

# Materials physics - Who we are and what we do



Jaakko Akola



Raffaella Cabriolu



Ton van Helvoort



Randi Holmestad



Magnus Nord



Morten Kildemo



Turid Reenaas

## Techniques and materials:

- Modelling and simulations of materials
- Thin film deposition and materials processing
- Optical characterization, polarimetry
- Transmission electron microscopy
- Programming, advanced data handling, machine learning
  
- Semiconductors, Metals and alloys, (Multi-)ferroic materials
- Nanoelectronics, Nanophotonics, Photovoltaics, ICT, catalysis.....

II-positions: Jesper Friis, Per Erik Vullum, David Zhe Gao  
~4 technicians, ~20 postdocs/PhD students, ~15 MSc students.. **All together approx. ~50 people**

**..via a project with us  
you can be part of one  
of these activities ...**

## A project within our section offers:

- Choice of a project that fits your interests and background
- Training in operating advanced scientific equipment
- Or simulation and quantification software (theory/modelling)
- "Big data" processing using Python
- Concrete tasks - industry relevant projects available
- Weekly meetings with supervisor during the project
- In some cases:
  - Being part of a large, dynamic scientific consortium
  - Possibility in extending the project to MSc/PhD
  - Summer job / internship in Japan
  - Collaborations with other departments, international...



<http://www.ntnu.edu/geminicentre/tem>

# Prof. Jaakko Akola

[jaakko.akola@ntnu.no](mailto:jaakko.akola@ntnu.no)

<https://www.ntnu.edu/employees/jaakko.akola>

## Main research interests:

- Atomistic and mesoscale simulations of **metal alloys** (DFT, Monte Carlo, phase field)
- DFT simulations of **semiconductors**
- Simulations (DFT) of **catalytic reactions**

## Projects offered 2022:

- Fingerprinting of atomistic defect sites in oxides via machine learning, relevance for **microelectronics applications** (one project)
- Machine learning of atomic migration and Kinetic MC for modelling of **precipitate formation** in Al (two projects)
- **Catalytic reactions of CO<sub>2</sub>** on metal clusters, production of synthetic fuels (one project)

## ALLDESIGN

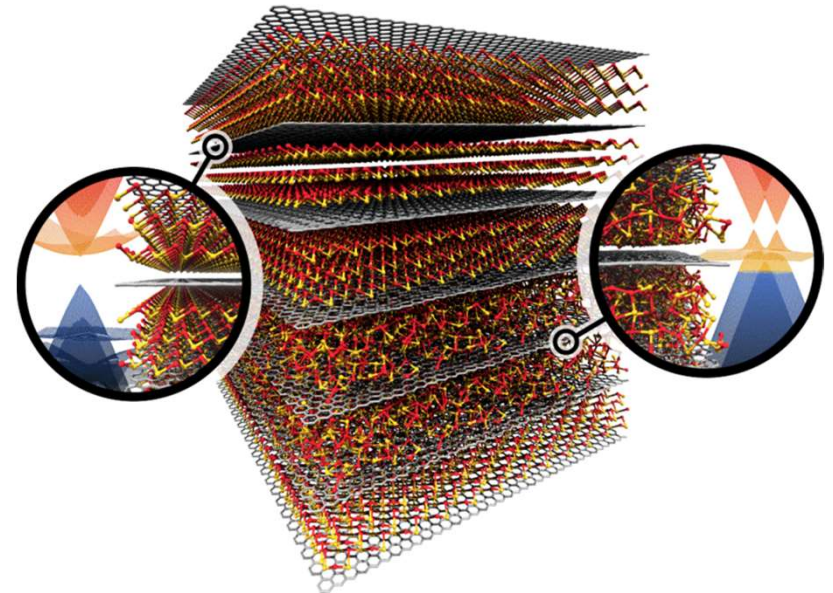
NTNU Digital Transformation project for aluminum alloys



$$E_0 = E[n_0] = \langle \Psi[n_0] | \hat{T} + \hat{V} + \hat{U} | \Psi[n_0] \rangle$$

$$V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2 n_s(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3 r' + V_{XC}[n_s(\vec{r})]$$

← DFT!



