	46 150.00	230 750.00	100.00	230 750.00	230 750.00	0.00	No	n/a
28. BASF	232 880.00	0.00	0.00	0.00	0.00	0.00	201 160.00	0.00	108 510.00	542 550.00	100.00	542 550.00	542 550.00	0.00	No	n/a
29. NVOLT	283 500.00	0.00	0.00	0.00	0.00	0.00	44 500.00	0.00	82 000.00	410 000.00	100.00	410 000.00	410 000.00	0.00	No	n/a
30. UNIBAS	266 063.00	0.00	0.00	0.00	0.00	0.00	105 000.00	0.00	92 765.75	463 828.75	100.00	463 828.75	463 828.75	0.00	No	n/a
31. ITU	294 936.00	0.00	0.00	0.00	0.00	0.00	33 500.00	0.00	82 109.00	410 545.00	100.00	410 545.00	410 545.00	0.00	No	n/a

DRAFT

ESTIMATED BUDGET FOR THE ACTION

	Estimated eligible[1] costs (per budget category)										EU contribution			Additional information		
	A. Direct personnel costs				B. Direct costs of subcontracting	*[C. Direct costs of fin. support]*	D. Other direct costs		E. Indirect costs[2]	Total costs	Reimbursement rate %	Maximum EU contribution[3]	Maximum grant amount[4]	Information for indirect costs	Information for auditors	Other information:
	A.1 Employees (or equivalent) A.2 Natural persons under direct contract A.3 Seconded persons *[A.6 Personnel for providing access to research infrastructure]*		A.4 SME owners without salary A.5 Beneficiaries that are natural persons without salary				D.1 Travel D.2 Equipment D.3 Other goods and services *[D.4 Costs of large research infrastructure]*	D.5 Costs of internally invoiced goods and services						Estimated costs of in-kind contributions not used on premises	Declaration of costs under Point D.4	Estimated costs of beneficiaries/ linked third parties not receiving funding/ international partners
Form of costs[6]	Actual	Unit[7]	Unit[8]		Actual	Actual	Actual	Unit[9]	Flat-rate[10] 25%							
	a	Total b	No hours	Total c	d	*[e]*	f	Total g	h = 0,25 x (a +b+c+f+g +*[i1]*[13]+*[i2]*[13]-n)	j = a+b+c+d +*[e]*+f+g+h +*[i1]*+*[i2]*	k	l	m	n	Yes/No	
32. 3DS	380 000.00	0.00	0.00	0.00	0.00	0.00	20 000.00	0.00	100 000.00	500 000.00	100.00	500 000.00	500 000.00	0.00	No	n/a
33. FZJ	585 990.00	0.00	0.00	0.00	0.00	0.00	48 000.00	0.00	158 497.50	792 487.50	100.00	792 487.50	792 487.50	0.00	No	n/a
34. SAFT	112 603.00	0.00	0.00	0.00	0.00	0.00	70 000.00	0.00	45 650.75	228 253.75	100.00	228 253.75	228 253.75	0.00	No	n/a
Total consortium	11 489 301.00	1 125 989.00			350 000.00	0.00	3 102 960.00	0.00	3 929 562.50	19 997 812.50		19 997 812.50	19 997 812.50			0.00

[1] See Article 6 for the eligibility conditions.
[2] Indirect costs already covered by an operating grant (received under any EU or Euratom funding programme; see Article 6.5.(b)) are ineligible under the GA. Therefore, a beneficiary/linked third party that receives an operating grant during the action's duration cannot declare indirect costs for the year(s)/reporting period(s) covered by the operating grant, unless it can demonstrate that the operating grant does not cover any costs of the action (see Article 6.2.E).
[3] This is the theoretical amount of EU contribution that the system calculates automatically (by multiplying all the budgeted costs by the reimbursement rate). This theoretical amount is capped by the 'maximum grant amount' (that the Commission decided to grant for the action) (see Article 5.1).
[4] The 'maximum grant amount' is the maximum grant amount decided by the Commission. It normally corresponds to the requested grant, but may be lower.
[5] Depending on its type, this specific cost category will or will not cover indirect costs. Specific unit costs that include indirect costs are: costs for energy efficiency measures in buildings, access costs for providing trans-national access to research infrastructure and costs for clinical studies.
[6] See Article 5 for the forms of costs.
[7] Unit : hours worked on the action; costs per unit (hourly rate) : calculated according to the beneficiary's usual accounting practice.
[8] See Annex 2a 'Additional information on the estimated budget' for the details (costs per hour (hourly rate)).
[9] Unit and costs per unit : calculated according to the beneficiary's usual accounting practices.
[10] Flat rate : 25% of eligible direct costs, from which are excluded: direct costs of subcontracting, costs of in-kind contributions not used on premises, direct costs of financial support, and unit costs declared under budget category F if they include indirect costs (see Article 6.2.E).
[11] See Annex 2a 'Additional information on the estimated budget' for the details (units, costs per unit).
[12] See Annex 2a 'Additional information on the estimated budget' for the details (units, costs per unit, estimated number of units, etc).
[13] Only specific unit costs that do not include indirect costs.
[14] See Article 9 for beneficiaries not receiving funding.
[15] Only for linked third parties that receive funding.

DRAFT

ANNEX 2a

ADDITIONAL INFORMATION ON THE ESTIMATED BUDGET

- **Instructions and footnotes in blue will not appear in the text generated by the IT system (since they are internal instructions only).**
- **For options *[*in square brackets*]*: the applicable option will be chosen by the IT system. Options not chosen will automatically not appear.**
- **For fields in [grey in square brackets] (even if they are part of an option as specified in the previous item): IT system will enter the appropriate data.**

⚠ **Transitory period: Until SyGMa fully supports Annex 2a, you must prepare it manually (using this template by choosing and deleting the options/entering the appropriate data).**
For the 'unit cost tables': either fill them out manually or use currently existing tables from Annex 1 or the proposal.
The document can then be uploaded in SyGMa and attached to the grant agreement.

Unit cost for SME owners/natural beneficiaries without salary

1. Costs for a *[*SME owner*][*beneficiary that is a natural person*]* not receiving a salary

Units: hours worked on the action

Amount per unit ('hourly rate'): calculated according to the following formula:

{the monthly living allowance for researchers in MSCA-IF actions / 143 hours}
multiplied by
{country-specific correction coefficient of the country where the beneficiary is established}

The monthly living allowance and the country-specific correction coefficients are set out in the Work Programme (section 3 MSCA) in force at the time of the call:

- for calls *before* Work Programme 2018-2020:
  - for the monthly living allowance: **EUR 4 650**
  - for the country-specific correction coefficients: see Work Programme 2014-2015 and Work Programme 2016-2017 (available on the Participant Portal Reference Documents page)
- for calls *under* Work Programme 2018-2020:
  - for the monthly living allowance: **EUR 4 880**
  - for the country-specific correction coefficients: see Work Programme 2018-2020 (available on the Participant Portal Reference Documents page)

[additional OPTION for beneficiaries/linked third parties that have opted to use the unit cost (in the proposal/with an amendment): For the following beneficiaries/linked third parties, the amounts per unit (hourly rate) are fixed as follows:

- beneficiary/linked third party [short name]: EUR [insert amount]
- beneficiary/linked third party [short name]: EUR [insert amount]

[same for other beneficiaries/linked third parties, if necessary] ***]***

Estimated number of units: see Annex 2

Energy efficiency measures unit cost

2. Costs for energy efficiency measures in buildings

Unit: m^2 of eligible 'conditioned' (i.e. built or refurbished) floor area

Amount per unit*: see (for each beneficiary/linked third party and BEST table) the 'unit cost table' attached

* Amount calculated as follows:
{EUR 0.1 x estimated total kWh saved per m² per year x 10}

Estimated number of units: see (for each beneficiary/linked third party and BEST table) the 'unit cost table' attached

Unit cost table (energy efficiency measures unit cost)[1]

Short name beneficiary/linked third party	BEST No	Amount per unit	Estimated No of units	Total unit cost (cost per unit x estimated no of units)

[1] Data from the 'building energy specification table (BEST)' that is part of the proposal and Annex 1.

Research infrastructure unit cost

3. Access costs for providing trans-national access to research infrastructure

Units[2]: see (for each access provider and installation) the 'unit cost table' attached

Amount per unit*: see (for each access provider and installation) the 'unit cost table' attached

* Amount calculated as follows:

$$\frac{\text{average annual total access cost to the installation (over past two years[3])}}{\text{average annual total quantity of access to the installation (over past two years[4])}}$$

Estimated number of units: see (for each access provider and installation) the 'unit cost table' attached

Unit cost table (access to research infrastructure unit cost)[5]

Short name access provider	Short name infrastructure	Installation		Unit of access	Amount per unit	Estimated No of units	Total unit cost (cost per unit x estimated no of units)
		No	Short name				

Clinical studies unit cost

4. Costs for clinical studies

Units: patients/subjects that participate in the clinical study

Amount per unit*: see (for each sequence (if any), clinical study and beneficiary/linked third party) the 'unit cost table' attached

* Amount calculated, for the cost components of each task, as follows:

For **personnel costs**:

For personnel costs of doctors: 'average hourly cost for doctors', i.e.:

$$\frac{\{\text{certified or auditable total personnel costs for doctors for year N-1}\}}{\{1720 * \text{number of full-time-equivalent for doctors for year N-1}\}}$$

multiplied by

estimated number of hours to be worked by doctors for the task (per participant)}

For personnel costs of other medical personnel: 'average hourly cost for other medical personnel', i.e.:

$$\frac{\{\text{certified or auditable total personnel costs for other medical personnel for year N-1}\}}{\{1720 * \text{number of full-time-equivalent for other medical personnel for year N-1}\}}$$

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2 Unit of access (e.g. beam hours, weeks of access, sample analysis) fixed by the access provider in proposal.

3 In exceptional and duly justified cases, the Commission/Agency may agree to a different reference period.

4 In exceptional and duly justified cases, the Commission/Agency may agree to a different reference period.

5 Data from the 'table on estimated costs/quantity of access to be provided' that is part of the proposal and Annex 1.

multiplied by
estimated number of hours to be worked by other medical personnel for the task (per participant)}

For personnel costs of technical personnel: 'average hourly cost for technical personnel', i.e.:

{certified or auditable total personnel costs for technical personnel for year N-1

{1720 * number of full-time-equivalent for technical personnel for year N-1}
multiplied by
estimated number of hours to be worked by technical personnel for the task (per participant)}

'total personnel costs' means actual salaries + actual social security contributions + actual taxes and other costs included in the remuneration, provided they arise from national law or the employment contract/equivalent appointing act

For **consumables**:

For each cost item: 'average price of the consumable', i.e.:

{{certified or auditable total costs of purchase of the consumable in year N-1

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total number of items purchased in year N-1}
multiplied by
estimated number of items to be used for the task (per participant)}

'total costs of purchase of the consumable' means total value of the supply contracts (including related duties, taxes and charges such as non-deductible VAT) concluded by the beneficiary for the consumable delivered in year N-1, provided the contracts were awarded according to the principle of best value- for-money and without any conflict of interests

For **medical equipment**:

For each cost item: 'average cost of depreciation and directly related services per unit of use', i.e.:

{{ certified or auditable total depreciation costs in year N-1 + certified or auditable total costs of purchase of services in year N-1 for the category of equipment concerned}

---

total capacity in year N-1
multiplied by
estimated number of units of use of the equipment for the task (per participant)}

'total depreciation costs' means total depreciation allowances as recorded in the beneficiary's accounts of year N-1 for the category of equipment concerned, provided the equipment was purchased according to the principle of best value for money and without any conflict of interests + total costs of renting or leasing contracts (including related duties, taxes and charges such as non-deductible VAT) in year N-1 for the category of equipment concerned, provided they do not exceed the depreciation costs of similar equipment and do not include finance fees

For **services**:

For each cost item: 'average cost of the service per study participant', i.e.:

{certified or auditable total costs of purchase of the service in year N-1

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total number of patients or subjects included in the clinical studies for which the service was delivered in year N-1}

'total costs of purchase of the service' means total value of the contracts concluded by the beneficiary (including related duties, taxes and charges such as non-deductible VAT) for the specific service delivered in year N-1 for the conduct of clinical studies, provided the contracts were awarded according to the principle of best value for money and without any conflict of interests

For **indirect costs**:

{{{cost component 'personnel costs' + cost component 'consumables' + cost component 'medical equipment'}

minus

{costs of in-kind contributions provided by third parties which are not used on the beneficiary's premises + costs of providing financial support to third parties (if any)}}

multiplied by

25%}

The estimation of the resources to be used must be done on the basis of the study protocol and must be the same for all beneficiaries/linked third parties/third parties involved.

The year N-1 to be used is the last closed financial year at the time of submission of the grant application.

Estimated number of units: see (for each clinical study and beneficiary/linked third party) the 'unit cost table' attached

Unit cost table: clinical studies unit cost[6]

Task, Direct cost categories	**Resource per patient**	**Costs year N-1 Beneficiary 1 [short name]**	**Costs year N-1 Linked third party 1a [short name]**	**Costs year N-1 Beneficiary 2 [short name]**	**Costs year N-1 Linked third party 2a [short name]**	**Costs year N-1 Third party giving in-kind contributions 1 [short name]**
Sequence No. 1						
Task No. 1 Blood sample						
(a) **Personnel costs:** - Doctors	n/a					
- Other Medical Personnel	Phlebotomy (nurse), 10 minutes	8,33 EUR	11,59 EUR	10,30 EUR	11,00 EUR	9,49 EUR
- Technical Personnel	Sample Processing (lab technician), 15 minutes	9,51 EUR	15,68 EUR	14,60 EUR	15,23 EUR	10,78 EUR
(b) **Costs of consumables**:	Syringe	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	Cannula	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	Blood container	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(c) **Costs of medical equipment**:	Use of -80° deep freezer, 60 days	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	Use of centrifuge, 15 minutes	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(d) **Costs of services**	Cleaning of XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(e) **Indirect costs** (25% flat-rate)		XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
Task No. 2						
…						
Amount per unit (unit cost sequence 1):		**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**
Sequence No. 2						
Task No. 1						

[6] Same table as in proposal and Annex 1.

