Materials Chemistry and Catalysis

Materials Chemistry and Catalysis (MCC)
research overview

Kris Helfferich & Ilja Janssen

PROTON

MCC

Materials Chemistry and Catalysis

3 full professors

3 assistant professors

9 technical/admin staff

4 postdocs

25 PhDs

6 MSc. students

1 BsC. student

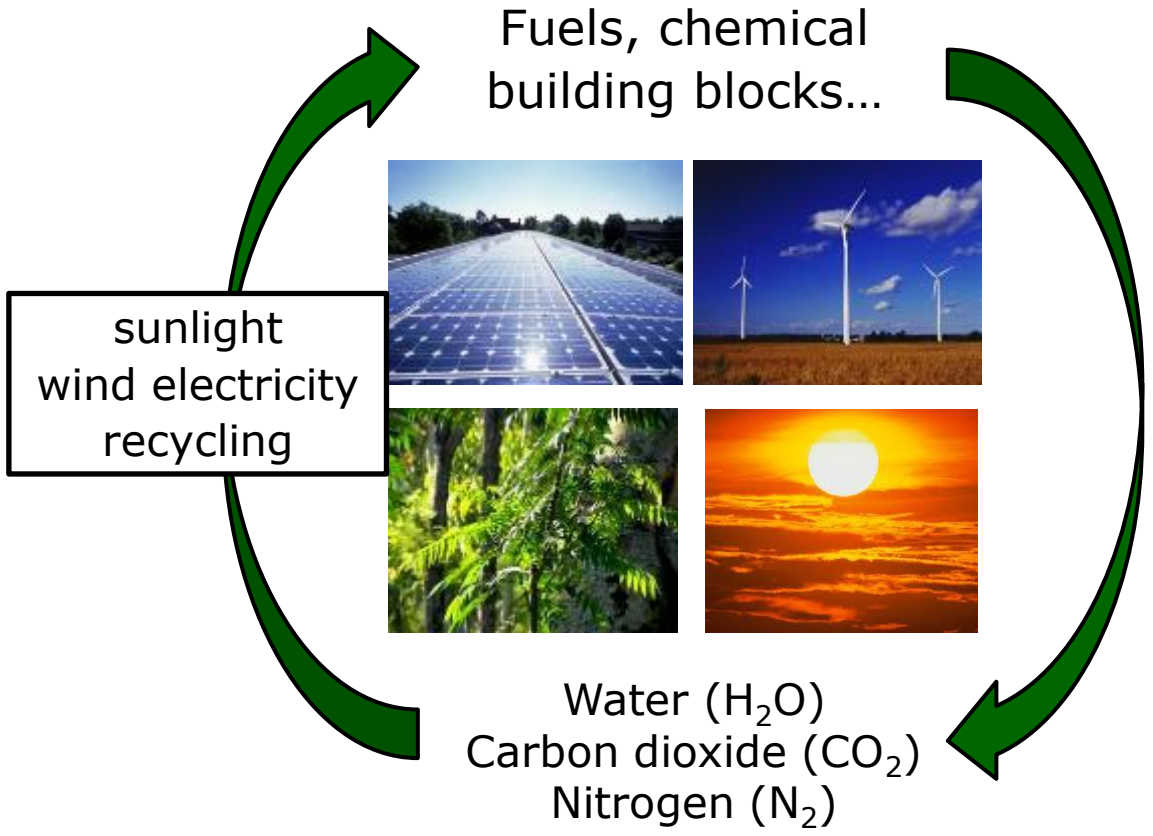
Our mission: Materials, Catalysis, Sustainability