# Assoc. prof. Raffaella Cabriolu

[raffaella.cabriolu@ntnu.no](mailto:raffaella.cabriolu@ntnu.no)

## Main research interests:

- Molecular simulation techniques for physical-chemistry applied problems.
- Rare events and Nucleation processes.
- Colloidal and Glassy systems.
- Nano-porus materials.
- Scientific software development.

## Project offered fall 2022:

- Understanding non-newtonian fluids.
- Mixing-Demixing and Phase transitions in colloidal systems.
- Dimensionality effect on thermal conductivity.



# Prof. Ton van Helvoort

[a.helvoort@ntnu.no](mailto:a.helvoort@ntnu.no),

<https://www.ntnu.edu/employees/a.helvoort>

TEM  
Gemini Centre

## Main research interests:

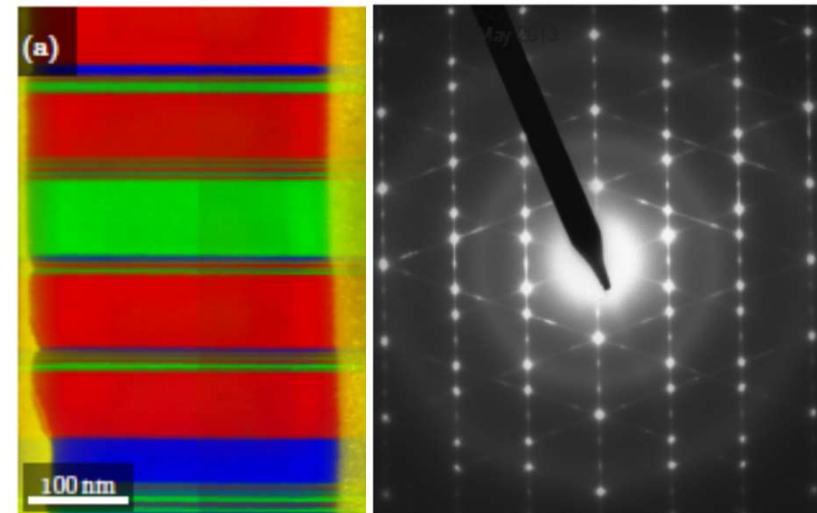
Application and development TEM, STEM, and SEM.

Electron microscopy novel data analysis  
(incl. machine learning) in open-source.

Electron crystallography: structure-property relations.

## Project offered H2022:

- Data mining electron diffraction data stacks
- Improving the accuracy electron spectroscopy
- TEM study of functional oxides and minerals



# Prof. Randi Holmestad

[randi.holmestad@ntnu.no](mailto:randi.holmestad@ntnu.no)

<https://www.ntnu.edu/employees/randi.holmestad>

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## Main research interests;

