SILVER ZEOLITE COMPOSITES - BASED LED: INSIGHTS FROM MULTISCALE MODELING AND ACCELERATING DISCOVERY BY ARTIFICIAL INTELLIGENCE.

A Data Management Plan created using DMPonline.be

Creator: Hung Tan Pham

Affiliation: KU Leuven (KUL)

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Project abstract:

Silver zeolite composite based LED (ZEOLED) devices are promising alternatives for current LEDs devices based on rare – earth metal complexes because of their good optical properties, and more importantly because they are made up of cheap abundant materials. However, the emissive properties and fundamental photodeactivation decays of the silver nanoclusters confined in zeolites are not fully understood yet. The current proposal devotes to fill this gap and by performing exhaustive computational modelling in complex environments and a high – throughput screening of a large chemistry space to identify novel silver zeolite materials with optimal photoluminescence properties. Computational protocols enabling to uncover the simultaneous effect of water molecules and counterbalancing ions on the photophysical properties of confined silver cluster, will be developed. Finally, the high–throughput screening of existing and hypothetical zeolite databases containing more than two million structures will be performed in search of novel excellent silver cluster zeolite materials.

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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: ***N****(ew data) or* ***E****(xisting data)*	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
Agn-Zeolites	photo properties of silver nanocluster confined in zeolites and their structural information	N	D	T		<100GB	
DeemDatabase	Theoretical zeolite frameworks	E	D	T		<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:

DeemDatabase: https://doi.org/10.1039/C0CP02255A

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

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).

Data sheets will be kept for all large datasets.

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

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)

How will the data be backed up?

- Personal back-ups I make (specify below)

Data will be stored on my desktop that provided by division.

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?

We set a strong password.

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

No extra-cost.

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

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

Cost will be covered by internal fund.

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 open data

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

Question not answered.

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.

- Other data repository (specify below)

we will use github.

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.

- MIT licence (code)

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.

- No

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

Free of charge

Responsibilities

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

I am in charge to manage data during the research project

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

I am in charge to manage data during the research project

Who will manage data preservation and sharing?

I am in charge to manage data during the research project

Who will update and implement this DMP?

I am in charge to manage data during the research project