DATA MANAGEMENT PLAN: KU LEUVEN PROJECT C14/22/103

ADMINISTRATIVE INFORMATION

Project title: Metal-doped carbon clusters as model systems for the chemical storage of hydrogen
Project Identifier: C14/22/103
Researchers: Ewald Janssens, Peter Lievens
Project summary: Hydrogen is expected to take as energy carrier a central role in the energy transition. The chemical storage of hydrogen in solid materials remains a critical point despite extensive research. Theoretically it is possible to realise high volumetric energy densities and reversible hydrogen charging kinetics in porous carbon materials that contain transition metal (TM) dopants, but there is a lack of fundamental understanding, particularly about the roles of the bonding between the metal catalyst and the carbon support, the clustering of the metal atoms, and the possible hydrogen spillover. Since fundamental chemical reaction steps take place at the level of individual atoms, insight can be garnered by investigating simplified cluster model systems under highly controlled conditions. In this project, we aim for atomistic and electronic level understanding of the interaction of hydrogen with binary TM-carbon clusters with TM = Sc, Ti, Nb, Rh, using a unique combination of experiments in molecular beams and accurate quantum chemical calculations.
Institution: KU Leuven

RESEARCH DATA SUMMARY

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

This project will generate new data. There is no personal data involved.

Type of data	Format	Volume	How created	WP
Mass spectra	.txt .csv	1-10 GB	Time-of-flight mass spectrometry measurements	1, 2
Infrared spectra	.txt .h5	10-50 GB	Infrared spectroscopy measurements at FELIX and at laboatory in Leuven	1, 2
TPD spectra and GC measurements	.dat .csv	1-10 GB	Gas chromatography spectra and temperature programmed desorption spectra	3
Quantum chemical calculations	.out .opj .dat	100 MB	Quantum chemical software packages: Gaussian, Orca, …	1-3
Relevant reviewed literature	.pdf, .bib	10-100 MB	Articles will be available at the KU Leuven digital library. The articles may be stored in pdf and the selection of articles can be exported as a .bib file using the reference manager Mendeley.	1-3
Lab books with written details about the different process trials, results, and observations.	Written in paper	1 drawer	Written by the researchers in the lab.	1-3
Physical samples	Physical	/	Fabricated by the researchers in the lab. Samples of the gas phase studies performed in WP 1 and 2 cannot be kept.	3

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

When research involves living animals, human participants, or when there is a possibility for dual use or misuse for unethical purposes, ethical approval needs to be obtained. Include your ethical approval reference number in the comment section.

- Not applicable

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so, please comment per dataset or data type where appropriate.

- No, but with following remark: Although tech transfer and valorisation are not direct goals of this project, if an opportunity presents itself, it will be discussed among the PIs involved in the project. The conclusions of that discussion will be appended to this data management plan.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

DOCUMENTATION AND METADATA

*Clearly describe what approach will be followed to capture the accompanying information necessary to keep **data understandable and usable**, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).*

- For each experiment, a detailed (electronic) logbook will be used (different logbooks for the different experimental setups). These logbooks will contain the date, a brief description of the performed experiment, the parameters used for each measurement, as well as the names of all the saved files. The names of the files will be structured in a comprehensible way: system studied/date/main parameters used.

- In addition, data will be stored in a folder per experimental setup, the type of investigated system and the corresponding date. In this way, by tracking the corresponding logbook notes, each file can be easily found on the local computers controlling the setup and on the server of the laboratory.

- The analysis files will contain notes describing the analysis procedure and mention which original data files are included. A readme file describing the goal of the experiment and the analysis procedure will be stored in the folder where the data is saved.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify which metadata standard will be used. If not, please specify which metadata will be created to make the data easier to find and reuse.

- No. In this research field, there is no formal metadata standard. However, the standardized steps described above will ensure that the data is easy to find and reuse.

DATA STORAGE & BACK-UP DURING THE RESEARCH PROJECT

Where will the data be stored?

- Shared network drive (R-drive)
- Personal network drive that is synchronized with OneDrive-KU Leuven.

How will the data be backed up?

- Data on personal computers is placed in OneDrive folders.
- The data stored on the local computers is continuously and automatically backed-up on local servers. This is taken care of by the IT responsibles of the department.

Is there currently sufficient storage & backup capacity during the project? If no or insufficient storage or backup capacities are available, explain how this will be taken care of.

- Yes: The amount of data that will be generated in this project should not exceed a few hundred GBs, which is small enough to be stored in local computers and on local servers.

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

- The data will be systematically transferred to the local server, with restricted access (managed by the IT responsible). Only the (co-)promotors and involved researchers have access to the shared folders where the data, analysis files and reports will be stored. Also, credentials are required to log in to local computers in the laboratories.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

- The costs are small. The departmental IT plan that is being rolled out will for each researcher cover a basic amount of data storage. Since data volumes in this project are not large, they are expected to fall within the offered amount.

DATA PRESERVATION AFTER THE END OF THE RESEARCH PROJECT

Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project? In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

- All data will be preserved for 10 years according to KU Leuven RDM policy

Where will these data be archived (stored and curated for the long-term)?

- Lab books will be stored in dedicated cabinets in the laboratories. Digital data will be retained on local data storage facilities. Physical samples used in WP3 will be stored in lab 01.05.

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

- The cost for data preservation during the retention period are comparable to the cost for storage and backup during the project. The same conditions apply.

DATA SHARING AND REUSE

Will the data (or part of the data) be made available for reuse after/during the project?
Please explain per dataset or data type which data will be made available.

- Depending on each specific research result, we will consider the option to make the data available as open data on RDR or another platform. This particularly makes sense for analyzed data like infrared spectra, mass spectra, and reaction kinetics data. Data that is not made available as open data, will be made available if requested by the editor or publisher of a scientific journal or upon request of an individual (e.g. a researcher who intends to reproduce an experiment).

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

- No

Where will the data be made available? .

- KU Leuven RDR (Research Data Repository)

  In a restricted access depository. Upon request and after the agreement of the project's PIs, all data can be made available on an open repository, for example if requested by the editor or publisher of a scientific journal or via restricted access upon request of an individual (e.g. a researcher who intends to reproduce an experiment).

When will the data be made available?

- Upon publication of research results and after agreement of the involved PIs (with a possible embargo time no longer than one year after the publication of the research)

Which data usage licenses are you going to provide?

- This is not decided yet and will be discussed case by case, but most likely we will opt for a CC license.

Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.

- Yes, a PID will be added upon deposit in a data repository

What are the expected costs for data sharing? How will these costs be covered?

- The cost of sharing is expected to be zero or low. In case there is a cost, it will be covered by working budget of the project.

RESPONSIBILITIES

Who will manage data documentation and metadata during the research project?

- Each researcher who collects data within the project, according to the standards that have been agreed upon.

Who will manage data storage and backup during the research project?

- Data storage and backup is managed by the departmental IT

Who will manage data preservation and sharing?

- Data preservation is managed by the departmental IT. Data sharing falls under the responsibility of the PIs: Ewald Janssens and Peter Lievens

Who will update and implement this DMP?

- The promotor of the project is responsible for the updating and implementation of this DMP.