Nanoengineering of multicomponent reversible graphene superlattices: Probing the fundamentals from the molecular level to the device scale.

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Project abstract:

The nanoarchitecture of 2D materials is of great interest in the scientific community and is recently exploited widely to tailor its electrical, chemical, optical, and mechanical properties. Chemical and photochemical reactions are the two promising methods to anchor the functional groups on 2D materials, in which the former reaction induces large-scale modification while the latter introduces spatially localized defects (sub-micron precision). Indeed, the precise control over the covalent functionalization of 2D materials at the molecular level still remains a challenging task due to the lack of molecular identity, spatial distribution, and density at the molecular level. In this proposal, a novel multicomponent reversible graphene superlattice consisting of both covalent and non-covalent bound moieties will be constructed with the aid of nano spectroscopy techniques such as TERS and nanoIR. The customized modulation of electrical and optical properties of the superlattice by exploiting the molecular switching events through external stimuli will enable the fabrication of multifunctional graphene substrates. The nano-spectroscopy techniques together with state-of-the-art surface analyzing techniques (AFM, STM, KPFM) permit real-time nanoscale chemical mapping and molecular visualization on the graphene layer. Furthermore, the synergy between STM/AFM imaging and time-resolved optical spectroscopy will be employed in this project in order to resolve the real-time ensembled dynamics of photoisomerization and the associated selfassembly of the photochromic molecules on the graphene layer. The sub-nanoscale molecular information will facilitate precise Fermi-level engineering. Finally, the feasibility of devising new flexible and transparent field-effect transistors (FET) devices using the newly architect graphene superlattices will be scrutinized.

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DPIA

DPIA

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

- Not applicable

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GDPR record

GDPR record

Have you registered personal data processing activities for this project?

- Not applicable

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Grant proposal

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1. Data summary

1.1 Types of data/other research outputs

Throughout the project, raw data will be generated from instruments. The data type will strongly depend on the individual instruments and their specific purposes, ranging from the spectroscopic data and their exported format (txt, ASCII, SPC), microscopic images (png, jpg), videos (avi), other instrumental images (.aist), analyzed data (OPJ, OPJU, jpg, pdf), and program (.mat).

The experimental raw data will be analyzed further with the aid of home-build programs.

Additionally, physical data including different graphene substrates, lab notes, and newly developed protocols will be generated during the project.

2. FAIR principles

2.1 Findability of data/research outputs

Data will be deposited in the Research Data Repository (RDR) and Leuven Institutional Repository and Information Archiving System (Lirias) platforms of KU Leuven. The data will be identified by a persistent identifier, RDR assigns digital object identifiers (DOIs) to uploaded datasets and makes them easily available. Large raw datasets (Raman, AFM, KPFM, STM and TERS mapping, raw compiled movies, etc.) used to pattern and characterize the graphene will remain available for at least five years in the in-house 10 TB server of the host laboratory (and freely available upon request to the corresponding authors). The materials/resources used or newly generated in the project will be stored in-house and will be freely available to the community upon request. The preprint of the scientific publication will also be made available through public repositories such as chemRxiv, arXiv, and Open Research Europe.

2.2 Accessibility of data/research outputs

The data will be made openly accessible in repositories without any restrictions as early as possible. The preprint of the scientific articles will be made available through public repositories such as ChemRxiv, arXiv, and Open Research Europe. The peer-reviewed work will be accessible under open licenses, specifically the Creative Commons Attribution International Public License (CC BY), and will also be archived in KU Leuven's Lirias repository system.

2.3 Interoperability of data/research outputs

The data will be deposited in a widely accepted and easily accessible format, such as txt, pdf, and MS Word/Excel (xlsx) file formats. Systematic file nomenclatures, incorporating dates (YYYY/MM/DD), experiment/project names, and experimental parameters, will be employed to name and categorize various files.