XXX						
(a) **Personnel costs:** - Doctors	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
- Other Medical Personnel	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
- Technical Personnel	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(b) **Costs of consumables**:	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(c) **Costs of medical equipment**:	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(d) **Costs of services**	XXX	XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
(e) **Indirect costs** (25% flat-rate)		XX EUR	XX EUR	XX EUR	XX EUR	XX EUR
Task No. 2						
…						
Amount per unit (unit cost sequence 2):		**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**
…						
Amount per unit (unit cost entire study):		**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**	**XX EUR**

]

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

UPPSALA UNIVERSITET (UU), established in VON KRAEMERS ALLE 4, UPPSALA 751 05, Sweden, VAT number: SE202100293201, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('2')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

KARLSRUHER INSTITUT FUER TECHNOLOGIE (KIT), established in KAISERSTRASSE 12, KARLSRUHE 76131, Germany, VAT number: DE266749428, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become ***beneficiary*** No ('3')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS), established in RUE MICHEL ANGE 3, PARIS 75794, France, VAT number: FR40180089013, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('4')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER (WWU), established in SCHLOSSPLATZ 2, MUENSTER 48149, Germany, VAT number: DE126118759, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('5')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES (CEA), established in RUE LEBLANC 25, PARIS 15 75015, France, VAT number: FR43775685019, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('6')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

KEMIJSKI INSTITUT (NIC), established in HAJDRIHOVA 19, LJUBLJANA 1000, Slovenia, VAT number: SI33840890, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('7')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

SINTEF AS (SINTEF), established in STRINDVEGEN 4, TRONDHEIM 7034, Norway, VAT number: NO919303808MVA, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('8')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

POLITECNICO DI TORINO (PDT), established in CORSO DUCA DEGLI ABRUZZI 24, TORINO 10129, Italy, VAT number: IT00518460019, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('9')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V. (Fraunhofer), established in HANSASTRASSE 27C, MUNCHEN 80686, Germany, VAT number: DE129515865, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('10')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

CHALMERS TEKNISKA HOEGSKOLA AB (CTH), established in -, GOETEBORG 41296, Sweden, VAT number: SE556479559801, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('11')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

POLITECHNIKA WARSZAWSKA (WUT), established in PLAC POLITECHNIKI 1, WARSZAWA 00 661, Poland, VAT number: PL5250005834, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('12')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS (CSIC), established in CALLE SERRANO 117, MADRID 28006, Spain, VAT number: ESQ2818002D, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('13')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

TECHNISCHE UNIVERSITEIT DELFT (TUD), established in STEVINWEG 1, DELFT 2628 CN, Netherlands, VAT number: NL001569569B01, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('14')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

CONSIGLIO NAZIONALE DELLE RICERCHE (CNR), established in PIAZZALE ALDO MORO 7, ROMA 00185, Italy, VAT number: IT02118311006, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('15')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL), established in BATIMENT CE 3316 STATION 1, LAUSANNE 1015, Switzerland, VAT number: CHE116075613TVA, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('16')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE (UCAM), established in TRINITY LANE THE OLD SCHOOLS, CAMBRIDGE CB2 1TN, United Kingdom, VAT number: GB823847609, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('17')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD (UOXF), established in WELLINGTON SQUARE UNIVERSITY OFFICES, OXFORD OX1 2JD, United Kingdom, VAT number: GB125506730, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('18')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

TARTU ULIKOOL (UT), established in ULIKOOLI 18, TARTU 50090, Estonia, VAT number: EE100030417, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('19')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

THE UNIVERSITY OF LIVERPOOL (ULIV), established in BROWNLOW HILL 765 FOUNDATION BUILDING, LIVERPOOL L69 7ZX, United Kingdom, VAT number: GB673598875, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('20')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

EUROPEAN SYNCHROTRON RADIATION FACILITY (ESRF), established in 71 AVENUE DES MARTYRS, GRENOBLE 38000, France, VAT number: FR60338723919, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('21')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

INSTITUT MAX VON LAUE - PAUL LANGEVIN (ILL), established in 71 AVENUE DES MARTYRS, GRENOBLE 38000, France, VAT number: FR01779555887, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become ***beneficiary*** No ('22')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

SYNCHROTRON SOLEIL SOCIETE CIVILE (SOLEIL), established in L ORME DES MERISIERS, SAINT AUBIN 91190, France, VAT number: FR27439684903, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('23')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

FUNDACION CIDETEC (CID), established in PASEO MIRAMON 196 PARQUE TECNOLOGICO DE MIRAMON, SAN SEBASTIAN 20014, Spain, VAT number: ESG20588588, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('24')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL (EMIRI), established in RUE DU MARAIS 31, BRUXELLES 1000, Belgium, VAT number: BE0500888006, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('25')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

UMICORE (UMI), established in RUE DU MARAIS 31, BRUXELLES 1000, Belgium, VAT number: BE0401574852, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('26')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

SOLVAY SA (SOLB), established in RUE DE RANSBEEK 310, BRUXELLES 1120, Belgium, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('27')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

BASF SE (BASF), established in CARL BOSCH STRASSE 38, LUDWIGSHAFEN AM RHEIN 67056, Germany, VAT number: DE149145247, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('28')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

NORTHVOLT AB (NVOLT), established in GAMLA BROGATAN 26, STOCKHOLM 111 20, Sweden, VAT number: SE559015889401, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('29')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

UNIVERSITAT BASEL (UNIBAS), established in PETERSPLATZ 1, BASEL 4051, Switzerland, VAT number: CHE115244907MWST, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('30')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

IT-UNIVERSITETET I KOBENHAVN (ITU), established in RUED LANGGAARDSVEJ 7, KOBENHAVN 2300, Denmark, VAT number: DK29057753, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('31')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

DASSAULT SYSTEMES DEUTSCHLAND GMBH (3DS), established in MEITNERSTRASSE 8, STUTTGART 70563, Germany, VAT number: DE147319694, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('32')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

FORSCHUNGSZENTRUM JULICH GMBH (FZJ), established in WILHELM JOHNEN STRASSE, JULICH 52428, Germany, VAT number: DE122624631, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('33')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ANNEX 3

ACCESSION FORM FOR BENEFICIARIES

SAFT (SAFT), established in 26 QUAI CHARLES PASQUA, LEVALLOIS PERRET 92300, France, VAT number: FR21383703873, ('the beneficiary'), represented for the purpose of signing this Accession Form by the undersigned,

hereby agrees

to become *beneficiary* No ('34')

in Grant Agreement No 957189 ('the Agreement')

between DANMARKS TEKNISKE UNIVERSITET **and** *the European Union ('the EU'), represented by the European Commission ('the Commission'),*

for the action entitled 'Battery Interface Genome - Materials Acceleration Platform (BIG-MAP)'.

and mandates

the coordinator *to submit and sign in its name and on its behalf any* ***amendments*** *to the Agreement, in accordance with Article 55.*

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement it in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the *beneficiary*

DRAFT

ⓘ print format A4 landscape

MODEL ANNEX 4 FOR H2020 GENERAL MGA — MULTI

FINANCIAL STATEMENT FOR *[BENEFICIARY [name]/ LINKED THIRD PARTY [name]]* FOR REPORTING PERIOD [reporting period]

	Eligible[1] costs (per budget category)														Receipts	EU contribution			Additional information
	A. Direct personnel costs				B. Direct costs of subcontracting	*[C. Direct costs of fin. support]*	D. Other direct costs			E. Indirect costs[2]	*[F. Costs of …]*			Total costs	Receipts	Reimbursement rate %	Maximum EU contribution[3]	Requested EU contribution	Information for indirect costs :
	A.1 Employees (or equivalent) A.2 Natural persons under direct contract A.3 Seconded persons *[A.6 Personnel for providing access to research infrastructure]*		A.4 SME owners without salary A.5 Beneficiaries that are natural persons without salary			*[C.1 Financial support]* *[C.2 Prizes]*	D.1 Travel D.2 Equipment D.3 Other goods and services	*[D.4 Costs of large research infrastructure]*	D.5 Costs of internally invoiced goods and services		*[F.1 Costs of …]*		*[F.2 Costs of …]*		Receipts of the action, to be reported in the last reporting period, according to Article 5.3.3				Costs of in-kind contributions not used on premises
Form of costs[4]	Actual	Unit	Unit		Actual	Actual	Actual	Actual	Unit	Flat-rate[5] 25%	Unit		*[Unit][Lump sum]*						
	a	Total b	No hours	Total c	d	*[e]*	f	*[g]*	Total h	i=0,25 x (a+b+c+f+*[g]* + h+ *[j 1]*[6] +*[j2]*[6] -p)	No units	Total *[j1]*	Total *[j2]*	k = a+b+c+d+*[e]* +*f* + *[g]* +h+ i + *[j1]* +*[j2]*	l	m	n	o	p
[short name beneficiary/linked third party]																			

The beneficiary/linked third party hereby confirms that:
The information provided is complete, reliable and true.
The costs declared are eligible (see Article 6).
The costs can be substantiated by adequate records and supporting documentation that will be produced upon request or in the context of checks, reviews, audits and investigations (see Articles 17, 18 and 22).
For the last reporting period: that all the receipts have been declared (see Article 5.3.3).

ⓘ Please declare all eligible costs, even if they exceed the amounts indicated in the estimated budget (see Annex 2). Only amounts that were declared in your individual financial statements can be taken into account lateron, in order to replace other costs that are found to be ineligible.

[1] See Article 6 for the eligibility conditions

[2] The indirect costs claimed must be free of any amounts covered by an operating grant (received under any EU or Euratom funding programme; see Article 6.2.E). If you have received an operating grant during this reporting period, you cannot claim indirect costs unless you can demonstrate that the operating grant does not cover any costs of the action.

[3] This is the *theoretical* amount of EU contribution that the system calculates automatically (by multiplying the reimbursement rate by the total costs declared). The amount you request (in the column 'requested EU contribution') may be less,

[4] See Article 5 for the forms of costs

[5] Flat rate : 25% of eligible direct costs, from which are excluded: direct costs of subcontracting, costs of in-kind contributions not used on premises, direct costs of financial support, and unit costs declared under budget category F if they include indirect costs (see Article 6.2.E)

[6] Only specific unit costs that do not include indirect costs

ANNEX 5

MODEL FOR THE CERTIFICATE ON THE FINANCIAL STATEMENTS

- **For options [*in italics in square brackets*]: choose the applicable option. Options not chosen should be deleted.**
- **For fields in [grey in square brackets]: enter the appropriate data**

TABLE OF CONTENTS

TERMS OF REFERENCE FOR AN INDEPENDENT REPORT OF FACTUAL FINDINGS ON COSTS DECLARED UNDER A GRANT AGREEMENT FINANCED UNDER THE HORIZON 2020 RESEARCH FRAMEWORK PROGRAMME

INDEPENDENT REPORT OF FACTUAL FINDINGS ON COSTS DECLARED UNDER A GRANT AGREEMENT FINANCED UNDER THE HORIZON 2020 RESEARCH FRAMEWORK PROGRAMME

Terms of Reference for an Independent Report of Factual Findings on costs declared under a Grant Agreement financed under the Horizon 2020 Research and Innovation Framework Programme

This document sets out the '**Terms of Reference (ToR)**' under which

[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]

agrees to engage

[**insert legal name of the auditor**] ('the Auditor')

to produce an independent report of factual findings ('the Report') concerning the Financial Statement(s)[1] drawn up by the *[Beneficiary] [Linked Third Party]* for the Horizon 2020 grant agreement [insert number of the grant agreement, title of the action, acronym and duration from/to] ('the Agreement'), and

to issue a Certificate on the Financial Statements' ('CFS') referred to in Article 20.4 of the Agreement based on the compulsory reporting template stipulated by the Commission.

The Agreement has been concluded under the Horizon 2020 Research and Innovation Framework Programme (H2020) between the Beneficiary and *[OPTION 1: the European Union, represented by the European Commission ('the Commission')][OPTION 2: the European Atomic Energy Community (Euratom,) represented by the European Commission ('the Commission')][OPTION 3: the [Research Executive Agency (REA)] [European Research Council Executive Agency (ERCEA)] [Innovation and Networks Executive Agency (INEA)] [Executive Agency for Small and Medium-sized Enterprises (EASME)] ('the Agency'), under the powers delegated by the European Commission ('the Commission').]*

The *[Commission] [Agency]* is mentioned as a signatory of the Agreement with the Beneficiary only. The *[European Union][Euratom][Agency]* is not a party to this engagement.

1.1 Subject of the engagement

The coordinator must submit to the *[Commission][Agency]* the final report within 60 days following the end of the last reporting period which should include, amongst other documents, a CFS for each beneficiary and for each linked third party that requests a total contribution of EUR 325 000 or more, as reimbursement of actual costs and unit costs calculated on the basis of its usual cost accounting practices (see Article 20.4 of the Agreement). The CFS must cover all reporting periods of the beneficiary or linked third party indicated above.

The Beneficiary must submit to the coordinator the CFS for itself and for its linked third party(ies), if the CFS must be included in the final report according to Article 20.4 of the Agreement.

