Chiral-induced spin selectivity effect at nano and single-molecule scales (CISSCA)

A Data Management Plan created using DMPonline.be

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Project abstract:

Chirality is often considered as a structural property of molecules, but the concept also applies to electrons because of their spin. Achiral at rest, they acquire a helicity (chirality) in the direction of motion. Consequently, electrons are filtered according to their spin when crossing chiral materials. This newly uncovered chiral-induced spin selectivity (CISS) effect is surprisingly large. Spin polarization up to 100% has been demonstrated paving the way to multiple applications in chemistry, such as improved control of enantioselective reactions and easier separation of enantiomers. Impacts are also expected in physics (spintronics) and biology (molecular recognition of biomolecules). To date, the spin-filtering mechanism and molecular materials structure-property relationships remain elusive. CISSCA aims at measuring CISS effect on well-defined self-assembled chiral monolayers on several spin-polarized interfaces to elucidate the role of molecular structure, orientation vs substrate, and order on the strength of spin-polarization, from the nano down to the single-molecule level. To face the challenge Y. Geerts (ULB) and S. De Feyter (KU Leuven) groups will team up. The former will design, synthesize, and supply tailored molecular systems to the latter that will measure spin-polarization by scanning tunneling microscopy and spectroscopy.

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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
		Please choose from the following options: • Generate new data • Reuse existing data	*Please choose from the following options:* • Digital • Physical	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .cvs,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
STM	scanning tunneling microscopy	Generate new data	digital	experimental	.mi	<1TB	
AFM	atomic force microscopy	Generate new data	digital	experimental	.ibw	<1TB	
AFM-IR	atomic force microscopy combined with infrared spectroscopy	Generate new data	digital	experimental	.dat	<1TB	
Hyperchem	Molecular models	Generate new data	digital	experimental	.hin	<100GB	
Raman	Raman spectroscopy data	Generate new data	digital	experimental	.tvb	<100GB	
Protocols	Protocols used for preparation of formulations and materials	Generate new data	digital	experimental	.docx	<100GB	
Samples	Samples of physisorbed self-assembled networks on graphite and covalently modified graphite substrates	Generate new data	physical	experimental			

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)? 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).

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 (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

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.

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

Where will the data be stored?

KUL:
Storage capacity/repository
During research:
- Co-worker takes backup of the data
- Instrument responsible takes daily backup of the data generated
- Data are transferred to university's central network drives (OneDrive)
- Data of published papers will be stored in KU Leuven Research Data Repository (RDR) After the research
- Data (including metadata) are stored on local drives
- Data are transferred to university's central network drives (OneDrive)
- Data of published papers will be stored in KU Leuven Research Data Repository (RDR)

How will the data be backed up?

KUL: The data will be stored on a personal hard drive and transferred to the university’s central servers.

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

There is room on local drives and university's central servers

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

KUL: The data will be securely stored in KU Leuven OneDrive, KU Leuven network drives, and RDR.

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

KUL: Standard every user has 2 TB on University's central network drive (OneDrive). This capacity can be extended to 5 TB without costs

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...).

KULeuven: Physical data in the form of samples will be retained for 5 years. Most samples will degrade with time and will not be usable after 5 years. Digital data will be
retained for 10 years.

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

KULeuven: Samples will be stored for 5 years in dedicated cabinets in the laboratories. Digital data will be retained for 10 years on local (KU Leuven) data storage facilities.

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).

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 an Open Access repository
- Yes, in a restricted access repository (after approval, institutional access only, …)

Yes, in an Open Access repository
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 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.

KUL: All data that will be made available will be accessible in and via the KU Leuven Research Data Repository

When will the data be made available?

After publication

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

KUL: CC-BY-4.0

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?

KUL. 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.

6. Responsibilities

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

The researchers who generate the data are usually responsible for documentation, metadata, storage and backup, whereas the supervisor of the project, in each university, has the end responsibility and manages long term preservation and sharing.

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Who will update and implement this DMP?

Steven De Feyter