2.4 Reusability of data/research outputs

Research outputs will be made available through open licenses (Creative Commons Attribution International Public Licence (CC BY))

3. Resources and responsibilities

3.1 Curation and storage/preservation costs

There will be no cost to make data and research outputs FAIR in this project, as repositories and other resources are provided by KU Leuven free of charge.

3.2 Person/team responsible for data management and quality assurance

The researcher is responsible for data management during the project. Regular meetings with the supervisor will be conducted to discuss the quality of the generated data and outputs. Additionally, frequent discussions in the group meetings will ensure quality control over the data collection process. Moreover, the project supervisor will ensure the long-term storage of the project data at KU Leuven.

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Full DMP

Version information

Action number

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Action acronym

MRGS-Nano-Spec.

Action title

Nanoengineering of multicomponent reversible graphene superlattices: Probing the fundamentals from the molecular level to the device scale.

DMP version number

v1.0

Date

12/01/2024

1. Data summary

1.1 Will you re-use any existing data and what will you re-use it for?

The Matlab program developed by the host laboratory will be reused for data analysis, specifically for Raman mapping on patterned graphene surfaces. Furthermore, the established protocol for direct laser patterning on graphene substrates, as published by the host lab, will be reused in this project to compare with newly developed patterning protocols on graphene.

1.2 What types and formats of data and other research outputs will the project generate or re-use?

During the project, raw data will be generated from instruments. The data type will strongly depend on the individual instruments and their specific purposes, ranging from the spectroscopic data and their exported format (txt, ASCII, SPC), microscopic images (png, jpg, tiff), videos (avi), other instrumental images (.aist), analyzed data (OPJ, OPJU, jpg, pdf), and program (.mat).
The experimental raw data will be analyzed further with the aid of home-build programs.
Additionally, physical data including graphene substrates, lab notes, and newly developed protocols will be generated during the project.

1.3 What is the purpose of the data generation or re-use and its relation to the objectives of the project?

Through this project, we aim to upscale the fundamental knowledge of spatially controlled nanopatterning on 2D materials and fabricate a novel photo-switchable hybrid graphene superlattice. To fulfill the proposed objectives, various spectroscopic and imaging data need to be acquired. During the chemical patterning of graphene, micro-Raman spectroscopy data, Raman images, optical images, AFM, and KPFM images will be acquired. In addition, nano-IR and Tip-enhanced Raman spectroscopy data will also generated in order to understand the spatial heterogeneity and density of the covalently anchored molecule on the patterned graphene layer. Furthermore, STM and AFM images and time-resolved optical spectroscopy data will also be generated to study the ensembled molecular dynamics of the photochromic molecule on the

graphene superlattices.

1.4 What is the expected size of the data that you intend to generate or re-use?

The size of the data is expected to be less than 10 TB.

1.5 What is the origin/provenance of the data, either generated or re-used?

The data originates from in-house equipments used to characterize and assess the samples.

1.6 To whom might your data be useful ('data utility'), outside your project?

The data will be highly beneficial for researchers and industrial scientists exploring the fabrication of novel 2D substrates for various applications.

2.1 FAIR data: Making data findable, including provisions for metadata

2.1.1 Will data and other research outputs be identified by a persistent identifier?

- Yes: describe below

We will use the RDR data repository of KU Leuven. The data will be identified by a persistent identifier DOI (from KU Leuven RDR, ChemRxiv, arXiv, etc.). The deposited data in the RDR repository will remain accessible even after the project concludes. Also, the DOI of the MSCA grant and other grants obtained will be indicated in the open-access preprints and publications.

2.1.2 Will rich metadata be provided to allow discovery?
What metadata will be created?
What disciplinary or general standards will be followed?
In case metadata standards do not exist in your discipline, please outline what type of metadata will be created and how.

We will use the RDR data repository of KU Leuven. A metadata standard is automatically applied upon depositing the data. The metadata model will include fields that are required, recommended, and optional. Using this data repository, the data sets will be findable and reusable. Systematic titles matching with the open-access preprints and publications will be used to ease the location of the datasets.

