## Plan Overview

*A Data Management Plan created using DMPonline.be*

**Title:** Layered Double Hydroxides in cement - water structuring and dynamics in novel cementitious binders revealed by NMR crystallography - LDH2O

**Creator:** Ruben Snellings

**Principal Investigator:** Ruben Snellings, n.n., n.n.

**Affiliation:** KU Leuven (KUL)

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

**Template:** FWO DMP (Flemish Standard DMP)

**Principal Investigator:** Ruben Snellings, n.n. n.n., n.n. n.n.

**Project abstract:**

Concrete, a composite material held together by hydrated cement, is the number one synthesized material by man-kind and responsible for 7% of global CO2 emissions. Calcium aluminate layered double hydroxides (LDH) are an important component of hydrated cement. Optimizing their composition and improving our knowledge on their structure and properties offers options to reduce the CO2 footprint of concrete and reduce resource depletion by prolonging the life of concrete structures and enabling its production in a more sustainable way. The LDH2O project focuses on resolving the structural role of water in cement LDH phases. Using NMR crystallography, a powerful combination of advanced NMR spectroscopy, diffraction and transmission electron microscopy techniques, the project will resolve new LDH structures and refine existing one. This will shed light on how the LDH interlayer architecture and hydration states are determined by the interlayer anion groups. This is important, as changes in the LDH structure and properties impact the way concrete responds to changes in temperature, humidity, or aggressive environments.

**ID:** 212294

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**End date:** 31-12-2028

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## DPIA

**DPIA**

- Not applicable

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## Application DMP

**Questionnaire**

The project will generate 1) analytical data of synthesized LDH phases (diffraction, NMR spectroscopy, Transmission Electron Microscopy,...). These datasets will be used to develop and validate structure models that will, in turn, generate data for thermodynamic databases; 2) experimental results, the interpreted data; 3) Reports (papers), presentations and posters; and 4) visualizations of the results (graphics).

The supervisor/spokesperson (Ruben Snellings) will be in charge of developing and implementing the data management plan and managing the data preservation. Data and metadata will be stored in a structured project folder located in a shared environment for project team members only (Teams/Sharepoint).

At the end of the project, all research data will be archived by the IT services (K-drive, ICTS, KU Leuven). Research data used in, or supporting published manuscripts will be publicly
shared by archiving in the KU Leuven Research Data Repository (RDR). All data will be retained for 10 years after the project in line with the KU Leuven RDM policy.

N/A

N/A

N/A

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## GDPR

**GDPR**

- Not applicable

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## FWO DMP (Flemish Standard DMP)

### 1. Research Data Summary

| | | | | 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:*<br>• Generate new data<br>• Reuse existing data | *Please choose from the following options:*<br>• Digital<br>• Physical | *Please choose from the following options:*<br>• Observational<br>• Experimental<br>• Compiled/aggregated data<br>• Simulation data<br>• Software<br>• Other<br>• NA | *Please choose from the following options:*<br>• .por, .xml, .tab, .csv,.pdf, .txt, .rtf, .dwg, .gml, …<br>• NA | *Please choose from the following options:*<br>• <100MB<br>• <1GB<br>• <100GB<br>• <1TB<br>• <5TB<br>• <10TB<br>• <50TB<br>• >50TB<br>• NA | |
| 1. analytical characterisation data of synthetic LDH phases | Datasets including diffraction, NMR spectroscopy, TEM, SEM, ICP-OES,... | New data | Digital | Observational and Experimental | .raw, .csv, .xls, .txt | <100 GB | - |
| 2.interpreted data for thermodynamic database | Solubility data, calculated thermodynamic properties | New data | Digital | Experimental and calculated data | .xls | <100 MB | |
| 3.Crystal structure information files | Crystal structure information: space group, atomic positions, occupancies,... | New data | Digital | Calculated data | .cif | <100 MB | |
| 4. Reports | Scientific papers, presentations and posters | New data | Digital | Compiled data | .pdf | <1 GB | |
| 5. Data visualization | Graphics | New data | Digital | Other | .ai, .tiff, .jpg | <1 GB | |

