
COVALENT CHIRAL FUNCTIONALIZATION OF GRAPHITE FOR ENANTIOSELECTIVE SEPARATION

A Data Management Plan created using DMPonline.be

Creators: Shammi Rana, Steven De Feyter

Affiliation: KU Leuven (KUL)

Funder: Fonds voor Wetenschappelijk Onderzoek - Research Foundation Flanders (FWO)

Template: FWO DMP (Flemish Standard DMP)

Principal Investigator: Shammi Rana

Grant number / URL: 12ZZO23N

ID: 200037

Start date: 01-01-2023

End date: 31-12-2024

Project abstract:

An object, or a molecule is said to be chiral if it can be distinguished from its mirror image. Chirality plays an important role in many areas of chemistry, biology, and physics. Many chemical processes involving solid surfaces such as catalysis, crystallization, adsorption, and so forth, are sensitive to chirality. Thus, surfaces are not only fertile playground studying chirality, but they can also be used to promote the separation of mirror image molecules, i.e. enantiomers, due to additional constraints created by the two-dimensional (2D) environment. Because of the reduced symmetry at the interface, these constraints enhance the expression of molecular chirality, allowing not only chiral molecules, but also prochiral molecules to produce chiral superstructures. Even so, recognition processes based on non-covalent interactions could be used to separate enantiomorphs in 2D systems. This new method could be used to resolve racemic mixtures. In this project, nanoconfinement conditions created using scanning probe nanolithography will reveal how the shape and size of the confinement, as well as the nanolithography process itself, affect the chirality of on-surface crystallization processes. Robust chiral surfaces will be created using covalent functionalization of graphite and applied for enantioselective separation. Also, bulk chiral graphitic materials will be synthesized and used as stationary phase in chiral chromatography. CHIRAL-SURF will allow me to pursue a highly innovative research line in surface science, providing me a perfect platform for my personal development in terms of research and training in a topic of key importance, i.e. chirality, and state-of-the-art imaging techniques. This project will also allow me to strengthen my team-working and leadership skills as well as widen my scientific network and collaborations. In summary, this research grant will be a positive turning point in my academic career towards scientific excellence.

Last modified: 01-06-2023

COVALENT CHIRAL FUNCTIONALIZATION OF GRAPHITE FOR ENANTIOSELECTIVE SEPARATION

FWO DMP (Flemish Standard DMP)

1. 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.

				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
		<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Generate new data Reuse existing data 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Digital Physical 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> Observational Experimental Compiled/aggregated data Simulation data Software Other NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> .por, .xml, .tab, .cvs, .pdf, .txt, .rtf, .dwg, .gml, ... NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <100MB <1GB <100GB <1TB <5TB <10TB <50TB >50TB NA 	
	Super-resolution microscopy images	Generate new data	Digital	<ul style="list-style-type: none"> Observational Experimental Compiled/aggregated data Simulation data Software 	.por, .xml, .tab, .cvs, .pdf, .txt, .rtf, .dwg, .gml, ...	<5TB	
	Raman Data	Generate new data	Digital	<ul style="list-style-type: none"> Observational Experimental Compiled/aggregated data Simulation data Software 	.txt, ASCII	<100GB	
	Experimental protocols, results, conclusions. Analyzed papers	Generate new data	Physical				Lab Note book
	Figures, datasets, drafts of research articles	Generate new data	Digital	<ul style="list-style-type: none"> Observational Experimental Compiled/aggregated data 	.por, .xml, .tab, .cvs, .pdf, .txt, .rtf, .dwg, .gml	<1TB	

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:

Existing data are not reuse in current research project.

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- 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

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 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

2. 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).

All collected data will be clearly labelled per experiment. A table with a summary for every experiment will be provided. This table contains: date at which data was acquired, sample description (Name of the compound, concentration and labelling), measurement parameters (Type of Instrument, substrate types), brief report of results and conclusion, suggestion towards follow-up experiment. Further, a detailed description of the used protocol to prepare the samples will be written and kept in the electronic lab journal (regular backups)

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- No

No metadata standard will be used. Necessary documentations on the creation of the data will be include in the same folder with the dataset:

Metadata generated automatically by the measurement setup, and is embedded in the microscopy/spectroscopy data.