Making existing processes cleaner, consume less energy and materials

Chemical products, medicines, plastics, fuels…

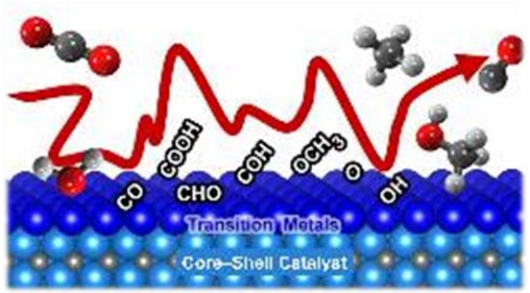
80-90% uses catalyst

Design and make new catalysts and energy materials for a sustainable future

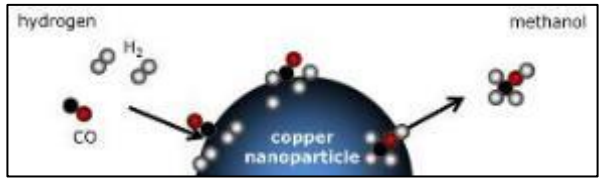


Materials and Catalysis Research

Our research focusses on sustainability

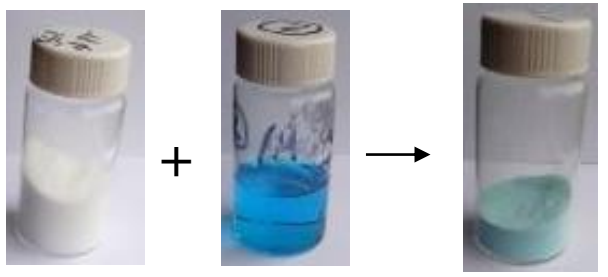


Testing



Characterization

Theory



Preparation

Scientific staff

Full Professors

Prof. Petra. E. de Jongh
Catalysts and energy materials

Prof. Frank M. de Groot
X-ray Spectroscopy of
Catalytic Nanomaterials

Prof. Krijn de Jong
emeritus

Assistant professors

Dr. Peter Ngene
Materials for energy
conversion and storage

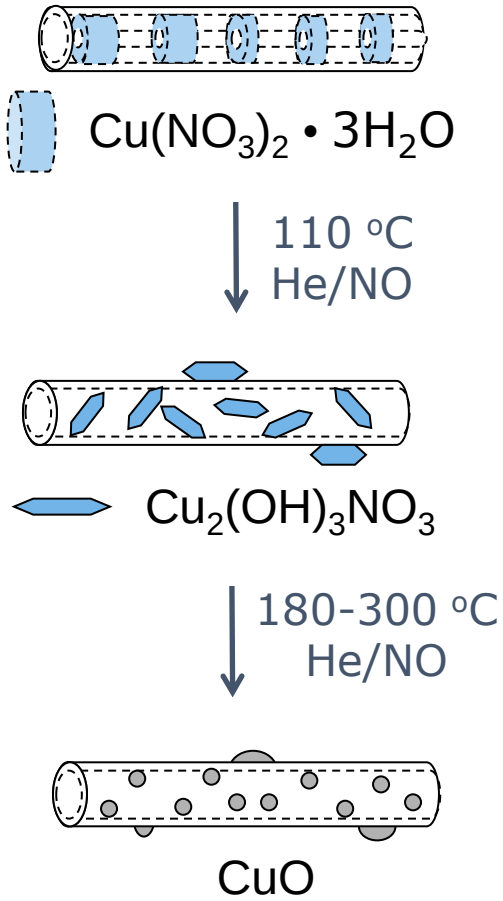
Dr. Nongnuch Artrith
Computational Materials
Science, Machine Learning