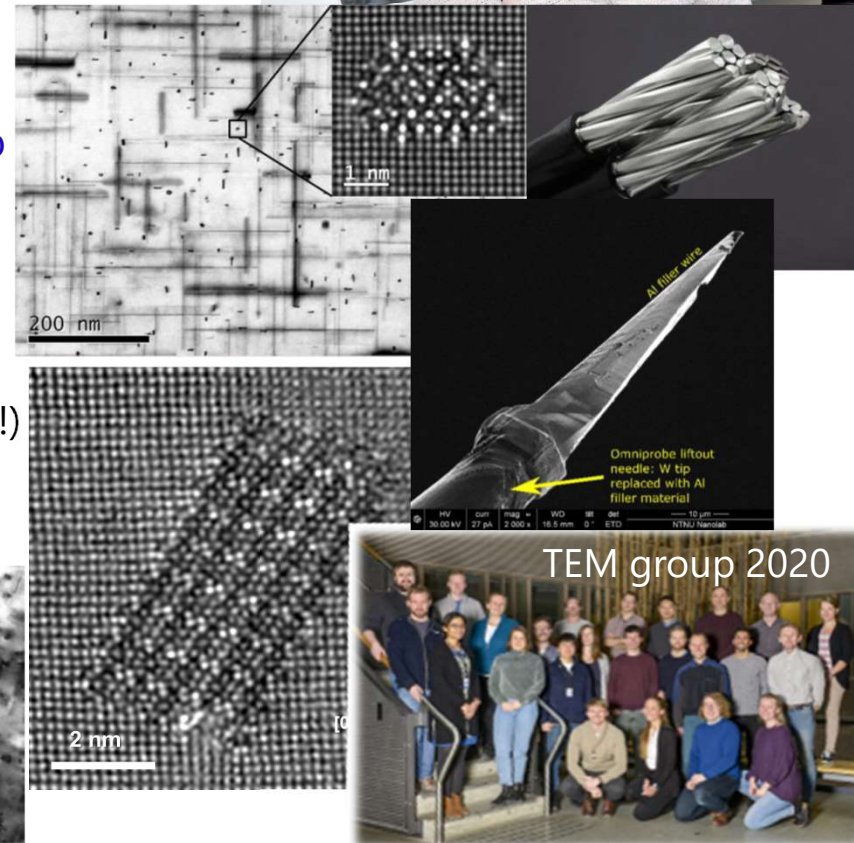
Materials physics and transmission **electron diffraction and microscopy** (TEM), materials microstructure and the **relation to macroscopic properties**.

## Projects offered 2022;

- **Aluminium alloys** (summer job or internship to Japan)
- **Multi-material joining** (summer job + if you want to work with FIB!)
- **Conductivity at the nanoscale** (with Ragnvald Mathiesen)
- **Catalysis/membranes** (with Tina Bergh/ Per Erik Vullum)
- **Strain measurements** (with SINTEF)

See all projects from the TEM group [here!](#)

<https://www.ntnu.edu/physics/temgemini>



# Assoc. prof. Magnus Nord

[magnus.nord@ntnu.no](mailto:magnus.nord@ntnu.no)

<https://www.ntnu.edu/employees/magnus.nord>

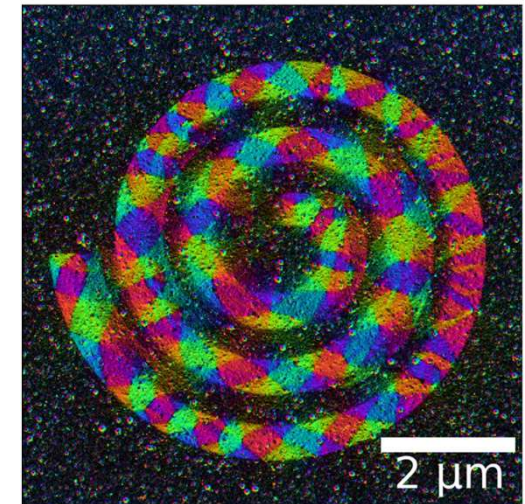
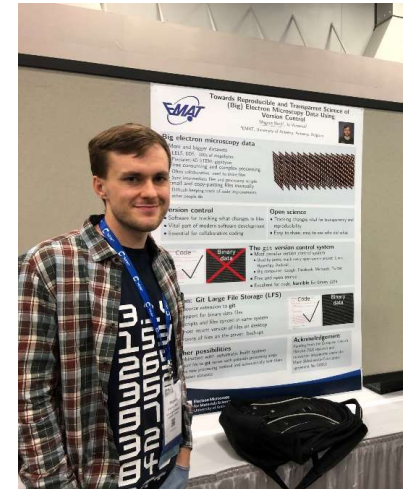
**TEM**  
Gemini Centre

## Main research interests:

- Development of TEM techniques using **new high speed cameras**
- **Image magnetic fields** in materials at nanometer length scales
- Developing "**Big data**" **processing software** using scientific Python
- **Open source** scientific software development

## Project offered 2022:

- ~~Nanoscale structural and magnetic studies of perovskite oxide thin films using TEM~~
- ~~Nanoscale imaging of ferromagnetic artificial spin ice structures using Transmission Electron Microscopy~~
- Electron microscopy of thin films for spintronics applications



TEM image of ferromagnetic domains in a spiral shaped nanostructured thin film. The colours showing the magnitude and direction of the magnetic domains.