2.1.3 Will search keywords be provided in the metadata to optimize the possibility for discovery and then potential re-use?

- Yes: describe below

Keywords will be provided through the different repository system.

2.1.4 Will metadata be offered in such a way that it can be harvested and indexed?

- Yes: describe below

This is ensured in the KU Leuven RDR repository platform.

2.2 FAIR data: Making data accessible

2.2.1 Will the data and other research outputs be deposited in a trusted repository?

- Yes: describe below

The research data and output will be deposited in the Research Data Repository (RDR) of KU Leuven. All documentation and published results will also be available through Lirias, the institutional repository of KU Leuven. Lirias also provides a gateway to materials stored on the Research Data Repository.

2.2.2 Have you explored appropriate arrangements with the identified repository where your data and other research outputs will be deposited?

- Yes

We will use RDR data repository of KU Leuven.

2.2.3 Does the repository ensure that the data and other research outputs are assigned an identifier? Will the repository resolve the identifier to a digital object?

Yes. Most data depositories used in this project use digital objective identifier (DOI).

2.2.4 Will all data and other research outputs be made openly available?

- Yes

2.2.5 Is an embargo applied to give time to publish or seek protection of the intellectual property (e.g. patents)?

- No

2.2.6 If an embargo is applied (see question 2.2.5), specify why and how long this will apply, bearing in mind that research data should be made available as soon as possible.

Not applicable

2.2.7 Will the data and other research outputs be accessible through a free and standardized access protocol?

- Yes: describe below

This ensured by the different repositories that will be used in this project, including the KU Leuven RDR.

2.2.8 If there are restrictions on use, how will access be provided to the data, both during and after the end of the project?

There will be no restrictions on use.

2.2.9 How will the identity of the person accessing the data be ascertained?

Not applicable.

2.2.10 Is there a need for a data access committee (e.g. to evaluate/approve access requests to personal/sensitive data)?

- No

2.2.11 Will metadata be made openly available and licenced under a public domain dedication CC0, as per the Grant Agreement? If not, please clarify why.

- Yes

Metadata will be made openly available and licensed under a public domain dedication open license (Creative Commons Attribution International Public License (CC BY)).

2.2.12 Will metadata contain information to enable the user to access the data?

- Yes

2.2.13 How long will the data remain available and findable? Will metadata be guaranteed to remain available after data is no longer available?

KU Leuven RDR ensures the storage of data at least for 10 years.

2.2.14 Will documentation or reference about any software needed to access or read the data be included? Will it be possible to include the relevant software (e.g. in open source code)?

Detailed Materials and Methods sections will be available in open-access preprints and publications, as well as in metadata file descriptions. These descriptions will explicitly outline the list of software used, references, DOIs, parameters, and more. The data will be provided in readily accessible formats (PDF, XLSX) and in file formats commonly employed in our discipline.

2.3 FAIR data: Making data interoperable

2.3.1
What data and metadata vocabularies, standards, formats or methodologies will you follow to make your data interoperable to allow data exchange and re-use within and across disciplines?
Will you follow community-endorsed interoperability best practices? Which ones?

All descriptors will be conveyed in a language easily understood by diverse disciplines, ensuring accessibility to a wider scientific community. Data will be deposited in a format that can be easily accessible for everyone (using txt files, MS Word/Excel, pdf).
All metadata and data vocabularies will be recognizable to any researcher working on our discipline as well as chemistry, and physical chemistry.
We will adhere to accepted standards for interoperability, as endorsed by the community and applicable to our specific field.

2.3.2 In case it is unavoidable that you use uncommon or generate project specific ontologies or vocabularies:
Will you provide mappings to more commonly used ontologies?

Will you openly publish the generated ontologies or vocabularies to allow reusing, refining or extending them?