Dr. Jessi van der Hoeven
Electron microscopy and
colloidal catalyst design

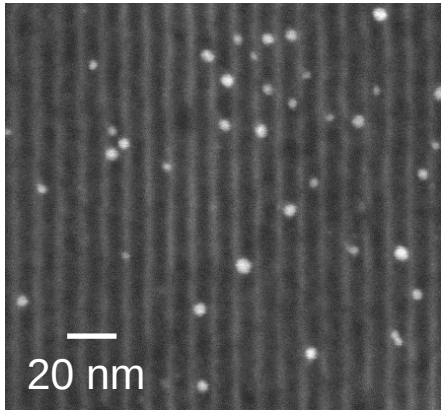
Prof. Petra de Jongh

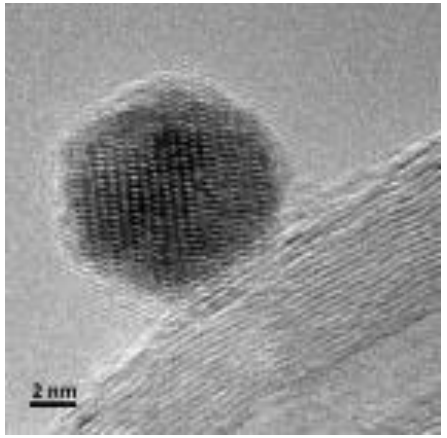
Preparation and testing of catalytic materials

Fundamentals of catalyst preparation



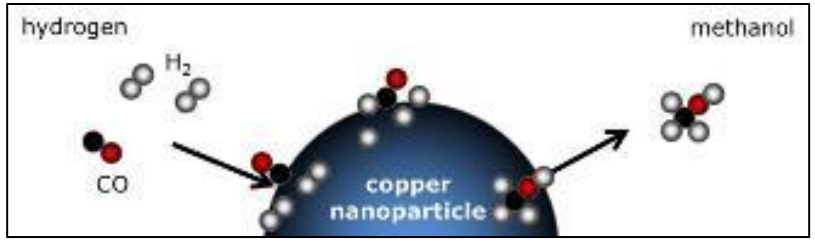
Catalyst Characterization





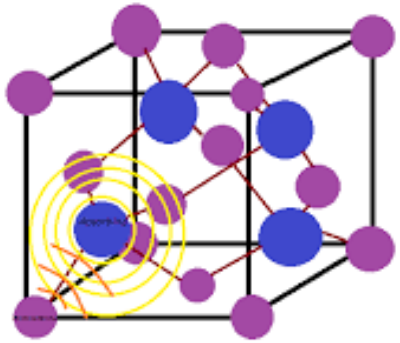
Testing under relevant conditions

- Methanol Synthesis
- CO_2/CO and H_2 to oxygenates, olefins, aromatics
- Selective oxidation
- Selective hydrogenation
- Electrocatalysis
- Battery materials
- Hydrogen