# Prof. Morten Kildemo

[morten.kildemo@ntnu.no](mailto:morten.kildemo@ntnu.no)

**web Page for activity:** <https://www.ntnu.edu/physics/nanophotonics-and-polarimetry>

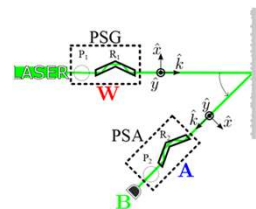
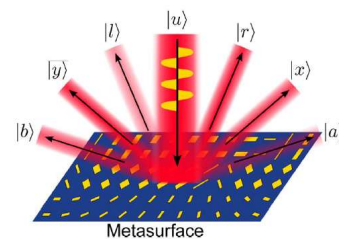
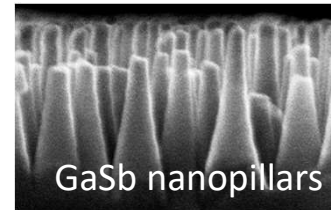
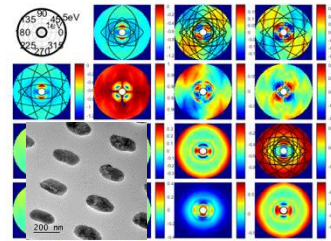
<https://www.ntnu.edu/employees/morten.kildemo>

## Main research interest:

**Design, nanomanufacture and metrology** (instrumentation) of novel optical functional materials ranging from nanostructures applied to Photovoltaic absorbers/ AR coatings and nanoplasmonic devices. Recently focused on so-called **metasurface**-based light-weight lenses, polarimetric components, holographic elements, vector beams etc., based on surfaces with **well- designed dielectric and/or plasmonic nano-resonators**. A new collaborative project in the group is to develop the field of **coupling of photons to magnons**, and another new collaborative project with CERN within **plasmonics** in high gradient accelerators.

## Projects 2022:

- **Manufacturing (and characterization)** of metasurface designs based on well-designed nanoresonators through structuring of a-Si and/or  $\text{TiO}_2$  thin films/layers (Nanolab).
- **Computational Modelling and design** of nano-optics structures through FDTD, FEM, RCWA for design of optical functions using metasurfaces.
- **Instrumentational projects in optics** : Characterization and modelling of metasurfaces and nano-optics on optical bench





# Prof. Turid Reenaas

[turid.reenaas@ntnu.no](mailto:turid.reenaas@ntnu.no)

<https://www.ntnu.edu/employees/turid.reenaas>

## Main research interest

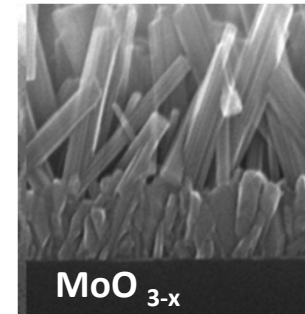
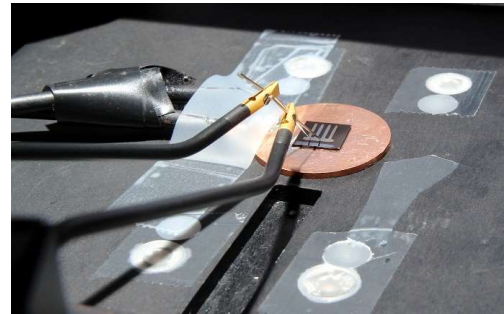
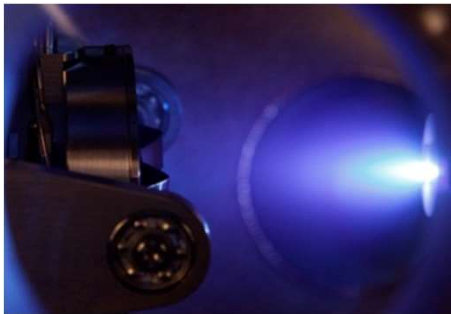
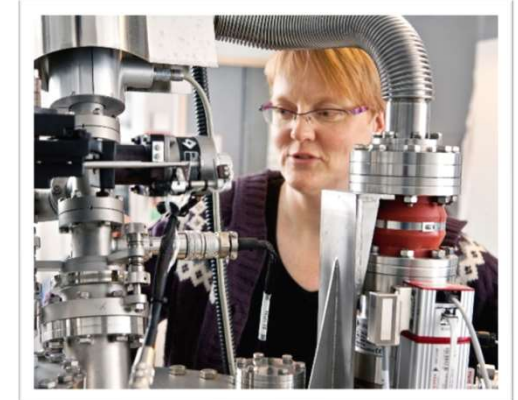
Intermediate band solar cells; theoretical efficiency approx. 49% compared to 33% for conventional solar cells

