
Chemical engineering of interfaces for tailored opto-electronic properties

A Data Management Plan created using DMPOnline.be

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Project abstract:

The interface is the device” is the famous quote with which H. Kroemer started his Nobel laureate lecture in 2000. Interfaces critically determine the functional properties and stability of materials. Therefore, tailoring interfaces is critical for the performance of electronic, optical, or electro-optical devices. A major challenge is to tailor the structural and functional defects that naturally define materials' interfaces. The project aims to rationally develop advanced chemical strategies for surface and interface engineering. The consortium will also build on its strong track record in developing microspectroscopic techniques to characterize the structural properties and the dynamic processes at the interfaces and use this information to rationally engineer the interface chemistry. Via this synergistic approach, the applicants will realize novel composite materials, with a potential for application in lighting, detectors, sensors, and photovoltaics.

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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.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: <i>N</i> (ew data) or <i>E</i> (xisting data)	Indicate: <i>D</i> (igital) or <i>P</i> (hysical)	Indicate: Audiovisual Images Sound Numerical Textual Model SOftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
STM	Scanning tunneling microscopy data	N	D	I	.mi	<1TB	
STS	Scanning tunneling spectroscopy data	N	D	N	.dat	<1TB	
AFM	Atomic Force microscopy data	N	D		.ibw	<1TB	
AFM-IR	Atomic Force microscopy-Infrared spectroscopy data	N	D	I, N	.dat	<1TB	
Raman	Raman spectroscopy data	N	D	N	.tvb	<100 GB	
CV	Cyclic voltammetry data	N	D	N	.dat,	<100 GB	
UV-Vis	optical absorption and emission spectroscopy	N	D	N	.dat, .txt, .asc, .sp	<100 GB	
XRD	X-ray diffraction data	N	D	N	.dat, .txt	<1 GB	
XPS	X-ray photoelectron spectroscopy data	N	D	N	.txt, .sp, .opj	<1 GB	
SHG spectroscopy	second harmonic generation data	N	D	N	.txt	<1 GB	
SPT	Single photon timing	N	D	N	.sdt	< 1TB	
Fluorescence microscopy	Fluorescence microscopy and spectroscopy data	N	D	N, I	.aist, .txt, .lsf	<100 GB	
Protocols	Protocols used for the preparation of formulations and materials	N	D	T	.docx	<1GB	
Graphite-related Samples	Samples of physisorbed self-assembled networks on graphite and covalently modified graphite substrates	N	P	Physical samples			
(perovskite) semiconductor samples	Nano- to micrometer-sized crystals and thin films	N	P	Physical samples			1 mL suspensions in 4 mL vials
Device-related data	Photodetector, LED prototypes	N	D & P	N and physical sets	.dat, .txt, .asc	< 100 GB	

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.

- No

NA

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

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).

In order to make sure all the data collected and stored will be reliable and reproducible, a text document describing the exact experimental conditions, including date, time, location of measurements, instruments, sample preparation protocol and measurement parameters etc. This file will be kept in the same folder where the data is stored. For the materials, a list of samples and the location where these are stored will be kept in researcher's logbook. A description of the sample's characteristics (e.g. sample name, solvent, quantity, date, concentration) will be added to allow rapid identification and reuse.

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

Since the data generated by various experimental instruments do not use a standard metadata, we are unable to use a common format. As a consequence, we have created our own file format that fits to our experimental data. Although most of the generated data files contain metadata specific for that experiment, this is not sufficient and we will supplement this information with a detailed text document (ASCII type) storing the necessary information for finding, understanding and reuse of data. The text file will be placed in every folder containing data or processed data. In the case of processed or analysed data, detailed descriptions on the analysis steps will also be included. The text file and the structure of the folders used to deposit data will have a standard format. This will allow other users to: repeat the experiments or find and retrieve data.

Data Storage & Back-up during the Research Project

Where will the data be stored?

- ManGO
- OneDrive (KU Leuven)
- Large Volume Storage
- Shared network drive (J-drive)

-Besides the above-mentioned storage, we will also take regular backups of the data on physical hard drives as an additional measure.

-Data of published papers will be stored in KULeuven Research Data Repository (RDR) After the research

How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution
- Personal back-ups I make (specify below)

Personal back-ups will be carried out by co-workers regularly on physical hard drives.

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

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

The data will be securely stored in KU Leuven OneDrive, KU Leuven network drives, and RDR. Data on KU Leuven servers are restricted to authorized users. OneDrive folders are shared only with relevant personnel, and J-Drive folders are password-protected.

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

Every user has a standard 2 TB capacity on the University's central network drive (OneDrive). This capacity can be extended to 5 TB without costs.

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)?

- KU Leuven RDR
- Large Volume Storage (longterm for large volumes)

The data will be archived in the K-drive volume offered by KULEuven.

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

Costs are expected to be moderate and will be covered by other running projects from the involved groups (in case of no running projects, accumulated reserves will be used).

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.

- Yes, as restricted data (upon approval, or institutional access only)

KUL: Data that are published will be made available via the KU Leuven Research Data Repository.

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

NA

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.

- No

Where will the data be made available?

If already known, please provide a repository per dataset or data type.

- KU Leuven RDR (Research Data Repository)

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.

- CC-BY 4.0 (data)

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?

Deposition of smaller datasets in data repositories is usually covered by the repository and for sharing physical data, the cost are typically paid by the researcher requesting the materials.

Responsibilities

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

Each PI is responsible for the data documentation & metadata.

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

Each PI is responsible for data storage & backup.

Who will manage data preservation and sharing?

Each PI is responsible for data preservation and sharing.

Who will update and implement this DMP?

Each PI is responsible updating & implementing this DMP.