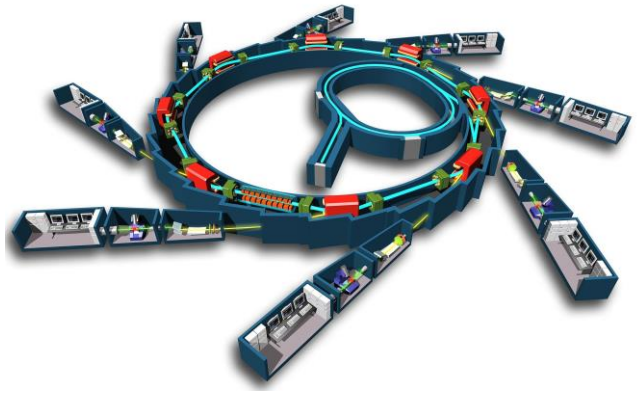


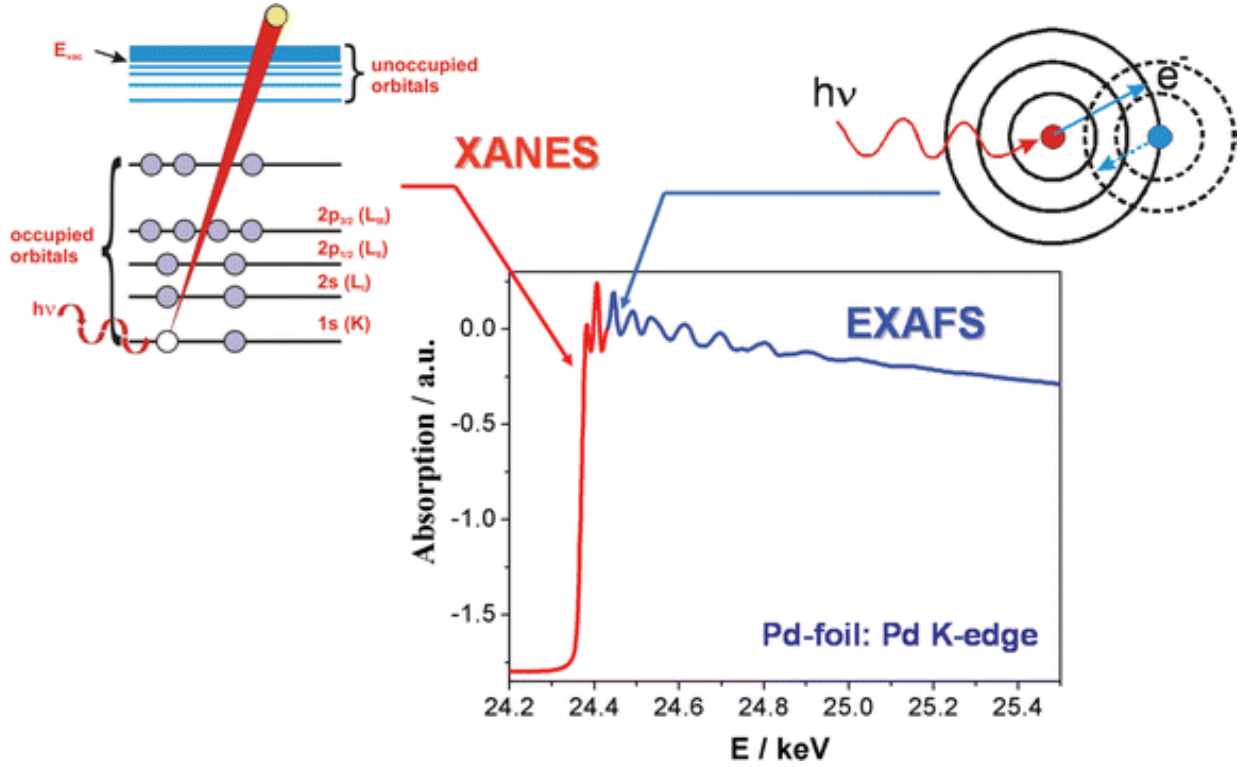
Prof. Frank de Groot

X-ray Spectroscopy: theory and *in situ* measurements



- Use X-ray spectroscopy to understand the electronic and structural properties of energy materials and heterogenous catalysts
- Develop or use theoretical models to interpret results from X-ray absorption spectroscopy





Dr. Peter Ngene

Materials for energy storage and conversion

- Preparation and characterization of materials for energy conversion and storage
- Batteries, H_2 storage, fuel cells, electrochemical CO_2 reduction

Hydrogen

Electricity

Next generation batteries (novel electrodes and solid electrolytes)

CO_2, N_2

Fuels/Chemical
NH_3

Fuel cells

Novel materials for reversible H_2 storage

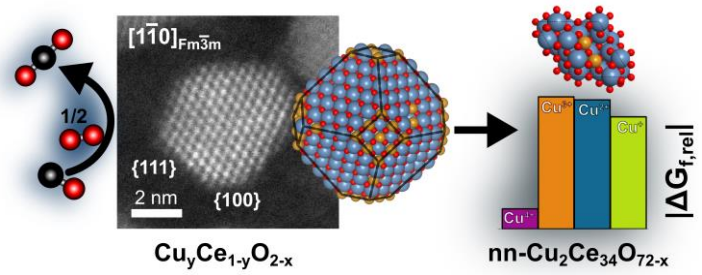
Computational Materials Science and Machine Learning

Modelling and computational discovery of energy materials and interpretation of experimental observations with atomistic first-principles methods and machine learning