## Project offered 2022

- Intermediate band solar cell [simulations](#)
- Pulsed laser [deposition and characterization](#) of doped  $\text{TiO}_2$  and non-stoichiometric  $\text{TiO}_{2-x}$
- [Processing/recrystallization](#) of implanted ( $\text{TiO}_2$  and Si) films and single crystals
- [Device fabrication and testing](#)

## Relevant characterization techniques

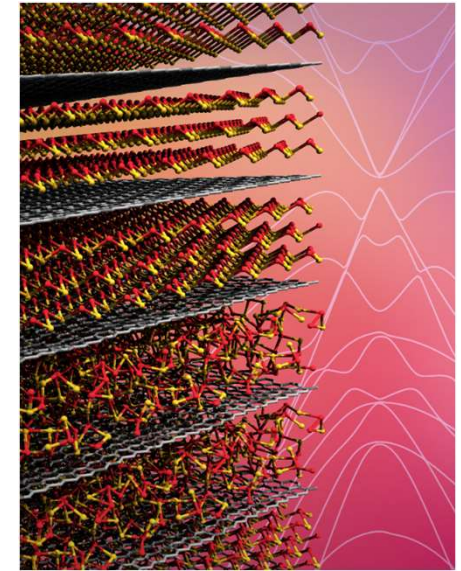
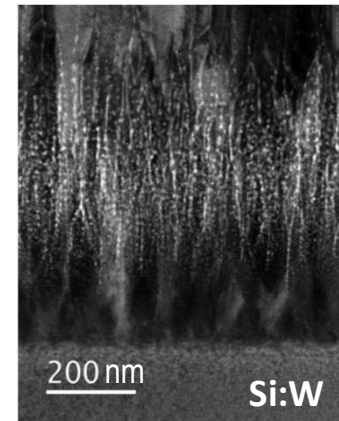
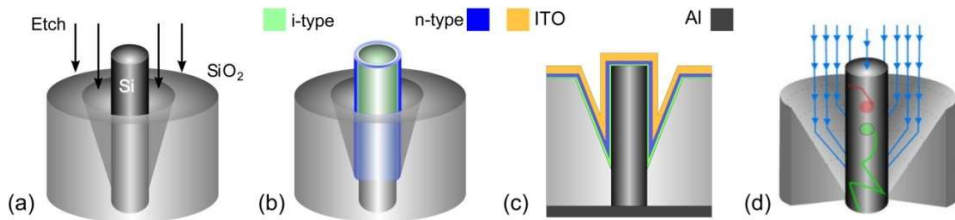
- electron microscopy (SEM, TEM),
- X-ray diffraction (HR-XRD),
- optical spectroscopy,
- photoelectron spectroscopy (XPS),
- surface topography (AFM, optical profilometer)



# Interested in learning more?

We invite you to meet us for coffee and waffles on Tuesday 5<sup>th</sup> April at 12.00 in R60 (E3-103) to get more detailed information about the projects.

..or contact us by email or phone!



$$E = E_0 + V_0 \sum_i \sigma_i + V_1 \sum_{\langle ij \rangle} \sigma_i \sigma_j + \dots$$