The CFS is composed of two separate documents:

- The Terms of Reference ('the ToR') to be signed by the *[Beneficiary] [Linked Third Party]* and the Auditor;

[1] By which costs under the Agreement are declared (see template 'Model Financial Statements' in Annex 4 to the Grant Agreement).

- The Auditor's Independent Report of Factual Findings ('the Report') to be issued on the Auditor's letterhead, dated, stamped and signed by the Auditor (or the competent public officer) which includes the agreed-upon procedures ('the Procedures') to be performed by the Auditor, and the standard factual findings ('the Findings') to be confirmed by the Auditor.

If the CFS must be included in the final report according to Article 20.4 of the Agreement, the request for payment of the balance relating to the Agreement cannot be made without the CFS. However, the payment for reimbursement of costs covered by the CFS does not preclude the Commission *[Agency,]* the European Anti-Fraud Office and the European Court of Auditors from carrying out checks, reviews, audits and investigations in accordance with Article 22 of the Agreement.

1.2 Responsibilities

The *[Beneficiary] [Linked Third Party]:*

- must draw up the Financial Statement(s) for the action financed by the Agreement in compliance with the obligations under the Agreement. The Financial Statement(s) must be drawn up according to the *[Beneficiary's] [Linked Third Party's]* accounting and book-keeping system and the underlying accounts and records;
- must send the Financial Statement(s) to the Auditor;
- is responsible and liable for the accuracy of the Financial Statement(s);
- is responsible for the completeness and accuracy of the information provided to enable the Auditor to carry out the Procedures. It must provide the Auditor with a written representation letter supporting these statements. The written representation letter must state the period covered by the statements and must be dated;
- accepts that the Auditor cannot carry out the Procedures unless it is given full access to the *[Beneficiary's] [Linked Third Party's]* staff and accounting as well as any other relevant records and documentation.

The Auditor:

- *[Option 1 by default:* is qualified to carry out statutory audits of accounting documents in accordance with Directive 2006/43/EC of the European Parliament and of the Council of 17 May 2006 on statutory audits of annual accounts and consolidated accounts, amending Council Directives 78/660/EEC and 83/349/EEC and repealing Council Directive 84/253/EEC or similar national regulations*]*.
- *[Option 2 if the Beneficiary or Linked Third Party has an independent Public Officer:* is a competent and independent Public Officer for which the relevant national authorities have established the legal capacity to audit the Beneficiary*]*.
- *[Option 3 if the Beneficiary or Linked Third Party is an international organisation:* is an [internal] [external] auditor in accordance with the internal financial regulations and procedures of the international organisation*]*.

The Auditor:

- must be independent from the Beneficiary *[and the Linked Third Party]*, in particular, it must not have been involved in preparing the *[Beneficiary's] [Linked Third Party's]* Financial Statement(s);
- must plan work so that the Procedures may be carried out and the Findings may be assessed;
- must adhere to the Procedures laid down and the compulsory report format;
- must carry out the engagement in accordance with this ToR;
- must document matters which are important to support the Report;
- must base its Report on the evidence gathered;
- must submit the Report to the *[Beneficiary] [Linked Third Party]*.

The Commission sets out the Procedures to be carried out by the Auditor. The Auditor is not responsible for their suitability or pertinence. As this engagement is not an assurance engagement, the Auditor does not provide an audit opinion or a statement of assurance.

1.3 Applicable Standards

The Auditor must comply with these Terms of Reference and with[2]:

- the International Standard on Related Services ('ISRS') 4400 *Engagements to perform Agreed-upon Procedures regarding Financial Information* as issued by the International Auditing and Assurance Standards Board (IAASB);
- the *Code of Ethics for Professional Accountants* issued by the International Ethics Standards Board for Accountants (IESBA). Although ISRS 4400 states that independence is not a requirement for engagements to carry out agreed-upon procedures, the *[Commission][Agency]* requires that the Auditor also complies with the Code's independence requirements.

The Auditor's Report must state that there is no conflict of interests in establishing this Report between the Auditor and the Beneficiary *[and the Linked Third Party]*, and must specify - if the service is invoiced - the total fee paid to the Auditor for providing the Report.

1.4 Reporting

The Report must be written in the language of the Agreement (see Article 20.7).

Under Article 22 of the Agreement, the Commission*[, the Agency],* the European Anti-Fraud Office and the Court of Auditors have the right to audit any work that is carried out under the action and for which costs are declared from [*the European Union*] [*Euratom*] budget. This includes work related to this engagement. The Auditor must provide access to all working papers (e.g. recalculation of hourly rates, verification of the time declared for the action) related to this assignment if the Commission *[, the Agency]*, the European Anti-Fraud Office or the European Court of Auditors requests them.

1.5 Timing

The Report must be provided by *[*dd Month yyyy*]*.

1.6 Other terms

[*The [Beneficiary] [Linked Third Party] and the Auditor can use this section to agree other specific terms, such as the Auditor's fees, liability, applicable law, etc. Those specific terms must not contradict the terms specified above.*]

[legal name of the Auditor]	[legal name of the *[Beneficiary][Linked Third Party]*]
[name & function of authorised representative]	[name & function of authorised representative]
[dd Month yyyy]	[dd Month yyyy]
Signature of the Auditor	Signature of the *[Beneficiary][Linked Third Party]*

[2] Supreme Audit Institutions applying INTOSAI-standards may carry out the Procedures according to the corresponding International Standards of Supreme Audit Institutions and code of ethics issued by INTOSAI instead of the International Standard on Related Services ('ISRS') 4400 and the Code of Ethics for Professional Accountants issued by the IAASB and the IESBA.

Independent Report of Factual Findings on costs declared under Horizon 2020 Research and Innovation Framework Programme

(To be printed on the Auditor's letterhead)

To
[name of contact person(s)], [Position]
[[*Beneficiary's*] [*Linked Third Party's*] name]
[Address]
[dd Month yyyy]

Dear [Name of contact person(s)],

As agreed under the terms of reference dated [dd Month yyyy]

with *[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')],*

we
[name of the auditor] ('the Auditor'),
established at
[full address/city/state/province/country],
represented by
[name and function of an authorised representative],

have carried out the procedures agreed with you regarding the costs declared in the Financial Statement(s)[3] of the *[Beneficiary] [Linked Third Party]* concerning the grant agreement [insert grant agreement reference: number, title of the action and acronym] ('the Agreement'),

with a total cost declared of
[total amount] EUR,

and a total of actual costs and unit costs calculated in accordance with the [*Beneficiary's*] [*Linked Third Party's*] usual cost accounting practices' declared of

[sum of total actual costs and total direct personnel costs declared as unit costs calculated in accordance with the *[Beneficiary's] [Linked Third Party's]* usual cost accounting practices] EUR

and **hereby provide our Independent Report of Factual Findings ('the Report')** using the compulsory report format agreed with you.

<u>The Report</u>

Our engagement was carried out in accordance with the terms of reference ('the ToR') appended to this Report. The Report includes the agreed-upon procedures ('the Procedures') carried out and the standard factual findings ('the Findings') examined.

[3] By which the Beneficiary declares costs under the Agreement (see template 'Model Financial Statement' in Annex 4 to the Agreement).

The Procedures were carried out solely to assist the *[Commission] [Agency]* in evaluating whether the *[Beneficiary's] [Linked Third Party's]* costs in the accompanying Financial Statement(s) were declared in accordance with the Agreement. The *[Commission] [Agency]* draws its own conclusions from the Report and any additional information it may require.

The scope of the Procedures was defined by the Commission. Therefore, the Auditor is not responsible for their suitability or pertinence. Since the Procedures carried out constitute neither an audit nor a review made in accordance with International Standards on Auditing or International Standards on Review Engagements, the Auditor does not give a statement of assurance on the Financial Statements.

Had the Auditor carried out additional procedures or an audit of the *[Beneficiary's] [Linked Third Party's]* Financial Statements in accordance with International Standards on Auditing or International Standards on Review Engagements, other matters might have come to its attention and would have been included in the Report.

Not applicable Findings

We examined the Financial Statement(s) stated above and considered the following Findings not applicable:

Explanation (to be removed from the Report):

*If a Finding was not applicable, it must be marked as '**N.A.**' ('Not applicable') in the corresponding row on the right-hand column of the table and means that the Finding did not have to be corroborated by the Auditor and the related Procedure(s) did not have to be carried out.*

The reasons of the non-application of a certain Finding must be obvious i.e.

i) if no cost was declared under a certain category then the related Finding(s) and Procedure(s) are not applicable;

ii) if the condition set to apply certain Procedure(s) are not met the related Finding(s) and those Procedure(s) are not applicable. For instance, for 'beneficiaries with accounts established in a currency other than euro' the Procedure and Finding related to 'beneficiaries with accounts established in euro' are not applicable. Similarly, if no additional remuneration is paid, the related Finding(s) and Procedure(s) for additional remuneration are not applicable.

List here all Findings considered not applicable for the present engagement and explain the reasons of the non-applicability.

….

Exceptions

Apart from the exceptions listed below, the *[Beneficiary] [Linked Third Party]* provided the Auditor all the documentation and accounting information needed by the Auditor to carry out the requested Procedures and evaluate the Findings.

Explanation (to be removed from the Report):

- *If the Auditor was not able to successfully complete a procedure requested, it must be marked as '**E**' ('Exception') in the corresponding row on the right-hand column of the table. The reason such as the inability to reconcile key information or the unavailability of data that prevents the Auditor from carrying out the Procedure must be indicated below.*
- *If the Auditor cannot corroborate a standard finding after having carried out the corresponding procedure, it must also be marked as '**E**' ('Exception') and, where possible, the reasons why the Finding was not fulfilled and its possible impact must be explained here below.*

List here any exceptions and add any information on the cause and possible consequences of each exception, if known. If the exception is quantifiable, include the corresponding amount.

….

Example (to be removed from the Report):

1. *The Beneficiary was unable to substantiate the Finding number 1 on … because ….*
2. *Finding number 30 was not fulfilled because the methodology used by the Beneficiary to calculate unit costs was different from the one approved by the Commission. The differences were as follows: …*
3. *After carrying out the agreed procedures to confirm the Finding number 31, the Auditor found a difference of _____ EUR. The difference can be explained by …*

Further Remarks

In addition to reporting on the results of the specific procedures carried out, the Auditor would like to make the following general remarks:

Example (to be removed from the Report):

1. *Regarding Finding number 8 the conditions for additional remuneration were considered as fulfilled because …*
2. *In order to be able to confirm the Finding number 15 we carried out the following additional procedures: ….*

Use of this Report

This Report may be used only for the purpose described in the above objective. It was prepared solely for the confidential use of the *[Beneficiary] [Linked Third Party]* and the [*Commission*] [*Agency*], and only to be submitted to the *[Commission] [Agency]* in connection with the requirements set out in Article 20.4 of the Agreement. The Report may not be used by the *[Beneficiary] [Linked Third Party]* or by the *[Commission] [Agency]* for any other purpose, nor may it be distributed to any other parties. The *[Commission] [Agency]* may only disclose the Report to authorised parties, in particular to the European Anti-Fraud Office (OLAF) and the European Court of Auditors.

This Report relates only to the Financial Statement(s) submitted to the *[Commission] [Agency]* by the *[Beneficiary] [Linked Third Party]* for the Agreement. Therefore, it does not extend to any other of the *[Beneficiary's] [Linked Third Party's]* Financial Statement(s).

There was no conflict of interest[4] between the Auditor and the Beneficiary *[and Linked Third Party]* in establishing this Report. The total fee paid to the Auditor for providing the Report was EUR _____ (including EUR_____ of deductible VAT).

We look forward to discussing our Report with you and would be pleased to provide any further information or assistance.

[legal name of the Auditor]
[name and function of an authorised representative]
[dd Month yyyy]
Signature of the Auditor

[4] A conflict of interest arises when the Auditor's objectivity to establish the certificate is compromised in fact or in appearance when the Auditor for instance:
- was involved in the preparation of the Financial Statements;
- stands to benefit directly should the certificate be accepted;
- has a close relationship with any person representing the beneficiary;
- is a director, trustee or partner of the beneficiary; or
- is in any other situation that compromises his or her independence or ability to establish the certificate impartially.

Agreed-upon procedures to be performed and standard factual findings to be confirmed by the Auditor

The European Commission reserves the right to i) provide the auditor with additional guidance regarding the procedures to be followed or the facts to be ascertained and the way in which to present them (this may include sample coverage and findings) or to ii) change the procedures, by notifying the Beneficiary in writing. The procedures carried out by the auditor to confirm the standard factual finding are listed in the table below.

If this certificate relates to a Linked Third Party, any reference here below to 'the Beneficiary' is to be considered as a reference to 'the Linked Third Party'.

The 'result' column has three different options: 'C', 'E' and 'N.A.':

- 'C' stands for 'confirmed' and means that the auditor can confirm the 'standard factual finding' and, therefore, there is no exception to be reported.
- 'E' stands for 'exception' and means that the Auditor carried out the procedures but cannot confirm the 'standard factual finding', or that the Auditor was not able to carry out a specific procedure (e.g. because it was impossible to reconcile key information or data were unavailable),
- 'N.A.' stands for 'not applicable' and means that the Finding did not have to be examined by the Auditor and the related Procedure(s) did not have to be carried out. The reasons of the non-application of a certain Finding must be obvious i.e. i) if no cost was declared under a certain category then the related Finding(s) and Procedure(s) are not applicable; ii) if the condition set to apply certain Procedure(s) are not met then the related Finding(s) and Procedure(s) are not applicable. For instance, for 'beneficiaries with accounts established in a currency other than the euro' the Procedure related to 'beneficiaries with accounts established in euro' is not applicable. Similarly, if no additional remuneration is paid, the related Finding(s) and Procedure(s) for additional remuneration are not applicable.

