Data Management Plan – FWO project G033724N

1. General Project Information	
Name Grant Holder & ORCID	Ewald Janssens (ORCID 0000-0002-5945-1194)
Contributor name(s) (+ ORCID) & roles	María J. López (University of Valladolid, Valladolid, Spain) (ORICD 0000-0001-7698-9327), non-Flemish co-supervisor Gaolei Hou (Xi'an Jiaotong University, Xi'an, China) (ORCID 0000-0003-1196-2777), non-Flemish co-supervisor
Project number [1] & title	ZKE5369, Mechanistic aspects of dehydrogenation reactions on metal-fullerene complexes
Funder(s) GrantID [2]	Research Foundation Flanders (FWO), project G033724N
Affiliation(s)	☒ KU Leuven ☐ Universiteit Antwerpen ☐ Universiteit Gent ☐ Universiteit Hasselt ☐ Vrije Universiteit Brussel ☐ Other:
Please provide a short project description	We will study water and ammonia dehydrogenation on neutral and cationic metal-fullerene clusters using gas phase reactivity experiments in a collision cell and in an ion trap. The reactants, intermediates, and reaction products will be characterized by visible light and infrared spectroscopy, and the reaction mechanisms will be modelled with quantum chemical calculations. This approach will provide atomic level understanding about the role played by the fullerene support and explore how cooperative metal-metal interaction in few-atom clusters can further modulate the dehydrogenation activity. The generated knowledge about the structure-reactivity relationship, structural fluxionality, and metalsupport interaction will provide guidance for the design of better dehydrogenation catalysts that can efficiently make use of scarce raw materials and generate green hydrogen. The project has four work packages: WP1: geometric structures of metal-fullerene clusters ($C_{60}M_n^+$; M = Pt, Ru, V, Fe, Co, Ni, n = 1–5) WP2: Reactivity of small clusters $M_n^{0,+}$ and $C_{60}M_n^+$ (M = Pt, V, Co, Ni) towards H_2O splitting WP3: Reactivity of small clusters $M_n^{0,+}$ and $C_{60}M_n^+$ (M = Ru, Fe, Co, Ni) towards NH_3 decomposition WP4: Project coordination and management, dissemination, and outreach activities

[1] "Project number" refers to the institutional project number. This question is optional. Applicants can only provide one project number.

[2] Funder(s) GrantID refers to the number of the DMP at the funder(s), here one can specify multiple GrantIDs if multiple funding sources were used.

2. 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 [3].

				ONLY FOR DIGITAL DATA	*ONLY FOR DIGITAL DATA*	*ONLY FOR DIGITAL DATA*	*ONLY FOR PHYSICAL DATA*
Dataset Name	**Description**	**New or Reused**	**Digital or Physical**	**Digital Data Type**	**Digital Data Format**	**Digital Data Volume (MB, GB, TB)**	**Physical Volume**
Mass spectra	Time-of-flight mass spectra; gas phase studies	New data	Digital	Numerical	.txt, .csc	1-10 GB	/
Spectroscopic data	Infrared spectra, visible absorption spectra; gas phase studies	New data	Digital	Numerical	.txt, .csc	1-10 GB	/
Relevant literature	The articles may be stored in pdf and the selection of articles can be exported as a .bib file using the reference manager Mendeley.	Reuse existing data	Digital	Textual	.pdf, .bib	100 MB -1 GB	/
Quantum chemical calculations	Output files from quantum chemical software packages: Gaussian, Orca, SIESTA	New data	Digital	Textual	.out, .opj .dat	< 100 GB	/
Lab books	Hand written (or typed) notes by researchers in lab with details about the different process trials, results, and observations.	New data	Digital or physical	Textual + Images	.doc	< 100 MB	Few logbooks

[3] Add rows for each dataset you want to describe.

GUIDANCE: *The data description forms the basis of your entire DMP, so make sure it is detailed and complete. It includes digital and physical data and encompasses the whole spectrum ranging from raw data to processed and analysed data including analysis scripts and code. Physical data are all materials that need proper management because they are valuable, difficult to replace and/or ethical issues are associated. Materials that are not considered data in an RDM context include your own manuscripts, theses and presentations; documentation is an integral part of your datasets and should described under documentation/metadata.* *RDM Guidance on data*	
If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type.	NA
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.	☐ Yes, human subject data; provide SMEC or EC approval number: ☐ Yes, animal data; provide ECD reference number: ☐ Yes, dual use; provide approval number: ☒ No Additional information:
Will you process personal data[4]? 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).	☐ Yes (provide PRET G-number or EC S-number below) ☒ No Additional information:
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.	☐ Yes ☒ No 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.

[4] See Glossary Flemish Standard Data Management Plan

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/Data transfer agreements, research collaboration agreements)? If so, please explain to what data they relate and what restrictions are in place.	☐ Yes ☒ No If yes, please explain:
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 to what data they relate and which restrictions will be asserted.	☒ Yes ☐ No If yes, please explain: the project involves external partners (see contributors on first page). A collaboration agreement is being concluded, which covers the protection and valorization of project results, including the data that lead to those results.