Dr. Nong Artrith

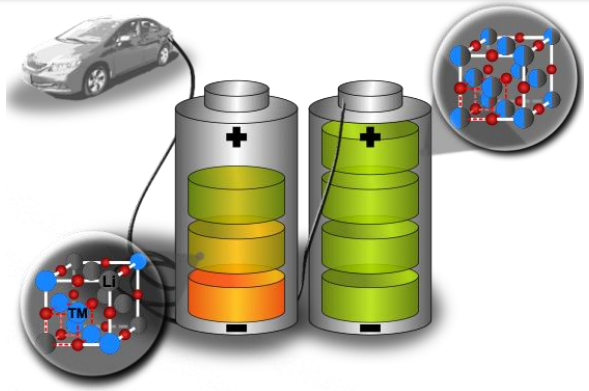
1. Machine Learning & Data Science

- Data from simulation and experiment (with collaborators)
- Accelerating DFT calculations
- Predicting materials properties
- Data mining for materials discovery



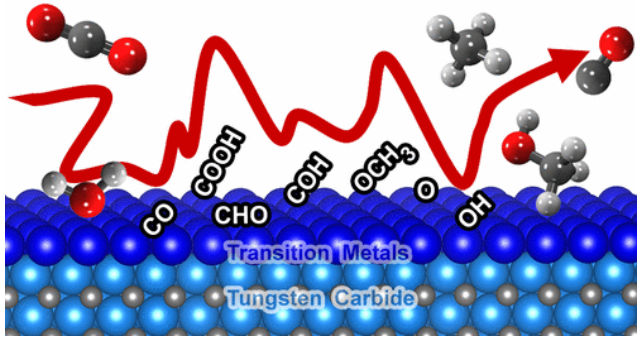
2. Energy Storage

- Storage for renewable energy
- Enable electric vehicles
- Improve portable electronics



3. Energy Conversion

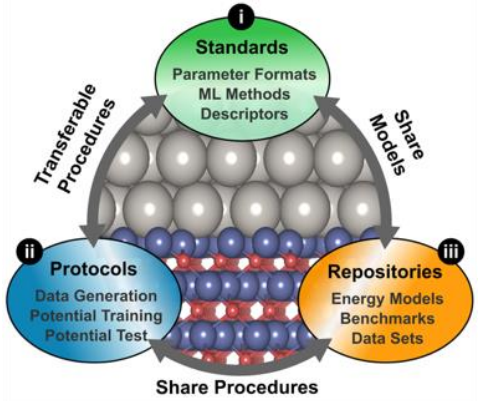
- Replace fossil fuels (oil/gas)
- Produce synthetic fuels using renewable energy



4. Method Development

- **Open-source** ML modeling tools

http://nartrith.atomistic.net aenet



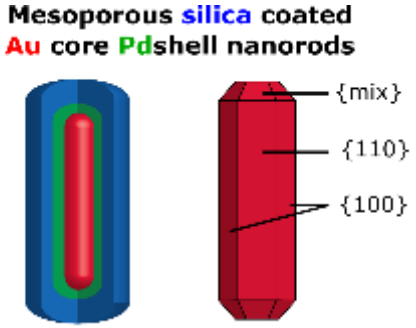
Colloidal Catalysts and Advanced Electron Microscopy

Focus on the design of new catalyst structures using colloid synthesis, and looking at them under operating conditions in the electron microscope