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
A	**ACTUAL PERSONNEL COSTS AND UNIT COSTS CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICE**		
	The Auditor draws a sample of persons whose costs were declared in the Financial Statement(s) to carry out the procedures indicated in the consecutive points of this section A. (*The sample should be selected randomly so that it is representative. Full coverage is required if there are fewer than 10 people (including employees, natural persons working under a direct contract and personnel seconded by a third party), otherwise the sample should have a minimum of 10 people, or 10% of the total, whichever number is the highest)* The Auditor sampled _____ people out of the total of _____ people.		

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
A.1	**PERSONNEL COSTS** For the persons included in the sample and working under an employment contract or equivalent act (general procedures for individual actual personnel costs and personnel costs declared as unit costs) To confirm standard factual findings 1-5 listed in the next column, the Auditor reviewed following information/documents provided by the Beneficiary: o a list of the persons included in the sample indicating the period(s) during which they worked for the action, their position (classification or category) and type of contract; o the payslips of the employees included in the sample; o reconciliation of the personnel costs declared in the Financial Statement(s) with the accounting system (project accounting and general ledger) and payroll system; o information concerning the employment status and employment conditions of personnel included in the sample, in particular their employment contracts or equivalent; o the Beneficiary's usual policy regarding payroll matters (e.g. salary policy, overtime policy, variable pay); o applicable national law on taxes, labour and social security and o any other document that supports the personnel costs declared. The Auditor also verified the eligibility of all components of the retribution (see Article 6 GA) and recalculated the personnel costs for employees included in the sample.	1) The employees were i) directly hired by the Beneficiary in accordance with its national legislation, ii) under the Beneficiary's sole technical supervision and responsibility and iii) remunerated in accordance with the Beneficiary's usual practices.	
		2) Personnel costs were recorded in the Beneficiary's accounts/payroll system.	
		3) Costs were adequately supported and reconciled with the accounts and payroll records.	
		4) Personnel costs did not contain any ineligible elements.	
		5) There were no discrepancies between the personnel costs charged to the action and the costs recalculated by the Auditor.	
	Further procedures if 'additional remuneration' is paid To confirm standard factual findings 6-9 listed in the next column, the Auditor: o reviewed relevant documents provided by the Beneficiary (legal form, legal/statutory	6) The Beneficiary paying "additional remuneration" was a non-profit legal entity.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	obligations, the Beneficiary's usual policy on additional remuneration, criteria used for its calculation, the Beneficiary's usual remuneration practice for projects funded under national funding schemes…); o recalculated the amount of additional remuneration eligible for the action based on the supporting documents received (full-time or part-time work, exclusive or non-exclusive dedication to the action, usual remuneration paid for projects funded by national schemes) to arrive at the applicable FTE/year and pro-rata rate (see data collected in the course of carrying out the procedures under A.2 'Productive hours' and A.4 'Time recording system'). *'ADDITIONAL REMUNERATION' MEANS ANY PART OF THE REMUNERATION WHICH EXCEEDS WHAT THE PERSON WOULD BE PAID FOR TIME WORKED IN PROJECTS FUNDED BY NATIONAL SCHEMES.* *IF ANY PART OF THE REMUNERATION PAID TO THE EMPLOYEE QUALIFIES AS "ADDITIONAL REMUNERATION" AND IS ELIGIBLE UNDER THE PROVISIONS OF ARTICLE 6.2.A.1, THIS CAN BE CHARGED AS ELIGIBLE COST TO THE ACTION UP TO THE FOLLOWING AMOUNT:* *(A) IF THE PERSON WORKS FULL TIME AND EXCLUSIVELY ON THE ACTION DURING THE FULL YEAR: UP TO EUR 8 000/YEAR;* *(B) IF THE PERSON WORKS EXCLUSIVELY ON THE ACTION BUT NOT FULL-TIME OR NOT FOR THE FULL YEAR: UP TO THE CORRESPONDING PRO-RATA AMOUNT OF EUR 8 000, OR* *(C) IF THE PERSON DOES NOT WORK EXCLUSIVELY ON THE ACTION: UP TO A PRO-RATA AMOUNT CALCULATED IN ACCORDANCE TO ARTICLE 6.2.A.1.*	7) The amount of additional remuneration paid corresponded to the Beneficiary's usual remuneration practices and was consistently paid whenever the same kind of work or expertise was required.	
		8) The criteria used to calculate the additional remuneration were objective and generally applied by the Beneficiary regardless of the source of funding used.	
		9) The amount of additional remuneration included in the personnel costs charged to the action was capped at EUR 8,000 per FTE/year (up to the equivalent pro-rata amount if the person did not work on the action full-time during the year or did not work exclusively on the action).	
	Additional procedures in case "unit costs calculated by the Beneficiary in accordance with its usual cost accounting practices" is applied: Apart from carrying out the procedures indicated above to confirm standard factual findings 1-5 and, if applicable, also 6-9, the Auditor carried out following procedures to confirm standard	10) The personnel costs included in the Financial Statement were calculated in accordance with the Beneficiary's usual cost accounting practice. This methodology was consistently	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	factual findings 10-13 listed in the next column: ○ obtained a description of the Beneficiary's usual cost accounting practice to calculate unit costs;. ○ reviewed whether the Beneficiary's usual cost accounting practice was applied for the Financial Statements subject of the present CFS; ○ verified the employees included in the sample were charged under the correct category (in accordance with the criteria used by the Beneficiary to establish personnel categories) by reviewing the contract/HR-record or analytical accounting records; ○ verified that there is no difference between the total amount of personnel costs used in calculating the cost per unit and the total amount of personnel costs recorded in the statutory accounts; ○ verified whether actual personnel costs were adjusted on the basis of budgeted or estimated elements and, if so, verified whether those elements used are actually relevant for the calculation, objective and supported by documents.	used in all H2020 actions.	
		11) The employees were charged under the correct category.	
		12) Total personnel costs used in calculating the unit costs were consistent with the expenses recorded in the statutory accounts.	
		13) Any estimated or budgeted element used by the Beneficiary in its unit-cost calculation were relevant for calculating personnel costs and corresponded to objective and verifiable information.	
	<u>For natural persons included in the sample and working with the Beneficiary under a direct contract other than an employment contract, such as consultants (no subcontractors).</u> To confirm standard factual findings 14-17 listed in the next column the Auditor reviewed following information/documents provided by the Beneficiary: ○ the contracts, especially the cost, contract duration, work description, place of work, ownership of the results and reporting obligations to the Beneficiary; ○ the employment conditions of staff in the same category to compare costs and; ○ any other document that supports the costs declared and its registration (e.g. invoices, accounting records, etc.).	14) The natural persons worked under conditions similar to those of an employee, in particular regarding the way the work is organised, the tasks that are performed and the premises where they are performed.	
		15) The results of work carried out belong to the Beneficiary, or, if not, the Beneficiary has obtained all necessary rights to fulfil its obligations as if those	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
		results were generated by itself.	
		16) Their costs were not significantly different from those for staff who performed similar tasks under an employment contract with the Beneficiary.	
		17) The costs were supported by audit evidence and registered in the accounts.	
	<u>For personnel seconded by a third party and included in the sample (not subcontractors)</u> To confirm standard factual findings 18-21 listed in the next column, the Auditor reviewed following information/documents provided by the Beneficiary: o their secondment contract(s) notably regarding costs, duration, work description, place of work and ownership of the results; o if there is reimbursement by the Beneficiary to the third party for the resource made available_(in-kind contribution against payment): any documentation that supports the costs declared (e.g. contract, invoice, bank payment, and proof of registration in its accounting/payroll, etc.) and reconciliation of the Financial Statement(s) with the accounting system (project accounting and general ledger) as well as any proof that the amount invoiced by the third party did not include any profit; o if there is no reimbursement by the Beneficiary to the third party for the resource made available (in-kind contribution free of charge): a proof of the actual cost borne by the Third Party for the resource made available free of charge to the Beneficiary such as a statement of costs incurred by the Third Party and proof of the registration in the Third Party's accounting/payroll;	18) Seconded personnel reported to the Beneficiary and worked on the Beneficiary's premises (unless otherwise agreed with the Beneficiary).	
		19) The results of work carried out belong to the Beneficiary, or, if not, the Beneficiary has obtained all necessary rights to fulfil its obligations as if those results were generated by itself..	
		If personnel is seconded against payment: 20) The costs declared were supported with documentation and recorded in the	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ any other document that supports the costs declared (e.g. invoices, etc.).	Beneficiary's accounts. The third party did not include any profit.	
		If personnel is seconded free of charge: 21) The costs declared did not exceed the third party's cost as recorded in the accounts of the third party and were supported with documentation.	
A.2	**PRODUCTIVE HOURS** To confirm standard factual findings 22-27 listed in the next column, the Auditor reviewed relevant documents, especially national legislation, labour agreements and contracts and time records of the persons included in the sample, to verify that: ○ the annual productive hours applied were calculated in accordance with one of the methods described below, ○ the full-time equivalent (FTEs) ratios for employees not working full-time were correctly calculated. If the Beneficiary applied method B, the auditor verified that the correctness in which the total number of hours worked was calculated and that the contracts specified the annual workable hours. If the Beneficiary applied method C, the auditor verified that the 'annual productive hours' applied when calculating the hourly rate were equivalent to at least 90 % of the 'standard annual workable hours'. The Auditor can only do this if the calculation of the standard annual workable	22) The Beneficiary applied method [*choose one option and delete the others*] [**A**: 1720 hours] [**B**: the 'total number of hours worked'] [**C**: 'standard annual productive hours' used correspond to usual accounting practices]	
		23) Productive hours were calculated annually.	
		24) For employees not working full-time the full-time equivalent (FTE) ratio was correctly applied.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	hours can be supported by records, such as national legislation, labour agreements, and contracts. *BENEFICIARY'S PRODUCTIVE HOURS' FOR PERSONS WORKING FULL TIME SHALL BE ONE OF THE FOLLOWING METHODS:* ***A.*** *1720 ANNUAL PRODUCTIVE HOURS (PRO-RATA FOR PERSONS NOT WORKING FULL-TIME)* ***B.*** *THE TOTAL NUMBER OF HOURS WORKED BY THE PERSON FOR THE BENEFICIARY IN THE YEAR (THIS METHOD IS ALSO REFERRED TO AS 'TOTAL NUMBER OF HOURS WORKED' IN THE NEXT COLUMN). THE CALCULATION OF THE TOTAL NUMBER OF HOURS WORKED WAS DONE AS FOLLOWS: ANNUAL WORKABLE HOURS OF THE PERSON ACCORDING TO THE EMPLOYMENT CONTRACT, APPLICABLE LABOUR AGREEMENT OR NATIONAL LAW PLUS OVERTIME WORKED MINUS ABSENCES (SUCH AS SICK LEAVE OR SPECIAL LEAVE).* ***C.*** *THE STANDARD NUMBER OF ANNUAL HOURS GENERALLY APPLIED BY THE BENEFICIARY FOR ITS PERSONNEL IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICES (THIS METHOD IS ALSO REFERRED TO AS 'STANDARD ANNUAL PRODUCTIVE HOURS' IN THE NEXT COLUMN). THIS NUMBER MUST BE AT LEAST 90% OF THE STANDARD ANNUAL WORKABLE HOURS.* *'ANNUAL WORKABLE HOURS' MEANS THE PERIOD DURING WHICH THE PERSONNEL MUST BE WORKING, AT THE EMPLOYER'S DISPOSAL AND CARRYING OUT HIS/HER ACTIVITY OR DUTIES UNDER THE EMPLOYMENT CONTRACT, APPLICABLE COLLECTIVE LABOUR AGREEMENT OR NATIONAL WORKING TIME LEGISLATION.*	*If the Beneficiary applied method B.* 25) The calculation of the number of 'annual workable hours', overtime and absences was verifiable based on the documents provided by the Beneficiary. 25.1) The Beneficiary calculates the hourly rates per full financial year following procedure A.3 (method B is not allowed for beneficiaries calculating hourly rates per month).	
		If the Beneficiary applied method C. 26) The calculation of the number of 'standard annual workable hours' was verifiable based on the documents provided by the Beneficiary.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
		27) The 'annual productive hours' used for calculating the hourly rate were consistent with the usual cost accounting practices of the Beneficiary and were equivalent to at least 90 % of the 'annual workable hours'.	
A.3	**HOURLY PERSONNEL RATES** <u>I) For unit costs calculated in accordance to the Beneficiary's usual cost accounting practice (unit costs):</u> If the Beneficiary has a "Certificate on Methodology to calculate unit costs " (CoMUC) approved by the Commission, the Beneficiary provides the Auditor with a description of the approved methodology and the Commission's letter of acceptance. The Auditor verified that the Beneficiary has indeed used the methodology approved. If so, no further verification is necessary. If the Beneficiary does not have a "Certificate on Methodology" (CoMUC) approved by the Commission, or if the methodology approved was not applied, then the Auditor: o reviewed the documentation provided by the Beneficiary, including manuals and internal guidelines that explain how to calculate hourly rates; o recalculated the unit costs (hourly rates) of staff included in the sample following the results of the procedures carried out in A.1 and A.2. <u>II) For individual hourly rates:</u> The Auditor: o reviewed the documentation provided by the Beneficiary, including manuals and internal guidelines that explain how to calculate hourly rates;	28) The Beneficiary applied [*choose one option and delete the other*]: [Option I: "Unit costs (hourly rates) were calculated in accordance with the Beneficiary's usual cost accounting practices"] [Option II: Individual hourly rates were applied]	
		For option I concerning unit costs and if the Beneficiary applies the methodology approved by the Commission (CoMUC): 29) The Beneficiary used the Commission-approved methodology to calculate hourly rates. It corresponded to the organisation's usual cost accounting practices and was applied consistently for all	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ recalculated the hourly rates of staff included in the sample (recalculation of all hourly rates if the Beneficiary uses annual rates, recalculation of three months selected randomly for every year and person if the Beneficiary uses monthly rates) following the results of the procedures carried out in A.1 and A.2; ○ (only in case of monthly rates) confirmed that the time spent on parental leave is not deducted, and that, if parts of the basic remuneration are generated over a period longer than a month, the Beneficiary has included only the share which is generated in the month.	activities irrespective of the source of funding.	
	"UNIT COSTS CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICES": *IT IS CALCULATED BY DIVIDING THE TOTAL AMOUNT OF PERSONNEL COSTS OF THE CATEGORY TO WHICH THE EMPLOYEE BELONGS VERIFIED IN LINE WITH PROCEDURE A.1 BY THE NUMBER OF FTE AND THE ANNUAL TOTAL PRODUCTIVE HOURS OF THE SAME CATEGORY CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH PROCEDURE A.2.*	*For option I concerning unit costs and if the Beneficiary applies a methodology not approved by the Commission:* 30) The unit costs re-calculated by the Auditor were the same as the rates applied by the Beneficiary.	
	HOURLY RATE FOR INDIVIDUAL ACTUAL PERSONAL COSTS: *IT IS CALCULATED FOLLOWING ONE OF THE TWO OPTIONS BELOW:* *A) [OPTION BY DEFAULT] BY DIVIDING THE ACTUAL ANNUAL AMOUNT OF PERSONNEL COSTS OF AN EMPLOYEE VERIFIED IN LINE WITH PROCEDURE A.1 BY THE NUMBER OF ANNUAL PRODUCTIVE HOURS VERIFIED IN LINE WITH PROCEDURE A.2 (FULL FINANCIAL YEAR HOURLY RATE);* *B) BY DIVIDING THE ACTUAL MONTHLY AMOUNT OF PERSONNEL COSTS OF AN EMPLOYEE VERIFIED IN LINE WITH PROCEDURE A.1 BY 1/12 OF THE NUMBER OF ANNUAL PRODUCTIVE HOURS VERIFIED IN LINE WITH PROCEDURE A.2.(MONTHLY HOURLY RATE).*	*For option II concerning individual hourly rates:* 31) The individual rates re-calculated by the Auditor were the same as the rates applied by the Beneficiary. 31.1) The Beneficiary used only one option (per full financial year or per month) throughout each financial year examined. 31.2) The hourly rates do not include additional remuneration.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
A.4	**TIME RECORDING SYSTEM** To verify that the time recording system ensures the fulfilment of all minimum requirements and that the hours declared for the action were correct, accurate and properly authorised and supported by documentation, the Auditor made the following checks for the persons included in the sample that declare time as worked for the action on the basis of time records: o description of the time recording system provided by the Beneficiary (registration, authorisation, processing in the HR-system); o its actual implementation; o time records were signed at least monthly by the employees (on paper or electronically) and authorised by the project manager or another manager; o the hours declared were worked within the project period; o there were no hours declared as worked for the action if HR-records showed absence due to holidays or sickness (further cross-checks with travels are carried out in B.1 below) ; o the hours charged to the action matched those in the time recording system. *ONLY THE HOURS WORKED ON THE ACTION CAN BE CHARGED. ALL WORKING TIME TO BE CHARGED SHOULD BE RECORDED THROUGHOUT THE DURATION OF THE PROJECT, ADEQUATELY SUPPORTED BY EVIDENCE OF THEIR REALITY AND RELIABILITY (SEE SPECIFIC PROVISIONS BELOW FOR PERSONS WORKING EXCLUSIVELY FOR THE ACTION WITHOUT TIME RECORDS).*	32) All persons recorded their time dedicated to the action on a **daily/ weekly/ monthly** basis using a **paper/computer-based** system. (*delete the answers that are not applicable)*	
		33) Their time-records were authorised at least monthly by the project manager or other superior.	
		34) Hours declared were worked within the project period and were consistent with the presences/absences recorded in HR-records.	
		35) There were no discrepancies between the number of hours charged to the action and the number of hours recorded.	
	<u>If the persons are working exclusively for the action and without time records</u> For the persons selected that worked exclusively for the action without time records, the Auditor verified evidence available demonstrating that they were in reality exclusively dedicated to the action and that the Beneficiary signed a declaration confirming that they have worked exclusively for the action.	36) The exclusive dedication is supported by a declaration signed by the Beneficiary and by any other evidence gathered.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
B	**COSTS OF SUBCONTRACTING**		
B.1	**The Auditor obtained the detail/breakdown of subcontracting costs and sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). To confirm standard factual findings 37-41 listed in the next column, the Auditor reviewed the following for the items included in the sample: o the use of subcontractors was foreseen in Annex 1; o subcontracting costs were declared in the subcontracting category of the Financial Statement; o supporting documents on the selection and award procedure were followed; o the Beneficiary ensured best value for money (key elements to appreciate the respect of this principle are the award of the subcontract to the bid offering best price-quality ratio, under conditions of transparency and equal treatment. In case an existing framework contract was used the Beneficiary ensured it was established on the basis of the principle of best value for money under conditions of transparency and equal treatment). In particular, i. if the Beneficiary acted as a contracting authority within the meaning of Directive 2004/18/EC (or 2014/24/EU) or of Directive 2004/17/EC (or 2014/25/EU), the Auditor verified that the applicable national law on public procurement was followed and that the subcontracting complied with the Terms and Conditions of the Agreement. ii. if the Beneficiary did not fall under the above-mentioned category the Auditor verified that the Beneficiary followed their usual procurement rules and respected the Terms and Conditions of the Agreement..	37) The use of claimed subcontracting costs was foreseen in Annex 1 and costs were declared in the Financial Statements under the subcontracting category.	
		38) There were documents of requests to different providers, different offers and assessment of the offers before selection of the provider in line with internal procedures and procurement rules. Subcontracts were awarded in accordance with the principle of best value for money. *(When different offers were not collected the Auditor explains the reasons provided by the Beneficiary under the caption "Exceptions" of the Report. The Commission will analyse this information to evaluate whether these costs might be accepted as eligible)*	
		39) The subcontracts were not awarded to other Beneficiaries	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	For the items included in the sample the Auditor also verified that: o the subcontracts were not awarded to other Beneficiaries in the consortium; o there were signed agreements between the Beneficiary and the subcontractor; o there was evidence that the services were provided by subcontractor;	of the consortium.	
		40) All subcontracts were supported by signed agreements between the Beneficiary and the subcontractor.	
		41) There was evidence that the services were provided by the subcontractors.	
C	**COSTS OF PROVIDING FINANCIAL SUPPORT TO THIRD PARTIES**		
C.1	**The Auditor obtained the detail/breakdown of the costs of providing financial support to third parties and sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). The Auditor verified that the following minimum conditions were met: a) the maximum amount of financial support for each third party did not exceed EUR 60 000, unless explicitly mentioned in Annex 1; b) the financial support to third parties was agreed in Annex 1 of the Agreement and the other provisions on financial support to third parties included in Annex 1 were respected.	42) All minimum conditions were met	