Not applicable

2.3.3 Will your data and other research outputs include qualified references to other data (e.g. other data from your project, or datasets from previous research)?

- Yes

When applicable.

2.4 FAIR data: Increase data re-use

2.4.1 How will you provide documentation needed to validate data analysis and facilitate data re-use?

Detailed information on methodology, experimental setup, measurement parameters, and data analyses will be provided in the README files. This will ensure that our data will be easy to reuse and understand.

2.4.2
Will your data and other research outputs be made freely available in the public domain to permit the widest re-use possible?
Will your data and other research outputs be licensed using standard reuse licenses, in line with the obligations set out in the Grant Agreement?

Yes, data will be made freely available on the different repositories, including KU Leuven RDR, under standard reuse licenses (Creative Commons Attributions International Public License (CC BY)).

2.4.3 Will the data and other research output produced in the project be useable by third parties, in particular after the end of the project?

- Yes

All data will be preserved for 10 years according to KU Leuven RDM policy. Open access data and the preprint will be available for reuse by the community, specifically in the context of controlled spatio-selective nanoengineering of 2D materials and the fabrication of photoswitchable graphene superlattices.

2.4.4 Will the provenance of the data and other research outputs be thoroughly documented using the appropriate standards?

- Yes

Appropriate standards commonly used in our field will applied to document research outputs and data.

2.4.5 Describe all relevant data quality assurance processes.

Regular meetings with project supervisors will ensure quality control over the data collection process. The conclusive research output and data will be subsequently deposited in a trusted open repository. Data access will be free, but modifications by others will be restricted to ensure data quality and security. KU Leuven has specific IT specifications for data storage and management. Tailored solutions are provided by the IT department based on factors like data confidentiality, storage space, the possibility of data sharing with colleagues, data type, metadata, etc. Additionally, standard data quality processes such as calibration, repeat measurements, and peer review will be adhered to.

3. Other research outputs

3.1 Do you have any additional information, that was not addressed in the previous sections, which you wish to provide regarding other research outputs that are generated or re-used throughout the project?

Not applicable to the work carried out in this project. If, at any point, this becomes the case, we will adhere to this policy.

4. Allocation of resources

4.1 What will the costs be for making data and other research outputs FAIR in your project?

There will be no costs to make data and research outputs FAIR in this project, as repositories and other resources are provided by KU Leuven free of charge.

4.2 How will these be covered?

Not applicable.

4.3 Who will be responsible for data management in your project?

The research Fellow will be responsible for the data management during the project. Furthermore, the supervisor and co-supervisor of the project will ensure the long-term storage of the data at KU Leuven.

4.4 How will long term preservation be ensured?

All data will be preserved for 10 years according to KU Leuven RDM policy. KU Leuven provides this free of charge.

5. Data security

5.1 What provisions are or will be in place for data security?

KU Leuven has IT specifications for data storage and management, including standard backups. The IT department provides tailored solutions to ensure that data is securely stored, and cannot be altered by an unauthorized entity. Throughout the data collection phase of the project (i.e., before data is made open), all data will be securely stored on a 2-factor authentication-protected KU Leuven OneDrive server. Backup copies will be stored on the password-protected KU Leuven internal server, and the two folders are synchronized automatically. Other repositories such as chemRxiv and arXiv also have identical rules according to their policies.

5.2 Will the data be safely stored in trusted repositories for long term preservation and curation?

- Yes

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

6. Ethics

6.1 Are there, or could there be, any ethics or legal issues that can have an impact on data sharing?

- No

6.2 Will informed consent for data sharing and long term preservation be included in questionnaires dealing with personal data?

- Not applicable

7. Other issues

7.1 Do you, or will you, make use of other national/funder/sectorial/departmental procedures for data management? If yes, which ones (please list and briefly describe them)?

- Yes: describe below

KU Leuven has well-established data management policies, which will be thoroughly followed.