3. 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). *RDM guidance on documentation and metadata*.	• 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. *REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.*	☐ Yes ☒ No If yes, please specify (where appropriate per dataset or data type) which metadata standard will be used: If no, please specify (where appropriate per dataset or data type) which metadata will be created: 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.

4. Data Storage & Back-up during the Research Project	
Where will the data be stored? *Consult the interactive KU Leuven storage guide to find the most suitable storage solution for your data.*	☒ Shared network drive (R-drive) ☐ Personal network drive (I-drive) ☒ OneDrive (KU Leuven) ☐ Sharepoint online ☐ Sharepoint on-premis ☐ Large Volume Storage ☐ Digital Vault ☐ Other:
How will the data be backed up? *WHAT STORAGE AND BACKUP PROCEDURES WILL BE IN PLACE TO PREVENT DATA LOSS?*	☒ Standard back-up provided by the departmental ICTS for my storage solution ☐ Personal back-ups I make (specify) ☐ Other (specify)

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.	☒ Yes ☐ No If no, please specify:
How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons? *CLEARLY DESCRIBE THE MEASURES (IN TERMS OF PHYSICAL SECURITY, NETWORK SECURITY, AND SECURITY OF COMPUTER SYSTEMS AND FILES) THAT WILL BE TAKEN TO ENSURE THAT STORED AND TRANSFERRED DATA ARE SAFE.* *Guidance on security for research data*	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 rolled out, covers for each researcher a basic amount of data storage. Since data volumes in this project are not so large, they are expected to fall within the offered amount.

5. Data Preservation after the end of the Research Project	
Which data will be retained for at least five 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...). *Guidance on data preservation*	☒ All data will be preserved for 10 years according to KU Leuven RDM policy ☐ All data will be preserved for 25 years according to CTC recommendations for clinical trials with medicinal products for human use and for clinical experiments on humans ☐ Certain data cannot be kept for 10 years (explain)

Where will these data be archived (stored and curated for the long-term)? *Dedicated data repositories are often the best place to preserve your data. Data not suitable for preservation in a repository can be stored using a KU Leuven storage solution, consult the interactive KU Leuven storage guide.*	☐ KU Leuven RDR ☐ Large Volume Storage (longterm for large volumes) ☒ Shared network drive (R-drive) ☒ Other (specifiy): physical Lab books will be stored in dedicated cabinets in the laboratories
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.

6. 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. *NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS AND USE MAY APPLY. AVAILABILITY IN THIS QUESTION THUS ENTAILS BOTH OPEN & RESTRICTED ACCESS. FOR MORE INFORMATION: HTTPS://WIKI.SURFNET.NL/DISPLAY/STANDARDS/INFO-EU-REPO/#INFOEUREPO-ACCESSRIGHTS*	☐ Yes, as open data ☒ Yes, as embargoed data (temporary restriction) ☒ Yes, as restricted data (upon approval, or institutional access only) ☐ No (closed access) ☐ Other, please specify:
If access is restricted, please specify who will be able to access the data and under what conditions.	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)? Please explain per dataset or data type where appropriate.	☐ Yes, privacy aspects ☐ Yes, intellectual property rights ☐ Yes, ethical aspects ☐ Yes, aspects of dual use ☐ Yes, other ☒ No If yes, please specify: /
Where will the data be made available? If already known, please provide a repository per dataset or data type.	☒ KU Leuven RDR ☐ Other data repository (specify) ☐ Other (specify)
When will the data be made available?	☒ Upon publication of research results and after the agreement of the project's PIs ☐ Specific date (specify) ☐ Other (specify)
Which data usage licenses are you going to provide? If none, please explain why. *A DATA USAGE LICENSE INDICATES WHETHER THE DATA CAN BE REUSED OR NOT AND UNDER WHAT CONDITIONS. IF NO LICENCE IS GRANTED, THE DATA ARE IN A GREY ZONE AND CANNOT BE LEGALLY REUSED. DO NOTE THAT YOU MAY ONLY RELEASE DATA UNDER A LICENCE CHOSEN BY YOURSELF IF IT DOES NOT ALREADY FALL UNDER ANOTHER LICENCE THAT MIGHT PROHIBIT THAT.* *Check the RDR guidance on licences for data and software sources code or consult the License selector tool to help you choose.*	☒ CC-BY 4.0 (data) ☐ Data Transfer Agreement (restricted data) ☐ MIT licence (code) ☐ GNU GPL-3.0 (code) ☐ Other (specify)

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, please provide it here. *INDICATE WHETHER YOU INTEND TO ADD A PERSISTENT AND UNIQUE IDENTIFIER IN ORDER TO IDENTIFY AND RETRIEVE THE DATA.*	☒ Yes, a PID will be added upon deposit in a data repository ☐ My dataset already has a PID ☐ No
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.

7. 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 PI: Ewald Janssens
Who will update and implement this DMP?	The promotor of the project is responsible for the updating and implementation of this DMP.