D	OTHER ACTUAL DIRECT COSTS		
D.1	**COSTS OF TRAVEL AND RELATED SUBSISTENCE ALLOWANCES** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is the highest*). The Auditor inspected the sample and verified that: o travel and subsistence costs were consistent with the Beneficiary's usual policy for travel. In this context, the Beneficiary provided evidence of its normal policy for travel costs (e.g. use of first class tickets, reimbursement by the Beneficiary on the basis of actual costs, a lump sum or per diem) to enable the Auditor to compare the travel costs charged with this policy; o travel costs are correctly identified and allocated to the action (e.g. trips are directly linked to the action) by reviewing relevant supporting documents such as minutes of meetings, workshops or conferences, their registration in the correct project account, their consistency with time records or with the dates/duration of the workshop/conference; o no ineligible costs or excessive or reckless expenditure was declared (see Article 6.5 MGA).	43) Costs were incurred, approved and reimbursed in line with the Beneficiary's usual policy for travels.	
		44) There was a link between the trip and the action.	
		45) The supporting documents were consistent with each other regarding subject of the trip, dates, duration and reconciled with time records and accounting.	
		46) No ineligible costs or excessive or reckless expenditure was declared.	
D.2	**DEPRECIATION COSTS FOR EQUIPMENT, INFRASTRUCTURE OR OTHER ASSETS** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is the highest*). For "equipment, infrastructure or other assets" [from now on called "asset(s)"] selected in the sample the Auditor verified that: o the assets were acquired in conformity with the Beneficiary's internal guidelines and procedures;	47) Procurement rules, principles and guides were followed.	
		48) There was a link between the grant agreement and the asset charged to the action.	
		49) The asset charged to the action was traceable to the accounting records and the underlying documents.	

	○ they were correctly allocated to the action (with supporting documents such as delivery note invoice or any other proof demonstrating the link to the action) ○ they were entered in the accounting system; ○ the extent to which the assets were used for the action (as a percentage) was supported by reliable documentation (e.g. usage overview table); The Auditor recalculated the depreciation costs and verified that they were in line with the applicable rules in the Beneficiary's country and with the Beneficiary's usual accounting policy (e.g. depreciation calculated on the acquisition value). The Auditor verified that no ineligible costs such as deductible VAT, exchange rate losses, excessive or reckless expenditure were declared (see Article 6.5 GA).	50) The depreciation method used to charge the asset to the action was in line with the applicable rules of the Beneficiary's country and the Beneficiary's usual accounting policy.	
		51) The amount charged corresponded to the actual usage for the action.	
		52) No ineligible costs or excessive or reckless expenditure were declared.	
D.3	**COSTS OF OTHER GOODS AND SERVICES** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). For the purchase of goods, works or services included in the sample the Auditor verified that: ○ the contracts did not cover tasks described in Annex 1; ○ they were correctly identified, allocated to the proper action, entered in the accounting system (traceable to underlying documents such as purchase orders, invoices and accounting); ○ the goods were not placed in the inventory of durable equipment; ○ the costs charged to the action were accounted in line with the Beneficiary's usual accounting practices; ○ no ineligible costs or excessive or reckless expenditure were declared (see Article 6 GA). In addition, the Auditor verified that these goods and services were acquired in conformity with	53) Contracts for works or services did not cover tasks described in Annex 1.	
		54) Costs were allocated to the correct action and the goods were not placed in the inventory of durable equipment.	
		55) The costs were charged in line with the Beneficiary's accounting policy and were adequately supported.	
		56) No ineligible costs or excessive or reckless expenditure were declared. For internal invoices/charges only the cost element was charged, without any mark-ups.	

	the Beneficiary's internal guidelines and procedures, in particular: o if Beneficiary acted as a contracting authority within the meaning of Directive 2004/18/EC (or 2014/24/EU) or of Directive 2004/17/EC (or 2014/25/EU), the Auditor verified that the applicable national law on public procurement was followed and that the procurement contract complied with the Terms and Conditions of the Agreement. o if the Beneficiary did not fall into the category above, the Auditor verified that the Beneficiary followed their usual procurement rules and respected the Terms and Conditions of the Agreement. For the items included in the sample the Auditor also verified that: o the Beneficiary ensured best value for money (key elements to appreciate the respect of this principle are the award of the contract to the bid offering best price-quality ratio, under conditions of transparency and equal treatment. In case an existing framework contract was used the Auditor also verified that the Beneficiary ensured it was established on the basis of the principle of best value for money under conditions of transparency and equal treatment); *SUCH GOODS AND SERVICES INCLUDE, FOR INSTANCE, CONSUMABLES AND SUPPLIES, DISSEMINATION (INCLUDING OPEN ACCESS), PROTECTION OF RESULTS, SPECIFIC EVALUATION OF THE ACTION IF IT IS REQUIRED BY THE AGREEMENT, CERTIFICATES ON THE FINANCIAL STATEMENTS IF THEY ARE REQUIRED BY THE AGREEMENT AND CERTIFICATES ON THE METHODOLOGY, TRANSLATIONS, REPRODUCTION.*	57) Procurement rules, principles and guides were followed. There were documents of requests to different providers, different offers and assessment of the offers before selection of the provider in line with internal procedures and procurement rules. The purchases were made in accordance with the principle of best value for money. *(When different offers were not collected the Auditor explains the reasons provided by the Beneficiary under the caption "Exceptions" of the Report. The Commission will analyse this information to evaluate whether these costs might be accepted as eligible)*	
D.4	**AGGREGATED CAPITALISED AND OPERATING COSTS OF RESEARCH INFRASTRUCTURE** The Auditor ensured the existence of a positive ex-ante assessment (issued by the EC Services) of the cost accounting methodology of the Beneficiary allowing it to apply the guidelines on direct costing for large research infrastructures in Horizon 2020.	58) The costs declared as direct costs for Large Research Infrastructures (in the appropriate line of the Financial Statement) comply with the methodology described in the positive ex-ante assessment report.	