Metadata generated for/during analysis of the data: analysis protocols for analysis code for MATLAB with necessary comment for the user to understand how the analysis is performed and how parameters can be changed.

3. Data storage & back-up during the research project

Where will the data be stored?

The data is stored on portable hard drives stored at different locations and at the enterprise cloud storage service "BOX" and KUL personnel's internet drives offered by KU Leuven. The accepted version of the final manuscripts (+ accessory datasets) are submitted in open access journals and in the KU Leuven library's depository. In addition, relevant data will be transferred to the self-mirrored long-term storage capacity by the KUL ICTS for long-term storage till at least 5 years after the project.

How will the data be backed up?

The data will be backed-up automatically for remote data storage on a daily basis in hard drive. Additionally, three copies of the data will be kept at different physical locations, such as portable hard drives every week.

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

5TB Storage and backup capacity is already present for approximately for the 3 years and can be extended further by purchasing additional portable hard drives or cloud data volumes.

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

Access to the data is restricted by online build-in safe logins and by physical restriction of access to the portable hear drives through the security system installed in the building of the affiliation.

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

A volume of 5 TB hard disk is anticipated for data storage, and it will result in a cost of approximately 300 Euros which will be covered from the bench fee of this grant.

4. 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...).

Only a selection of relevant data will be preserved. Selection of data destined for long-term storage will be assessed by the applicant and the promotor on a yearly basis. Naturally, all data and metadata used/linked to published articles, will be preserved in the university library depository.

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

The selected data will be stored on the university's central servers for at least 10 years, confirm the KU Leuven RDM policy. In addition, the selected data will be preserved on minimum 3 different portable hard drives which are kept locked at different locations under the supervision of the promotor.

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

Costs for the retention of data on portable hard drives is already made. The long-term data storage of ICTS costs approximately 150 euros per year per 2TB. This storage has been set up for the research group, the shared cost will depend on the actual data generated from this project. A volume of 5 TB is anticipated, that will result in a cost of approximately 300 Euros to be covered from the bench fee of this grant.

5. Data sharing and reuse

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

- Yes, in a restricted access repository (after approval, institutional access only, ...)

If access is restricted, please specify who will be able to access the data and under what conditions.

The data will continue to be stored in a protected environment, similar as to before the end of the project. However, requests to access the data can be made via email to the promotor or Postdoc, who will decide upon this request after consultation with the promotor and co-authors of articles and after the possible receiver has signed a data sharing agreement.

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 in the comment section per dataset or data type where appropriate.

- No

Where will the data be made available? If already known, please provide a repository per dataset or data type.

The data can be made available via email to the promotor or Postdoc, who will decide upon this request after consultation with the promotor and co-authors of articles and after the possible receiver has signed a data sharing agreement.

When will the data be made available?

Upon publication of research results.

Which data usage licenses are you going to provide? If none, please explain why.

None

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- Yes

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

How data will be shared, will depend upon the type of the requested data. Data will always be shared in a protected environment; after the receiver signed a data sharing agreement.

6. Responsibilities

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

The responsible person during the project is the applicant himself, under supervision of the promoter.

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

After completion of the project, the responsible person will be the promoter.

Who will manage data preservation and sharing?

The responsible person is the applicant himself, under supervision of the promoter. After completion of the project, the responsible person is the promoter.

Who will update and implement this DMP?

The applicant and PI bears the end responsibility of updating & implementing this DMP.

COVALENT CHIRAL FUNCTIONALIZATION OF GRAPHITE FOR ENANTIOSELECTIVE SEPARATION

Application DMP

Questionnaire

Describe the datatypes (surveys, sequences, manuscripts, objects ...) the research will collect and/or generate and /or (re)use. (use up to 700 characters)

Question not answered.

Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)

Question not answered.

What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)

Question not answered.

Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)

Question not answered.

Which other issues related to the data management are relevant to mention? (use up to 700 characters)

Question not answered.

COVALENT CHIRAL FUNCTIONALIZATION OF GRAPHITE FOR ENANTIOSELECTIVE SEPARATION

DPIA

DPIA

Have you performed a DPIA for the personal data processing activities for this project?

Question not answered.

COVALENT CHIRAL FUNCTIONALIZATION OF GRAPHITE FOR ENANTIOSELECTIVE SEPARATION

GDPR

GDPR

Have you registered personal data processing activities for this project?

Question not answered.