Dr. Jessi van der Hoeven

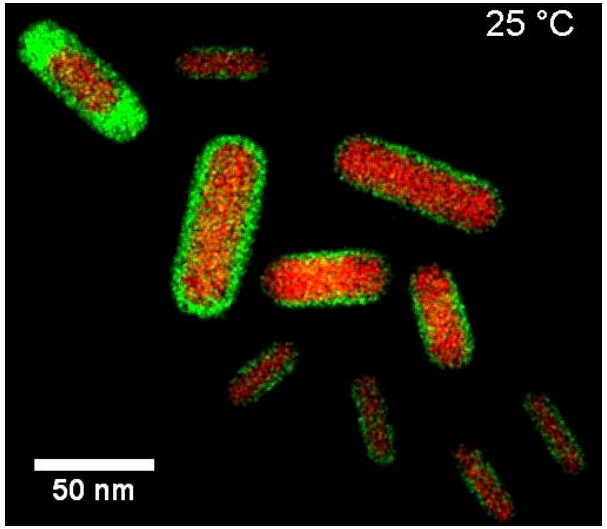
Colloid synthesis

of atomically precise model catalysts

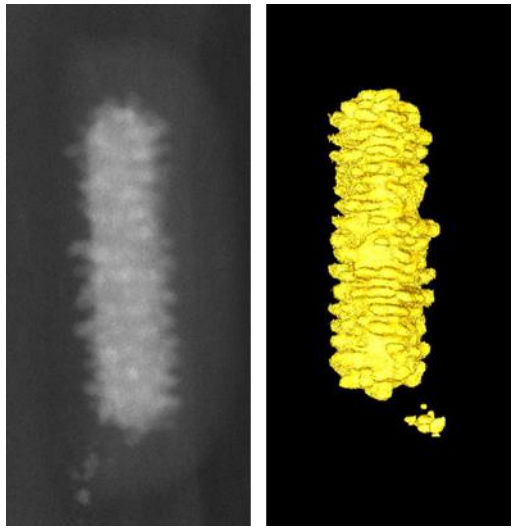


Electron Microscopy

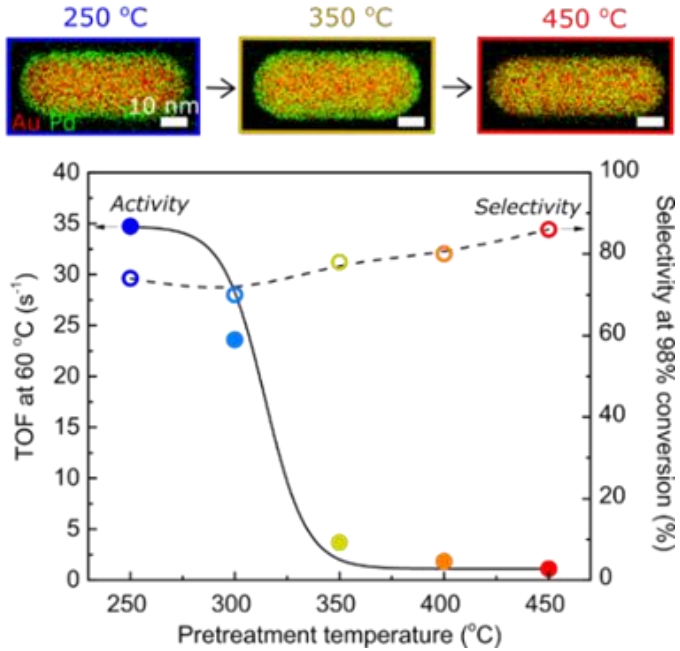
In situ



3D visualization



Reactor studies



As a student …..

- You are welcome in our group.
- You will have a challenging and exciting research project.
- You can get acquainted with all aspects of research (synthesis, characterisation, application, theory), but can choose to focus on a specific aspect.
- You can find information on https://materialschemistryandcatalysis.org/ → have a look at the pages of the PhD students and postdocs.
- You can mail Peter Ngene for more information on available projects.
- You are advised to follow Advanced Catalysis and Synthesis of heterogeneous catalysts and energy materials if you are interested in doing a masters project.