	In the cases that a positive ex-ante assessment has been issued *(see the standard factual findings 58-59 on the next column)***,** The Auditor ensured that the beneficiary has applied consistently the methodology that is explained and approved in the positive ex ante assessment; ***In the cases that a positive ex-ante assessment has NOT been issued*** *(see the standard factual findings 60 on the next column),* The Auditor verified that no costs of Large Research Infrastructure have been charged as direct costs in any costs category; ***In the cases that a draft ex-ante assessment report has been issued with recommendation for further changes*** *(see the standard factual findings 60 on the next column),* • The Auditor followed the same procedure as above (when a positive ex-ante assessment has NOT yet been issued) and paid particular attention (testing reinforced) to the cost items for which the draft ex-ante assessment either rejected the inclusion as direct costs for Large Research Infrastructures or issued recommendations.	59) Any difference between the methodology applied and the one positively assessed was extensively described and adjusted accordingly. 60) The direct costs declared were free from any indirect costs items related to the Large Research Infrastructure.	
D.5	**Costs of internally invoiced goods and services** **The Auditor sampled cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). To confirm standard factual findings 61-65 listed in the next column, the Auditor: ○ obtained a description of the Beneficiary's usual cost accounting practice to calculate costs of internally invoiced goods and services (unit costs); ○ reviewed whether the Beneficiary's usual cost accounting practice was applied for the Financial Statements subject of the present CFS; ○ ensured that the methodology to calculate unit costs is being used in a consistent manner, based on objective criteria, regardless of the source of funding; ○ verified that any ineligible items or any costs claimed under other budget categories, in particular indirect costs, have not been taken into account when calculating the costs of	61) The costs of internally invoiced goods and services included in the Financial Statement were calculated in accordance with the Beneficiary's usual cost accounting practice. 62) The cost accounting practices used to calculate the costs of internally invoiced goods and services were applied by the Beneficiary in a consistent manner based on objective criteria regardless of the source of funding. 63) The unit cost is calculated using the actual costs for the good or service recorded in the Beneficiary's accounts, excluding any ineligible cost or costs included in other	

	internally invoiced goods and services (see Article 6 GA); ○ verified whether actual costs of internally invoiced goods and services were adjusted on the basis of budgeted or estimated elements and, if so, verified whether those elements used are actually relevant for the calculation, and correspond to objective and verifiable information. ○ verified that any costs of items which are not directly linked to the production of the invoiced goods or service (e.g. supporting services like cleaning, general accountancy, administrative support, etc. not directly used for production of the good or service) have not been taken into account when calculating the costs of internally invoiced goods and services. ○ verified that any costs of items used for calculating the costs internally invoiced goods and services are supported by audit evidence and registered in the accounts.	budget categories. 64) The unit cost excludes any costs of items which are not directly linked to the production of the invoiced goods or service. 65) The costs items used for calculating the actual costs of internally invoiced goods and services were relevant, reasonable and correspond to objective and verifiable information.	
E	**USE OF EXCHANGE RATES**		
E.1	a) For Beneficiaries with accounts established in a currency other than euros **The Auditor sampled _____ cost items selected randomly and verified that the exchange rates used for converting other currencies into euros were in accordance with the following rules established in the Agreement** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest)*: *COSTS RECORDED IN THE ACCOUNTS IN A CURRENCY OTHER THAN EURO SHALL BE CONVERTED INTO EURO AT THE AVERAGE OF THE DAILY EXCHANGE RATES PUBLISHED IN THE C SERIES OF OFFICIAL JOURNAL OF THE EUROPEAN UNION (https://www.ecb.int/stats/exchange/eurofxref/html/index.en.html), DETERMINED OVER THE CORRESPONDING REPORTING PERIOD.* *IF NO DAILY EURO EXCHANGE RATE IS PUBLISHED IN THE OFFICIAL JOURNAL OF THE EUROPEAN UNION FOR THE CURRENCY IN QUESTION, CONVERSION SHALL BE MADE AT THE AVERAGE OF THE MONTHLY ACCOUNTING RATES ESTABLISHED BY THE COMMISSION AND PUBLISHED ON ITS WEBSITE (http://ec.europa.eu/budget/contracts_grants/info_contracts/inforeuro/inforeuro_en.cfm),*	66) The exchange rates used to convert other currencies into Euros were in accordance with the rules established of the Grant Agreement and there was no difference in the final figures.	

	DETERMINED OVER THE CORRESPONDING REPORTING PERIOD.		
	b) For Beneficiaries with accounts established in euros **The Auditor sampled _____ cost items selected randomly and verified that the exchange rates used for converting other currencies into euros were in accordance with the following rules established in the Agreement** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest)*: *COSTS INCURRED IN ANOTHER CURRENCY SHALL BE CONVERTED INTO EURO BY APPLYING THE BENEFICIARY'S USUAL ACCOUNTING PRACTICES.*	67) The Beneficiary applied its usual accounting practices.	

[legal name of the audit firm]
[name and function of an authorised representative]
[dd Month yyyy]
<Signature of the Auditor>

ANNEX 6

MODEL FOR THE CERTIFICATE ON THE METHODOLOGY

- **For options [*in italics in square brackets*]: choose the applicable option. Options not chosen should be deleted.**
- **For fields in [grey in square brackets]: enter the appropriate data.**

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TERMS OF REFERENCE FOR AN AUDIT ENGAGEMENT FOR A METHODOLOGY CERTIFICATE IN CONNECTION WITH ONE OR MORE GRANT AGREEMENTS FINANCED UNDER THE HORIZON 2020 RESEARCH AND INNOVATION FRAMEWORK PROGRAMME

INDEPENDENT REPORT OF FACTUAL FINDINGS ON THE METHODOLOGY CONCERNING GRANT AGREEMENTS FINANCED UNDER THE HORIZON 2020 RESEARCH AND INNOVATION FRAMEWORK PROGRAMME

Terms of reference for an audit engagement for a methodology certificate in connection with one or more grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme

This document sets out the '**Terms of Reference (ToR)**' under which

[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]

agrees to engage

[**insert legal name of the auditor**] ('the Auditor')

to produce an independent report of factual findings ('the Report') concerning the *[Beneficiary's] [Linked Third Party's]* usual accounting practices for calculating and claiming direct personnel costs declared as unit costs ('the Methodology') in connection with grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme.

The procedures to be carried out for the assessment of the methodology will be based on the grant agreement(s) detailed below:

[title and number of the grant agreement(s)] ('the Agreement(s)')

The Agreement(s) has(have) been concluded between the Beneficiary and *[OPTION 1: the European Union, represented by the European Commission ('the Commission')][OPTION 2: the European Atomic Energy Community (Euratom,) represented by the European Commission ('the Commission')][OPTION 3: the [Research Executive Agency (REA)] [European Research Council Executive Agency (ERCEA)] [Innovation and Networks Executive Agency (INEA)] [Executive Agency for Small and Medium-sized Enterprises (EASME)] ('the Agency'), under the powers delegated by the European Commission ('the Commission').].*

The *[Commission] [Agency]* is mentioned as a signatory of the Agreement with the Beneficiary only. The *[European Union] [Euratom] [Agency]* is not a party to this engagement.

1.1 Subject of the engagement

According to Article 18.1.2 of the Agreement, beneficiaries *[and linked third parties]* that declare direct personnel costs as unit costs calculated in accordance with their usual cost accounting practices may submit to the *[Commission] [Agency]*, for approval, a certificate on the methodology ('CoMUC') stating that there are adequate records and documentation to prove that their cost accounting practices used comply with the conditions set out in Point A of Article 6.2.

The subject of this engagement is the CoMUC which is composed of two separate documents:

- the Terms of Reference ('the ToR') to be signed by the *[Beneficiary] [Linked Third Party]* and the Auditor;

- the Auditor's Independent Report of Factual Findings ('the Report') issued on the Auditor's letterhead, dated, stamped and signed by the Auditor which includes; the standard statements ('the Statements') evaluated and signed by the *[Beneficiary] [Linked Third Party]*, the agreed-upon procedures ('the Procedures') performed by the Auditor and the standard factual findings

('the Findings') assessed by the Auditor. The Statements, Procedures and Findings are summarised in the table that forms part of the Report.

The information provided through the Statements, the Procedures and the Findings will enable the Commission to draw conclusions regarding the existence of the *[Beneficiary's] [Linked Third Party's]* usual cost accounting practice and its suitability to ensure that direct personnel costs claimed on that basis comply with the provisions of the Agreement. The Commission draws its own conclusions from the Report and any additional information it may require.

1.2 Responsibilities

The parties to this agreement are the *[Beneficiary] [Linked Third Party]* and the Auditor.

The *[Beneficiary] [Linked Third Party]:*

- is responsible for preparing financial statements for the Agreement(s) ('the Financial Statements') in compliance with those Agreements;
- is responsible for providing the Financial Statement(s) to the Auditor and enabling the Auditor to reconcile them with the *[Beneficiary's] [Linked Third Party's]* accounting and bookkeeping system and the underlying accounts and records. The Financial Statement(s) will be used as a basis for the procedures which the Auditor will carry out under this ToR;
- is responsible for its Methodology and liable for the accuracy of the Financial Statement(s);
- is responsible for endorsing or refuting the Statements indicated under the heading 'Statements to be made by the Beneficiary/ Linked Third Party' in the first column of the table that forms part of the Report;
- must provide the Auditor with a signed and dated representation letter;
- accepts that the ability of the Auditor to carry out the Procedures effectively depends upon the *[Beneficiary] [Linked Third Party]* providing full and free access to the *[Beneficiary's] [Linked Third Party's]* staff and to its accounting and other relevant records.

The Auditor:

- *[Option 1 by default: is qualified to carry out statutory audits of accounting documents in accordance with Directive 2006/43/EC of the European Parliament and of the Council of 17 May 2006 on statutory audits of annual accounts and consolidated accounts, amending Council Directives 78/660/EEC and 83/349/EEC and repealing Council Directive 84/253/EEC or similar national regulations].*
- *[Option 2 if the Beneficiary or Linked Third Party has an independent Public Officer: is a competent and independent Public Officer for which the relevant national authorities have established the legal capacity to audit the Beneficiary].*
- *[Option 3 if the Beneficiary or Linked Third Party is an international organisation: is an [internal] [external] auditor in accordance with the internal financial regulations and procedures of the international organisation].*

The Auditor:

- must be independent from the Beneficiary *[and the Linked Third Party]*, in particular, it must not have been involved in preparing the Beneficiary's *[and Linked Third Party's]* Financial Statement(s);
- must plan work so that the Procedures may be carried out and the Findings may be assessed;
- must adhere to the Procedures laid down and the compulsory report format;
- must carry out the engagement in accordance with these ToR;
- must document matters which are important to support the Report;
- must base its Report on the evidence gathered;
- must submit the Report to the *[Beneficiary] [Linked Third Party]*.

The Commission sets out the Procedures to be carried out and the Findings to be endorsed by the Auditor. The Auditor is not responsible for their suitability or pertinence. As this engagement is not an assurance engagement the Auditor does not provide an audit opinion or a statement of assurance.

1.3 Applicable Standards

The Auditor must comply with these Terms of Reference and with[1]:

- the International Standard on Related Services ('ISRS') 4400 *Engagements to perform Agreed-upon Procedures regarding Financial Information* as issued by the International Auditing and Assurance Standards Board (IAASB);
- the *Code of Ethics for Professional Accountants* issued by the International Ethics Standards Board for Accountants (IESBA). Although ISRS 4400 states that independence is not a requirement for engagements to carry out agreed-upon procedures, the Commission requires that the Auditor also complies with the Code's independence requirements.

The Auditor's Report must state that there was no conflict of interests in establishing this Report between the Auditor and the Beneficiary *[and the Linked Third Party]* that could have a bearing on the Report, and must specify – if the service is invoiced - the total fee paid to the Auditor for providing the Report.

1.4 Reporting

The Report must be written in the language of the Agreement (see Article 20.7 of the Agreement).

Under Article 22 of the Agreement, the Commission, *[the Agency]*, the European Anti-Fraud Office and the Court of Auditors have the right to audit any work that is carried out under the action and for which costs are declared from *[the European Union] [Euratom]* budget. This includes work related to this engagement. The Auditor must provide access to all working papers related to this assignment if the Commission*[, the Agency]*, the European Anti-Fraud Office or the European Court of Auditors requests them.

1.5 Timing

The Report must be provided by [dd Month yyyy].

1.6 Other Terms

[The [Beneficiary] [Linked Third Party] and the Auditor can use this section to agree other specific terms, such as the Auditor's fees, liability, applicable law, etc. Those specific terms must not contradict the terms specified above.]

[legal name of the Auditor]	[legal name of the [Beneficiary] [Linked Third Party]]
[name & title of authorised representative]	[name & title of authorised representative]
[dd Month yyyy]	[dd Month yyyy]
Signature of the Auditor	Signature of the *[Beneficiary] [Linked Third Party]*

[1] Supreme Audit Institutions applying INTOSAI-standards may carry out the Procedures according to the corresponding International Standards of Supreme Audit Institutions and code of ethics issued by INTOSAI instead of the International Standard on Related Services ('ISRS') 4400 and the Code of Ethics for Professional Accountants issued by the IAASB and the IESBA.

Independent report of factual findings on the methodology concerning grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme

(To be printed on letterhead paper of the auditor)

To
[name of contact person(s)], [Position]
[[Beneficiary's] [Linked Third Party's] name]
[Address]
[dd Month yyyy]

Dear [Name of contact person(s)],

As agreed under the terms of reference dated [dd Month yyyy]

with *[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]*,

we

[name of the auditor] ('the Auditor'),

established at

[full address/city/state/province/country],

represented by

[name and function of an authorised representative],

have carried out the agreed-upon procedures ('the Procedures') and provide hereby our Independent Report of Factual Findings ('the Report'), concerning the *[Beneficiary's] [Linked Third Party's]* usual accounting practices for calculating and declaring direct personnel costs declared as unit costs ('the Methodology').

You requested certain procedures to be carried out in connection with the grant(s)

[title and number of the grant agreement(s)] ('the Agreement(s)').

The Report

Our engagement was carried out in accordance with the terms of reference ('the ToR') appended to this Report. The Report includes: the standard statements ('the Statements') made by the *[Beneficiary] [Linked Third Party]*, the agreed-upon procedures ('the Procedures') carried out and the standard factual findings ('the Findings') confirmed by us.

