# DMP title

**Project Name** Catalytic upgrading of polyolefins via oxygenation and in-chain ester formation using Ti and Sn zeolite catalysts - FWO DMP - DMP title

**Grant Title** 1S85822N

**Principal Investigator / Researcher** Robin Lemmens

**Project Data Contact** +32496347927; robin.lemmens1@kuleuven.be

**Description** Plastic wastes are so far underexplored as feedstocks for producing upcycled materials. This project, focusing on the large available mass of end-of-life polyolefins, aims at selective oxidation of these hydrocarbon-type materials. As a first option, alcohol (and ketone) groups are created along the polyolefin chain. For this, selective Ti-containing zeolites and clean oxidants (e.g. hydrogen peroxide) are applied at mild temperatures, avoiding the adverse aspects of free radical autoxidations. Polyolefins with a small degree of hydroxylation offer great perspectives, e.g. regarding coatability, while preserving most attractive properties of the original polyolefins. Secondly, the ketone groups on the polyolefins are further converted to in-chain esters via a Baeyer-Villiger reaction. Such reaction is enabled by Sn-doped zeolites, using again peroxides. This results in polyethylene-derived polyesters, with attractive new properties like easy degradation by chemolysis, or even self-healing. For both major reaction types, the architecture of the zeolites is adapted to deal with the polymeric nature of the dissolved reactants. Catalyst-polymer interactions are studied in detail, also to facilitate recovery and reuse of the heterogeneous catalysts. Finally, key characteristics of the isolated reaction products (e.g. functionalization, thermal and structural properties) are recorded to facilitate future market adoption of these new materials.

**Institution** KU Leuven

## 1. General Information

### Name applicant

Robin Lemmens

### FWO Project Number & Title

1S85822N

Catalytic upgrading of polyolefins via oxygenation and in-chain ester formation using Ti and Sn zeolite catalysts

### Affiliation

- KU Leuven

## 2. Data description

### Will you generate/collect new data and/or make use of existing data?

- Generate new data

### Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow and per WP or objective of the project. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

Procedures for performing reactions, for synthesizing catalysts and initial observations of these experiments will be gathered. Such procedures will also result in raw data files containing chromatographic data (GC-FID, GC-MS) and material characterization data (XRD, physisorption and chemisorption data or spectroscopic analysis via UV-Vis, NMR etc.). These will be processed in excel files, summaries and presentations, finally culminating in manuscripts and/or patents. The combined virtual volume of these datasets will be limited (< 10 GB), and will consist mostly of data files containing GC chromatograms (up to 5 GB).

Examples:

| Type of data | Format | Volume | How created |
|---|---|---|---|
| X-ray diffractaction patterns | .xrdml | 20 kB | XRD spectroscopy of synthesized catalysts |
| UV-vis spectra | .csv | < 1 MB | UV-Vis spectropscopy of synthesized catalysts |
| GC chromatograms | .gcd | < 2 MB | GC analysis of worked-up reaction samples |
| NMR spectra | / | 256 kB | NMR spectroscopy of synthesized products |

## 3. Legal and ethical issues

**Will you use personal data? If so, shortly describe the kind of personal data you will use. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registering the fact that you process personal data is a legal obligation.**

- No

Privacy Registry Reference:
Short description of the kind of personal data that will be used:

**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, add the reference to the formal approval by the relevant ethical review committee(s)**

- No

**Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for what data and which restrictions will be asserted?**

- Yes

The methods and reactor configurations developed in this project have potential for valorization, which will be subjected for discussion during the project. Patents will be submitted, transferred and valorized with the assistance of the intellectual property unit of KU Leuven Research & Development (LRD).

**Do existing 3rd party agreements restrict dissemination or exploitation of the data you (re)use? If so, to what data do they relate and what restrictions are in place?**

- No

## 4. Documentation and metadata

**What documentation will be provided to enable reuse of the data collected/generated in this project?**

Details to reproduce reaction procedures are described in a personal lab booklet. Upon presentation or publication of data, procedures are described in sufficient detail to enable a reproduction of the generated results for an experienced user. ReadMe-files or recording methods for advanced characterization are stored in parallel with generated data.

**Will a metadata standard be used? If so, describe in detail which standard will be used. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.**

- No

Although no metadata standard is available for the advanced characterization in this project,

most techniques store a non-standardized ReadMe-file containing recording parameters and file information in parallel with recorded datasets. Alternatively, some datasets contain metadata headers on recording parameters (e.g. XRD diffractograms). The data will be stored and named in a consistent manner with unambiguous identifiers. Descriptions of experiments and materials are kept in physical lab notes for each identifier. The data will be processed and summarized in a comprehensive excel worksheet with references to the identifiers. The resulting summaries will culminate in presentations, and finally in manuscripts and/or patents.

## 5. Data storage and backup during the FWO project

**Where will the data be stored?**

Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from ‘Box’. KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space of up to 100 GB for each user.

**How is backup of the data provided?**

By using the cloud storage of ‘Box’, digital data will be stored in parallel on the cloud and on the personal computer of the applicant, guaranteeing back-up for this data. Most raw data is also stored and frequently backed up off-line on external hard drives.

**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

The cloud storage provides a storage space up to 100 GB for each user, while the project is expected to generate less than 10 GB.

**What are the expected costs for data storage and back up during the project? How will these costs be covered?**

Data storage costs on Box are included in an internal service contract with the KU Leuven IT support service (SET-IT). No additional costs are expected for the storage of data. In case additional costs do arise, they will be covered by the project budget or reserve funds.

**Data security: how will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

The data will be stored in the university's secure environment for private data. An Enterprise Box account 3 for cloud storage ensures a secure environment.

## 6. Data preservation after the FWO project

**Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state the reasons for this (legal or contractual restrictions, physical preservation issues, ...).**

All data will be retained for the expected 5 year period after the end of the project.

**Where will the data be archived (= stored for the longer term)?**

Upon termination of the contract, the data will be transferred and stored on an external hard drive (Samsung Portable SSD T5 1 TB), managed by Annelies Van Vlasselaer.

**What are the expected costs for data preservation during the retention period of 5 years? How will the costs be covered?**

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Given the cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project’s consumable expenses or covered by reserve funds.

## 7. Data sharing and reuse

**Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?**

- No

**Which data will be made available after the end of the project?**

Upon publication of the research results, the full datasets will be made available upon reasonable request.

**Where/how will the data be made available for reuse?**

- Upon request by mail

**When will the data be made available?**

Upon publication of the research results

**Who will be able to access the data and under what conditions?**

Only uses for research purposes will be allowed and commercial reuse will be excluded.

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

No additional costs are expected as the data can be shared via online platforms (e.g. WeTransfer) or the already budgeted storage cloud from Box. If additional costs would occur they will be covered from reserve funds.

## 8. Responsibilities

**Who will be responsible for data documentation & metadata?**

The applicant (Robin Lemmens).

**Who will be responsible for data storage & back up during the project?**

The applicant (Robin Lemmens), his supervisor (Dirk De Vos) and Annelies Van Vlasselaer.

**Who will be responsible for ensuring data preservation and reuse ?**

The supervisor (Dirk De Vos) and Annelies Van Vlasselaer.

**Who bears the end responsibility for updating & implementing this DMP?**

The applicant (Robin Lemmens) and his supervisor (Dirk De Vos) bear the end responsibility of updating & implementing this DMP.