LETTERS
https://doi.org/10.1038/s41563-021-00996-3
nature materials

Check for updates

Unlocking synergy in bimetallic catalysts by core–shell design

Jessi E. S. van der Hoeven[1,2], Jelena Jelic[1], Liselotte A. Olthof[1,2], Giorgio Totarella[1], Relinde J. A. van Dijk-Moes[2], Jean-Marc Krafft[4], Catherine Louis[4], Felix Studt[3,5], Alfons van Blaaderen[2]✉ and Petra E. de Jongh[1]✉

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Contents lists available at ScienceDirect

Catalysis Today

journal homepage: www.elsevier.com/locate/cattod

Check for updates

Copper sulfide derived nanoparticles supported on carbon for the electrochemical reduction of carbon dioxide

Christina H.M. van Oversteeg[a,b,1], Marisol Tapia Rosales[a,1], Kristiaan H. Helfferich[a], Mahnaz Ghiasi[a], Johannes D. Meeldijk[a], Nienke J. Firet[c], Peter Ngene[a], Celso de Mello Donegá[b], Petra E. de Jongh[a,*]

www.afm-journal.de

Designing Highly Conductive Sodium-Based Metal Hydride Nanocomposites: Interplay between Hydride and Oxide Properties

*Laura M. de Kort, Oscar E. Brandt Corstius, Valerio Gulino, Andrei Gurinov, Marc Baldus, and Peter Ngene**

Journal of Catalysis 394 (2021) 307–315

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Journal of Catalysis

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Manganese oxide promoter effects in the copper-catalyzed hydrogenation of ethyl acetate

Rolf Beerthuis[a,1], Nienke L. Visser[a,1], Jessi E.S. van der Hoeven[a,b], Peter Ngene[a], Jon M.S. Deeley[c], Glenn J. Sunley[c], Krijn P. de Jong[a], Petra E. de Jongh[a,*]

Effect of Pore Confinement of $NaNH_2$ and KNH_2 on Hydrogen Generation from Ammonia

Fei Chang,[†] Han Wu,[†] Robby van der Pluijm,[†] Jianping Guo,[‡] Peter Ngene,*[,†] and Petra E. de Jongh*[,†]

Stability of Colloidal Iron Oxide Nanoparticles on Titania and Silica Support

Nynke A. Krans, Dónal L. van Uunen, Caroline Versluis, Achim Iulian Dugulan, Jiachun Chai, Jan P. Hofmann, Emiel J. M. Hensen, Jovana Zečević, and Krijn P. de Jong*

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Questions?

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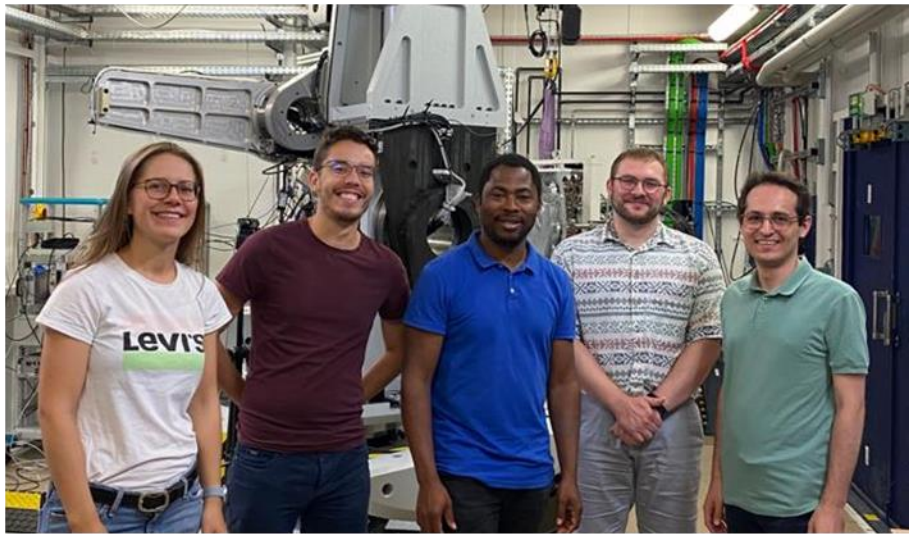
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