The engagement involved carrying out the Procedures and assessing the Findings and the documentation requested appended to this Report, the results of which the Commission uses to draw conclusions regarding the acceptability of the Methodology applied by the *[Beneficiary] [Linked Third Party]*.

The Report covers the methodology used from [dd Month yyyy]. In the event that the *[Beneficiary] [Linked Third Party]* changes this methodology, the Report will not be applicable to any Financial Statement[1] submitted thereafter.

The scope of the Procedures and the definition of the standard statements and findings were determined solely by the Commission. Therefore, the Auditor is not responsible for their suitability or pertinence.

Since the Procedures carried out constitute neither an audit nor a review made in accordance with International Standards on Auditing or International Standards on Review Engagements, we do not give a statement of assurance on the costs declared on the basis of the *[Beneficiary's] [Linked Third Party's]* Methodology. Had we carried out additional procedures or had we performed an audit or review in accordance with these standards, other matters might have come to its attention and would have been included in the Report.

Exceptions

Apart from the exceptions listed below, the *[Beneficiary] [Linked Third Party]* agreed with the standard Statements and provided the Auditor all the documentation and accounting information needed by the Auditor to carry out the requested Procedures and corroborate the standard Findings.

List here any exception and add any information on the cause and possible consequences of each exception, if known. If the exception is quantifiable, also indicate the corresponding amount.

…..

Explanation of possible exceptions in the form of examples (to be removed from the Report):

i. the [Beneficiary] [Linked Third Party] did not agree with the standard Statement number … because…;

ii. the Auditor could not carry out the procedure … established because …. (e.g. due to the inability to reconcile key information or the unavailability or inconsistency of data);

iii. the Auditor could not confirm or corroborate the standard Finding number … because ….

Remarks

We would like to add the following remarks relevant for the proper understanding of the Methodology applied by the [Beneficiary] [Linked Third Party] or the results reported:

Example (to be removed from the Report):

Regarding the methodology applied to calculate hourly rates …

Regarding standard Finding 15 it has to be noted that …

The [Beneficiary] [Linked Third Party] explained the deviation from the benchmark statement XXIV concerning time recording for personnel with no exclusive dedication to the action in the following manner: …

Annexes

Please provide the following documents to the auditor and annex them to the report when submitting this CoMUC to the Commission:

[1] Financial Statement in this context refers solely to Annex 4 of the Agreement by which the Beneficiary declares costs under the Agreement.

1. Brief description of the methodology for calculating personnel costs, productive hours and hourly rates;
2. Brief description of the time recording system in place;
3. An example of the time records used by the [*Beneficiary] [Linked Third Party*];
4. Description of any budgeted or estimated elements applied, together with an explanation as to why they are relevant for calculating the personnel costs and how they are based on objective and verifiable information;
5. A summary sheet with the hourly rate for direct personnel declared by the [*Beneficiary*] [*Linked Third Party*] and recalculated by the Auditor for each staff member included in the sample (the names do not need to be reported);
6. A comparative table summarising for each person selected in the sample a) the time claimed by the [*Beneficiary*] [*Linked Third Party*] in the Financial Statement(s) and b) the time according to the time record verified by the Auditor;
7. A copy of the letter of representation provided to the Auditor.

Use of this Report

This Report has been drawn up solely for the purpose given under Point 1.1 Reasons for the engagement.

The Report:

- is confidential and is intended to be submitted to the Commission by the [*Beneficiary*] [*Linked Third Party*] in connection with Article 18.1.2 of the Agreement;
- may not be used by the [*Beneficiary*] [*Linked Third Party*] or by the Commission for any other purpose, nor distributed to any other parties;
- may be disclosed by the Commission only to authorised parties, in particular the European Anti-Fraud Office (OLAF) and the European Court of Auditors.
- relates only to the usual cost accounting practices specified above and does not constitute a report on the Financial Statements of the [*Beneficiary*] [*Linked Third Party*].

No conflict of interest[2] exists between the Auditor and the Beneficiary *[and the Linked Third Party*] that could have a bearing on the Report. The total fee paid to the Auditor for producing the Report was EUR _____ (including EUR _____ of deductible VAT).

We look forward to discussing our Report with you and would be pleased to provide any further information or assistance which may be required.

Yours sincerely

[legal name of the Auditor]
[name and title of the authorised representative]
[dd Month yyyy]
Signature of the Auditor

[2] A conflict of interest arises when the Auditor's objectivity to establish the certificate is compromised in fact or in appearance when the Auditor for instance:
- was involved in the preparation of the Financial Statements;
- stands to benefit directly should the certificate be accepted;
- has a close relationship with any person representing the beneficiary;
- is a director, trustee or partner of the beneficiary; or
- is in any other situation that compromises his or her independence or ability to establish the certificate impartially.

Statements to be made by the Beneficiary/Linked Third Party ('the Statements') and Procedures to be carried out by the Auditor ('the Procedures') and standard factual findings ('the Findings') to be confirmed by the Auditor

The Commission reserves the right to provide the auditor with guidance regarding the Statements to be made, the Procedures to be carried out or the Findings to be ascertained and the way in which to present them. The Commission reserves the right to vary the Statements, Procedures or Findings by written notification to the Beneficiary/Linked Third Party to adapt the procedures to changes in the grant agreement(s) or to any other circumstances.

If this methodology certificate relates to the Linked Third Party's usual accounting practices for calculating and claiming direct personnel costs declared as unit costs any reference here below to 'the Beneficiary' is to be considered as a reference to 'the Linked Third Party'.

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
A. Use of the Methodology I. The cost accounting practice described below has been in use since *[*dd Month yyyy*]*. II. The next planned alteration to the methodology used by the Beneficiary will be from [dd Month yyyy*]*.	**Procedure:** ✓ The Auditor checked these dates against the documentation the Beneficiary has provided. **Factual finding:** 1. The dates provided by the Beneficiary were consistent with the documentation.
B. Description of the Methodology III. The methodology to calculate unit costs is being used in a consistent manner and is reflected in the relevant procedures. *[Please describe the methodology your entity uses to calculate personnel costs, productive hours and hourly rates, present your description to the Auditor and annex it to this certificate]* *[If the statement of section "B. Description of the methodology" cannot be endorsed by the Beneficiary or there is no written methodology to calculate unit costs it should be listed here below and reported as exception by the Auditor in the main Report of Factual Findings:* - *…]*	**Procedure:** ✓ The Auditor reviewed the description, the relevant manuals and/or internal guidance documents describing the methodology. **Factual finding:** 2. The brief description was consistent with the relevant manuals, internal guidance and/or other documentary evidence the Auditor has reviewed. 3. The methodology was generally applied by the Beneficiary as part of its usual costs accounting practices.

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
C. **Personnel costs** <u>General</u> IV. The unit costs (hourly rates) are limited to salaries including during parental leave, social security contributions, taxes and other costs included in the remuneration required under national law and the employment contract or equivalent appointing act; V. Employees are hired directly by the Beneficiary in accordance with national law, and work under its sole supervision and responsibility; VI. The Beneficiary remunerates its employees in accordance with its usual practices. This means that personnel costs are charged in line with the Beneficiary's usual payroll policy (e.g. salary policy, overtime policy, variable pay) and no special conditions exist for employees assigned to tasks relating to the European Union or Euratom, unless explicitly provided for in the grant agreement(s); VII. The Beneficiary allocates its employees to the relevant group/category/cost centre for the purpose of the unit cost calculation in line with the usual cost accounting practice; VIII. Personnel costs are based on the payroll system and accounting system. IX. Any exceptional adjustments of actual personnel costs resulted from relevant budgeted or estimated elements and were based on objective and verifiable information. *[Please describe the 'budgeted or estimated elements' and their relevance to personnel costs, and explain how they were reasonable and based on objective and verifiable information, present your explanation to the Auditor and annex it to this certificate].* X. Personnel costs claimed do not contain any of the following ineligible costs: costs related to return on capital; debt and debt service charges; provisions for future losses or debts; interest owed; doubtful debts; currency exchange losses; bank costs charged by the Beneficiary's bank for transfers from the Commission/Agency; excessive or reckless expenditure; deductible VAT or costs incurred during suspension of the implementation of the action. XI. Personnel costs were not declared under another EU or Euratom grant	**Procedure:** *The Auditor draws a sample of employees to carry out the procedures indicated in this section C and the following sections D to F.* *[The Auditor has drawn a random sample of 10 employees assigned to Horizon 2020 action(s). If fewer than 10 employees are assigned to the Horizon 2020 action(s), the Auditor has selected all employees assigned to the Horizon 2020 action(s) complemented by other employees irrespective of their assignments until he has reached 10 employees.].* For this sample: ✓ the Auditor reviewed all documents relating to personnel costs such as employment contracts, payslips, payroll policy (e.g. salary policy, overtime policy, variable pay policy), accounting and payroll records, applicable national tax , labour and social security law and any other documents corroborating the personnel costs claimed; ✓ in particular, the Auditor reviewed the employment contracts of the employees in the sample to verify that: i. they were employed directly by the Beneficiary in accordance with applicable national legislation; ii. they were working under the sole technical supervision and responsibility of the latter; iii. they were remunerated in accordance with the Beneficiary's usual practices; iv. they were allocated to the correct group/category/cost centre for the purposes of calculating the unit cost in line with the Beneficiary's usual cost accounting practices; ✓ the Auditor verified that any ineligible items or any costs claimed under other costs categories or costs covered by other types of grant or by other grants financed from the European Union budget have not been taken into account when calculating the personnel costs; ✓ the Auditor numerically reconciled the total amount of personnel costs used to calculate the unit cost with the total amount of personnel costs recorded in the statutory accounts and the payroll system.

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
(including grants awarded by a Member State and financed by the EU budget and grants awarded by bodies other than the Commission/Agency for the purpose of implementing the EU or Euratom budget in the same period, unless the Beneficiary can demonstrate that the operating grant does not cover any costs of the action). <u>If additional remuneration as referred to in the grant agreement(s) is paid</u> XII. The Beneficiary is a non-profit legal entity; XIII. The additional remuneration is part of the beneficiary's usual remuneration practices and paid consistently whenever the relevant work or expertise is required; XIV. The criteria used to calculate the additional remuneration are objective and generally applied regardless of the source of funding; XV. The additional remuneration included in the personnel costs used to calculate the hourly rates for the grant agreement(s) is capped at EUR 8 000 per full-time equivalent (reduced proportionately if the employee is not assigned exclusively to the action). *[If certain statement(s) of section "C. Personnel costs" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor in the main Report of Factual Findings:* *- ...]*	✓ to the extent that actual personnel costs were adjusted on the basis of budgeted or estimated elements, the Auditor carefully examined those elements and checked the information source to confirm that they correspond to objective and verifiable information; ✓ if additional remuneration has been claimed, the Auditor verified that the Beneficiary was a non-profit legal entity, that the amount was capped at EUR 8 000 per full-time equivalent and that it was reduced proportionately for employees not assigned exclusively to the action(s). ✓ the Auditor recalculated the personnel costs for the employees in the sample. **Factual finding:** 4. All the components of the remuneration that have been claimed as personnel costs are supported by underlying documentation. 5. The employees in the sample were employed directly by the Beneficiary in accordance with applicable national law and were working under its sole supervision and responsibility. 6. Their employment contracts were in line with the Beneficiary's usual policy; 7. Personnel costs were duly documented and consisted solely of salaries, social security contributions (pension contributions, health insurance, unemployment fund contributions, etc.), taxes and other statutory costs included in the remuneration (holiday pay, thirteenth month's pay, etc.); 8. The totals used to calculate the personnel unit costs are consistent with those registered in the payroll and accounting records; 9. To the extent that actual personnel costs were adjusted on the basis of budgeted or estimated elements, those elements were relevant for calculating the personnel costs and correspond to objective and verifiable information. The budgeted or estimated elements used are: — (indicate the elements and their values). 10. Personnel costs contained no ineligible elements; 11. Specific conditions for eligibility were fulfilled when additional

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
	remuneration was paid: a) the Beneficiary is registered in the grant agreements as a non-profit legal entity; b) it was paid according to objective criteria generally applied regardless of the source of funding used and c) remuneration was capped at EUR 8 000 per full-time equivalent (or up to up to the equivalent pro-rata amount if the person did not work on the action full-time during the year or did not work exclusively on the action).
D. Productive hours XVI. The number of productive hours per full-time employee applied is *[delete as appropriate]*: A. 1720 productive hours per year for a person working full-time (corresponding pro-rata for persons not working full time). B. the total number of hours worked in the year by a person for the Beneficiary C. the standard number of annual hours generally applied by the beneficiary for its personnel in accordance with its usual cost accounting practices. This number must be at least 90% of the standard annual workable hours. <u>If method B is applied</u> XVII. The calculation of the total number of hours worked was done as follows: annual workable hours of the person according to the employment contract, applicable labour agreement or national law plus overtime worked minus absences (such as sick leave and special leave). XVIII. 'Annual workable hours' are hours during which the personnel must be working, at the employer's disposal and carrying out his/her activity or duties under the employment contract, applicable collective labour agreement or national working time legislation. XIX. The contract (applicable collective labour agreement or national working time legislation) do specify the working time enabling to calculate the annual workable hours.	**Procedure (same sample basis as for Section C: Personnel costs):** ✓ The Auditor verified that the number of productive hours applied is in accordance with method A, B or C. ✓ The Auditor checked that the number of productive hours per full-time employee is correct. ✓ If method B is applied the Auditor verified i) the manner in which the total number of hours worked was done and ii) that the contract specified the annual workable hours by inspecting all the relevant documents, national legislation, labour agreements and contracts. ✓ If method C is applied the Auditor reviewed the manner in which the standard number of working hours per year has been calculated by inspecting all the relevant documents, national legislation, labour agreements and contracts and verified that the number of productive hours per year used for these calculations was at least 90 % of the standard number of working hours per year. **Factual finding:** <u>General</u> 12. The Beneficiary applied a number of productive hours consistent with method A, B or C detailed in the left-hand column. 13. The number of productive hours per year per full-time employee was accurate. <u>If method B is applied</u> 14. The number of 'annual workable hours', overtime and absences was

