Plan Overview

A Data Management Plan created using DMPonline

Title: Hot! Hot! Hot! Fundamentals of Plasmon Catalysis

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Project abstract:

Noble metal nanoparticles made of gold, silver, and copper are used as catalysts in a wide range of processes. Recently, it has been shown that irradiating such nanoparticles with light can significantly improve their catalytic activity and selectivity, a result that could have a tremendous impact on the chemical industry. The observed optical modulation of the electronic properties of nanostructured catalysts is due to the excitation of plasmon resonances, which are collective oscillations of the nanoparticle’s free electrons. However, despite increasing experimental efforts, the exact physical mechanism behind the observed plasmon enhancement of catalysis is still a topic of intense debate. In this proposal I will quantitatively discriminate between competing mechanisms of optical activation of catalysis, by comparing the electron transfer rates in model catalytic reactions in the dark and under plasmon resonance excitation. In particular, I will measure the reaction conversion rate on nanocatalysts with well-defined size, shape, composition, and surface chemistry, while selectively turning off each “hot” activation mechanism, by rational choice of the optical and chemical parameters. Furthermore, I will use a super-resolution microscopy approach to spatially reconstruct the distribution of catalytic events at the surface of individual nanoparticles, which will allow a direct visual discrimination between the competing mechanisms of plasmon activation of catalysis.

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Hot! Hot! Hot! Fundamentals of Plasmon Catalysis

General Information

Name applicant and project number

Andrea Baldi
Vidi project 680-47-550

Name of data management support staff consulted during the preparation of this plan and date of consultation.

1) Elisa Rodenburg, RDM Support Desk, University Library, Vrije Universiteit Amsterdam
2) Dr. Brett G. Olivier, Email: rdm.beta@vu.nl, Faculty of Science - Data Stewards, Vrije Universiteit Amsterdam
Consulted on January 19, 2021

1. What data will be collected or produced, and what existing data will be re-used?

1.1 Will you re-use existing data for this research?

If yes: explain which existing data you will re-use and under which terms of use.

- No

1.2 If new data will be produced: describe the data you expect your research will generate and the format and volumes to be collected or produced.

PhD #1 will work on chemical synthesis and optical characterisation of colloidal suspensions. These tasks involve the following data and data formats:
- textual laboratory notebooks
- optical spectra: .txt files and .xls spreadsheets
PhD #2 will work on nanolithography sample preparation and super-resolution microscopy imaging. These tasks involve the following data and data formats:
- textual laboratory notebooks
- .tiff images and .spe files
The .spe files will be converted to data spreadsheets using our own Matlab scripts. We will also use free data analysis softwares, including ImageJ and ThunderSTORM.

1.3. How much data storage will your project require in total?

- >1000 GB

In the past 3 years my research group has generated roughly 15 TB of data.
Most of these come from super-resolution microscopy experiments that require collecting microscope images at rates as high as 10 frames per second for several hours. This typically generates several (1-5) GB of data per experiment.

2. What metadata and documentation will accompany the data?

2.1 Indicate what documentation will accompany the data.

Metadata is typically written in lab notebooks or in readme.txt files saved in the same folder as the data.
The file structure of the group is as follows:
- Raw data is stored in folders with the researcher's name
- each researcher's folders contains several project folders
- each project folder contains several experiment folders named "yyyy-mm-dd_..."

When we prepare our results for publication, we take pictures of the notebooks and save them together with the data and we also summarise the metadata in readme.txt files that explain how the data has been acquired (setups, softwares, versions, etc.), analyzed, and stored.
Analysis (Matlab) scripts are typically commented to explain the different steps.

2.2 Indicate which metadata will be provided to help others identify and discover the data.

Typically data is accompanied by readme.txt files and/or (pictures of) laboratory notebooks.
For data appearing in publications, each article has a replication package folder containing a readme.txt file. The typical (DataCite compatible) content of a readme.txt file is as follows:
Title of the publication:
Authors:
Journal including volume and page numbers:
Date of publication:
Description:
Keywords:
Date:
Commercial software used in the data analysis:
Open access software used in the data analysis:
Structure of the folder:
Each article folder is further divided into "figure folders", which contain subfolders with the raw data and a readme.txt file describing how the raw data displayed in the figure has been acquired, analysed, converted, and plotted.

3. How will data and metadata be stored and backed up during the research?

3.1 Describe where the data and metadata will be stored and backed up during the project.

- Institution networked research storage

3.2 How will data security and protection of sensitive data be taken care of during the research?

- Not applicable (no sensitive data)

4. How will you handle issues regarding the processing of personal information and intellectual property rights and ownership?

4.1 Will you process and/or store personal data during your project?

If yes, how will compliance with legislation and (institutional) regulation on personal data be ensured?

- No

4.2 How will ownership of the data and intellectual property rights to the data be managed?

There are no such restrictions on the data.

5. How and when will data be shared and preserved for the long term?

5.1 How will data be selected for long-term preservation?

- All data resulting from the project will be preserved for at least 10 years

5.2 Are there any (legal, IP, privacy related, security related) reasons to restrict access to the data once made publicly available, to limit which data will be made publicly available, or to not make part of the data publicly available?

If yes, please explain.

- No

5.3 What data will be made available for re-use?

- All data resulting from the project will be made available

5.4 When will the data be available for re-use, and for how long will the data be available?

- Data available as soon as article is published

5.5 In which repository will the data be archived and made available for re-use, and under which license?

We will use one of the three long-term storage options available at the VU for example:

- DataversNL (provides unique identifiers and DOI's)
- Archstor (VU Institutional archive, data is findable by unique URN through the PURE research portal)
- Zenodo.org (provides DOI's)

An appropriate licence will be selected when published data is archived, for example, the Creative CommonsCC-BY 4.0 licence.

5.6 Describe your strategy for publishing the analysis software that will be generated in this project.

Most data will be published as is, or analysed using free software tools, such as ImageJ and ThunderSTORM.
Some data analysis will be performed using our own Matlab scripts. We are considering the option of sharing the scripts in GitHub.

6. Data management costs

6.1 What resources (for example financial and time) will be dedicated to data management and ensuring that data will be FAIR (Findable, Accessible, Interoperable, Re-usable)?

Data replication packages, including readme.txt files, raw data, and processed data will be created for each published article and PhD thesis. This typically costs 1 day of work to the first author of the manuscript.

The costs of data storage will be roughly €0.20/GB/year and will be covered by the group's annual budget.