NA

- No

- No

- No

- No

- No

**2. Documentation and Metadata**

We will use an excel log file and an experiment form to capture documentation accompanying measurement data (dataset 1). For measurement data, following information will be typically included in the log file, the experiment form or the data file, where applicable:
- Name of file or dataset
- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description of the dataset,
- Sample information: raw materials, synthesis procedure
- Number of files included
- List with names of files, description, date of creation
- Software used to generate data
- Software needed to open files
- Naming convention for file names
- Storage location(s)
- Aim for which the data were collected - reference to experiment form
- Data collection method, instrument, instrument settings
- Data processing method
- Confidentiality information
- Full names and definitions for column and rows
- Explanation of abbreviations
- Units of measurement
- Publications based on this dataset
- Relationship to other datasets
- References to datasets used to create the dataset

For simulation or calculated results (datasets 2,3), following data will typically be recorded in a log file:
- Name of file or dataset
- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description of the dataset, simulation/calculation information
- Number of files included
- List with names of files, description, date of creation
- File Formats
- Software used to generate data
- Software needed to open files
- Naming convention for file names
- Storage location(s)
- Rationale why the data were produced

- Confidentiality information
- Full names and definitions for column and rows
- Explanation of abbreviations
- Units of measurement
- Publications based on this dataset
- Relationship to other datasets
- References to publications used to create the dataset

For reports and graphics (datasets 4,5), following data will typically be recorded in a log file:

- Name of file or dataset
- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description
- File Formats
- Software used to generate data
- Software needed to open files
- Naming convention for file names
- Storage location(s)
- Reason why the file was produced
- Confidentiality information
- Explanation of abbreviations
- Relationship to underlying datasets
- References to other publications used to create the file

- Yes

The KU Leuven RDR metadata standard DataCite will be used.

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

- OneDrive (KU Leuven)/ Internal back-up service (RWTH Aachen) for local data storage
- Sharepoint online for collaboration
- During the project data will be stored in a structured Sharepoint folder. This will be structured for collaboration, sharing and storage of data, giving all team members access to the project information and data.

Standard back-up provided by KU Leuven ICTS

- Yes

The project will not generate excessive data volumes (<100 GB) as such the data can be covered under the data allowances provided by KU Leuven to its researchers without cost. If the data volume would exceed the personal allowances (500 GB), additional storage space will be purchased and provided by the PI.

The sharepoint is only made accessible to the research team members. Access is given by the project coordinator.

At this stage, KU Leuven centrally covers the costs related to data storage and backup of the Sharepoint.
RWTH Aachen will generate only small data volumes (dataset 2), hence no costs will be incurred.

#### 4. Data preservation after the end of the research project

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

- Shared network drive (J-drive): All project data will be stored on the secured archiving drive maintained by the IT services of the Department of Earth and Environmental Sciences.
- KU Leuven RDR: Research data used in or supporting published manuscripts will be publicly shared by archiving in the KU Leuven Research Data Repository (RDR).

We expect that the total size of data will not exceed 500 GB, which is comprised within the KU Leuven data storage drives and sharepoint allocations without cost.

#### 5. Data sharing and reuse

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

Dataset 1 will be made a accessible upon approval (restricted access) - this constitutes the "raw data" which may still need to be validated and/or published.
Datasets 2,3,4,5 will be made openly available - as publications, supporting information and through the RDR.

Dataset 1: data will be released to trusted users/research teams upon review of their request - this may require concluding a data transfer agreement.

- No

KU Leuven RDR (Research Data Repository)

Upon publication of research results
Finished, yet unpublished data will be made available latest 12 months after the end of the project, this time delay would allow for publication of late manuscripts.

CC-BY 4.0 (data)
Data Transfer Agreement (restricted data)

- Yes

We don't expect additional costs as the total volume of finished datasets will likely not exceed 50 GB, which is in line with RDR free allowance.

**6. Responsibilities**

Both ESRs and the post-doc will be responsible for implementing the data documentation and metadata management rules.

The project researchers, supervised by the PI and co-PI

The project supervisor: Ruben Snellings

The project PI, Ruben Snellings