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
<u>If method C is applied</u> XX. The standard number of productive hours per year is that of a full-time equivalent. XXI. The number of productive hours per year on which the hourly rate is based i) corresponds to the Beneficiary's usual accounting practices; ii) is at least 90 % of the standard number of workable (working) hours per year. XXII. Standard workable (working) hours are hours during which personnel are at the Beneficiary's disposal preforming the duties described in the relevant employment contract, collective labour agreement or national labour legislation. The number of standard annual workable (working) hours that the Beneficiary claims is supported by labour contracts, national legislation and other documentary evidence. *[If certain statement(s) of section "D. Productive hours" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* - *...]*	verifiable based on the documents provided by the Beneficiary and the calculation of the total number of hours worked was accurate. 15. The contract specified the working time enabling to calculate the annual workable hours. <u>If method C is applied</u> 16. The calculation of the number of productive hours per year corresponded to the usual costs accounting practice of the Beneficiary. 17. The calculation of the standard number of workable (working) hours per year was corroborated by the documents presented by the Beneficiary. 18. The number of productive hours per year used for the calculation of the hourly rate was at least 90 % of the number of workable (working) hours per year.
E. Hourly rates The hourly rates are correct because: XXIII. Hourly rates are correctly calculated since they result from dividing annual personnel costs by the productive hours of a given year and group (e.g. staff category or department or cost centre depending on the methodology applied) and they are in line with the statements made in section C. and D. above. *[If the statement of section 'E. Hourly rates' cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* - *...]*	**Procedure** ✓ The Auditor has obtained a list of all personnel rates calculated by the Beneficiary in accordance with the methodology used. ✓ The Auditor has obtained a list of all the relevant employees, based on which the personnel rate(s) are calculated. For 10 employees selected at random (same sample basis as Section C: Personnel costs): ✓ The Auditor recalculated the hourly rates. ✓ The Auditor verified that the methodology applied corresponds to the usual accounting practices of the organisation and is applied consistently for all activities of the organisation on the basis of objective criteria irrespective of the source of funding. **Factual finding:**

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	19. No differences arose from the recalculation of the hourly rate for the employees included in the sample.
F. Time recording XXIV. Time recording is in place for all persons with no exclusive dedication to one Horizon 2020 action. At least all hours worked in connection with the grant agreement(s) are registered on a **daily/weekly/monthly** basis *[delete as appropriate]* using a **paper/computer-based system** *[delete as appropriate]*; XXV. For persons exclusively assigned to one Horizon 2020 activity the Beneficiary has either signed a declaration to that effect or has put arrangements in place to record their working time; XXVI. Records of time worked have been signed by the person concerned (on paper or electronically) and approved by the action manager or line manager at least monthly; XXVII. Measures are in place to prevent staff from: i. recording the same hours twice, ii. recording working hours during absence periods (e.g. holidays, sick leave), iii. recording more than the number of productive hours per year used to calculate the hourly rates, and iv. recording hours worked outside the action period. XXVIII. No working time was recorded outside the action period; XXIX. No more hours were claimed than the productive hours used to calculate the hourly personnel rates. *[Please provide a brief description of the time recording system in place together with the measures applied to ensure its reliability to the Auditor and annex it to the*	**Procedure** ✓ The Auditor reviewed the brief description, all relevant manuals and/or internal guidance describing the methodology used to record time. The Auditor reviewed the time records of the random sample of 10 employees referred to under Section C: Personnel costs, and verified in particular: ✓ that time records were available for all persons with not exclusive assignment to the action; ✓ that time records were available for persons working exclusively for a Horizon 2020 action, or, alternatively, that a declaration signed by the Beneficiary was available for them certifying that they were working exclusively for a Horizon 2020 action; ✓ that time records were signed and approved in due time and that all minimum requirements were fulfilled; ✓ that the persons worked for the action in the periods claimed; ✓ that no more hours were claimed than the productive hours used to calculate the hourly personnel rates; ✓ that internal controls were in place to prevent that time is recorded twice, during absences for holidays or sick leave; that more hours are claimed per person per year for Horizon 2020 actions than the number of productive hours per year used to calculate the hourly rates; that working time is recorded outside the action period; ✓ the Auditor cross-checked the information with human-resources records to verify consistency and to ensure that the internal controls have been effective. In addition, the Auditor has verified that no more hours were charged to Horizon 2020 actions per person per year than the number of productive hours per year used to calculate the hourly rates, and verified that

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
present certificate[1]]. *[If certain statement(s) of section "F. Time recording" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* *- …]*	no time worked outside the action period was charged to the action. **Factual finding:** 20. The brief description, manuals and/or internal guidance on time recording provided by the Beneficiary were consistent with management reports/records and other documents reviewed and were generally applied by the Beneficiary to produce the financial statements. 21. For the random sample time was recorded or, in the case of employees working exclusively for the action, either a signed declaration or time records were available; 22. For the random sample the time records were signed by the employee and the action manager/line manager, at least monthly. 23. Working time claimed for the action occurred in the periods claimed; 24. No more hours were claimed than the number productive hours used to calculate the hourly personnel rates; 25. There is proof that the Beneficiary has checked that working time has not been claimed twice, that it is consistent with absence records and the number of productive hours per year, and that no working time has been claimed outside the action period. 26. Working time claimed is consistent with that on record at the human-resources department.

[1] The description of the time recording system must state among others information on the content of the time records, its coverage (full or action time-recording, for all personnel or only for personnel involved in H2020 actions), its degree of detail (whether there is a reference to the particular tasks accomplished), its form, periodicity of the time registration and authorisation (paper or a computer-based system; on a daily, weekly or monthly basis; signed and countersigned by whom), controls applied to prevent double-charging of time or ensure consistency with HR-records such as absences and travels as well as it information flow up to its use for the preparation of the Financial Statements.

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
[official name of the *[Beneficiary] [Linked Third Party]****]*** ***[name and title of authorised representative]*** ***[dd Month yyyy]*** ***<Signature of the*** *[Beneficiary] [Linked Third Party]****>***	***[official name of the Auditor]*** ***[name and title of authorised representative]*** ***[dd Month yyyy]*** ***<Signature*** *of the Auditor****>***

EUROPEAN COMMISSION
Directorate-General for Communications Networks, Content and Technology

CNECT.C – Digital Excellence and Science Infrastructure
C.4 – Flagships

GRANT AGREEMENT DATA SHEET

GrantAgreement (GA) No: 957189

Acronym: BIG-MAP

Title: Battery Interface Genome - Materials Acceleration Platform

Call/Topic: Novel methodologies for autonomous discovery of advanced battery chemistries

Type of action: Research and Innovation action

Granted by: European Union

Consortium agreement required: Yes

Collaboration agreement required: Yes

Coordination agreement required: No

Duration (in months): 36

Starting Date: 1 September 2020

Justification: A fixed starting data for all LC-BAT-12/13/14/15-2020 projects has been agreed with the Project Officer.

End date: 31 August 2023

Reimbursement rate: 100% of the action's eligible costs

Total costs (including non-EU funded)	Total costs	Maximum grant amount	Forms of costs
19 997 812.50	19 997 812.50	19 997 812.50	Unit, actual, flat rate, unit

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Prefinancing and guarantees:

Prefinancing amount	Guarantee fund Amount
15 998 250.00	999 890.63

Bank account (IBAN, BIC) for payments: DK9730004180011773

Reporting periods:

No	Month From	Month To
1	1	18
2	19	36

Obligation to keep records (in years): 5

Right to carry out reviews (up to number of years: 2

Right to carry out audits (up to number of years): 2

Extension of audit findings from other grants to this grant (no later than number of years): 2

Evaluation of the impact of the action (up to number of years): 5

List of beneficiaries and linked third parties and international partners:

Beneficiary/linked third party/ international partner	Role	PIC	Full official name	Country	Total costs (including non-EU funded)	Max. reimb. rate	Max Grant Amount
1 - DTU	CO	999990655	DANMARKS TEKNISKE UNIVERSITET	DK	2 704 992.50	100.00%	2 704 992.50
2 - UU	BEN	999985029	UPPSALA UNIVERSITET	SE	919 263.75	100.00%	919 263.75
3 - KIT	BEN	990797674	KARLSRUHER INSTITUT FUER TECHNOLOGIE	DE	1 375 000.00	100.00%	1 375 000.00
4 - CNRS	BEN	999997930	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS	FR	1 005 285.00	100.00%	1 005 285.00
UPJV	LinkTP	998207116	UNIVERSITE DE	FR	43 750.00	100.00%	43 750.00

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Beneficiary/linked third party/ international partner	Role	PIC	Full official name	Country	Total costs (including non-EU funded)	Max. reimb. rate	Max Grant Amount
			PICARDIE JULES VERNE				
5 - WWU	BEN	999853691	WESTFAELISCHE WILHELMS-UNIVERSITAET MUENSTER	DE	299 500.00	100.00%	299 500.00
6 - CEA	BEN	999992401	COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES	FR	803 107.50	100.00%	803 107.50
7 - NIC	BEN	998756718	KEMIJSKI INSTITUT	SI	399 500.00	100.00%	399 500.00
8 - SINTEF	BEN	910945140	SINTEF AS	NO	625 000.00	100.00%	625 000.00
9 - PDT	BEN	999977754	POLITECNICO DI TORINO	IT	210 025.00	100.00%	210 025.00
10 - Fraunhofer	BEN	999984059	FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.	DE	549 993.75	100.00%	549 993.75
11 - CTH	BEN	999980373	CHALMERS TEKNISKA HOEGSKOLA AB	SE	549 875.00	100.00%	549 875.00
12 - WUT	BEN	999884052	POLITECHNIKA WARSZAWSKA	PL	382 500.00	100.00%	382 500.00
13 - CSIC	BEN	999991722	AGENCIA ESTATAL CONSEJO SUPERIOR DEINVESTIGACIONES CIENTIFICAS	ES	384 858.75	100.00%	384 858.75
14 - TUD	BEN	999977366	TECHNISCHE UNIVERSITEIT DELFT	NL	349 185.00	100.00%	349 185.00
15 - CNR	BEN	999979500	CONSIGLIO NAZIONALE DELLE RICERCHE	IT	240 000.00	100.00%	240 000.00
16 - EPFL	BEN	999973971	ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE	CH	860 000.00	100.00%	860 000.00
17 - UCAM	BEN	999977172	THE CHANCELLOR MASTERS AND SCHOLARSOF THE UNIVERSITY OF CAMBRIDGE	UK	964 266.25	100.00%	964 266.25
18 - UOXF	BEN	999984350	THE CHANCELLOR,	UK	484 785.00	100.00%	484 785.00

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Beneficiary/linked third party/ international partner	Role	PIC	Full official name	Country	Total costs (including non-EU funded)	Max. reimb. rate	Max Grant Amount
			MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD				
19 - UT	BEN	999895013	TARTU ULIKOOL	EE	249 375.00	100.00%	249 375.00
20 - ULIV	BEN	999980567	THE UNIVERSITY OF LIVERPOOL	UK	649 727.50	100.00%	649 727.50
21 - ESRF	BEN	999484121	EUROPEAN SYNCHROTRON RADIATION FACILITY	FR	448 750.00	100.00%	448 750.00
22 - ILL	BEN	999933522	INSTITUT MAX VON LAUE - PAUL LANGEVIN	FR	391 000.00	100.00%	391 000.00
23 - SOLEIL	BEN	998721507	SYNCHROTRON SOLEIL SOCIETE CIVILE	FR	511 875.00	100.00%	511 875.00
24 - CID	BEN	999461229	FUNDACION CIDETEC	ES	524 250.00	100.00%	524 250.00
25 - EMIRI	BEN	946820687	ENERGY MATERIALS INDUSTRIAL RESEARCH INITIATIVE AISBL	BE	285 000.00	100.00%	285 000.00
26 - UMI	BEN	999893461	UMICORE	BE	208 532.50	100.00%	208 532.50
27 - SOLB	BEN	998067921	SOLVAY SA	BE	230 750.00	100.00%	230 750.00
28 - BASF	BEN	999829926	BASF SE	DE	542 550.00	100.00%	542 550.00
29 - NVOLT	BEN	909661830	NORTHVOLT AB	SE	410 000.00	100.00%	410 000.00
30 - UNIBAS	BEN	999907914	UNIVERSITAT BASEL	CH	463 828.75	100.00%	463 828.75
31 - ITU	BEN	998273464	IT-UNIVERSITETET I KOBENHAVN	DK	410 545.00	100.00%	410 545.00
32 - 3DS	BEN	947393181	DASSAULT SYSTEMES DEUTSCHLAND GMBH	DE	500 000.00	100.00%	500 000.00
33 - FZJ	BEN	999980470	FORSCHUNGSZENTRUM JULICH GMBH	DE	792 487.50	100.00%	792 487.50
34 - SAFT	BEN	963494405	SAFT	FR	228 253.75	100.00%	228 253.75

GA options:

Article 2 – Complementary grant

Article 6.2.D.2 – Equipment costs – depreciation

Article 6.2.D.4 – Large research infrastructure (LRI) costs

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Article 14 – Linked third parties
Article 29.3 – Actions that participate in the Open Research Data Pilot
Article 30.3 – EU right to object to transfers or licensing – EU grants
Article 31.5 – Access rights to results for EU – EU grants
Article 57.2 – Dispute settlement – non-EU beneficiaries

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