NANOcenter consortium

Electron Microscopy for Materials Science

CMT Condensed Matter Theory

PLASMANT Plasma, Laser Ablation and Surface Modelling Antwerp

Quick rundown:

- Represents the internationally renowned expertise in nanoscience at the University of Antwerp.

- It consists of three participating groups that are international leaders in their subfield:
  - ⇨ EMAT: electron microscopy center for materials research
  - ⇨ CMT: meso- and nano-scale materials modelling
  - ⇨ PLASMANT: Atomic scale surface simulations as well as macroscale plasma simulations.

- 11 Professors, ~100 researchers at PhD/Post-doc level
  Since 2012: 1500 publications with 150 in high impact journals (impact factor >10)
  4 ERC's hosted
  4 EU infrastructure projects + 1 Marie curie ITN

- Goal: better understanding of materials through advanced characterization supported by computer simulation of (nano)structures and their properties

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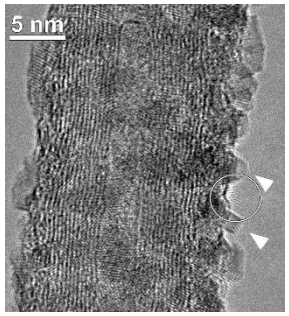
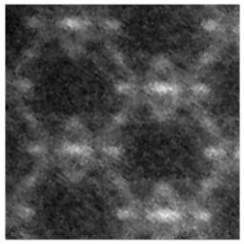
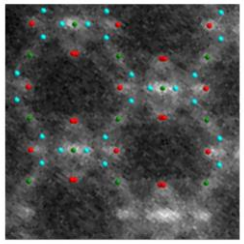
- Observation of microstructure, size and shape of particles, detecting coating layers, crystallinity, soft material imaging (HAADF-STEM, HRTEM, Cryo-TEM, electron diffraction)

HR-image of a CNT

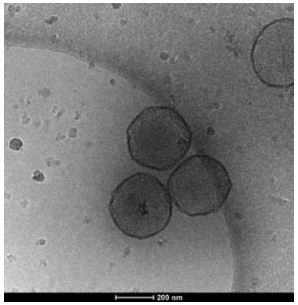


Imaging zeolite pore structure



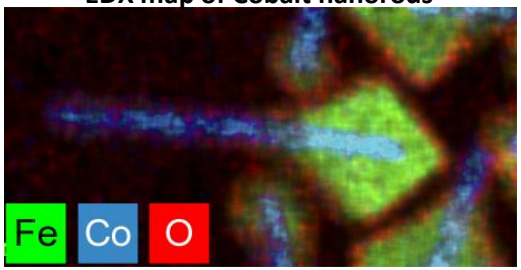


Cryo image of PMA beads

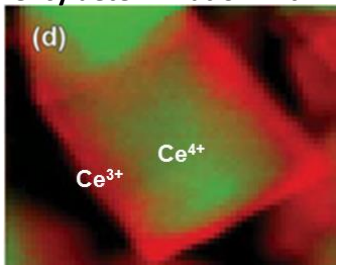


- Combination with analysis of local chemical composition (EDX, EELS)

EDX map of Cobalt nanorods



Valency determination with EELS



⇨ Materials: Nanoparticles, steels and alloys, polymers, battery materials, glass,...

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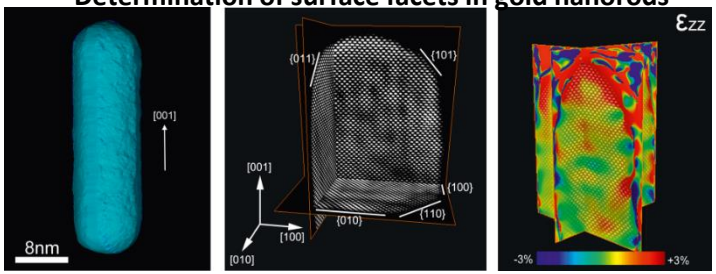
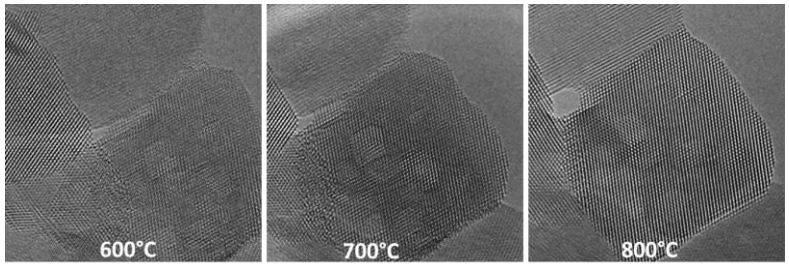
- 3D imaging through tomography

Determination of surface facets in gold nanorods

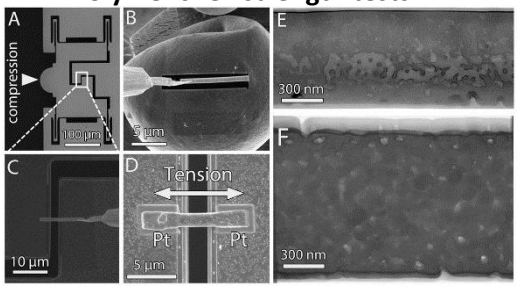


- In situ measurements: heating/cooling, mechanical & electrical

Sintering of Ceria particles

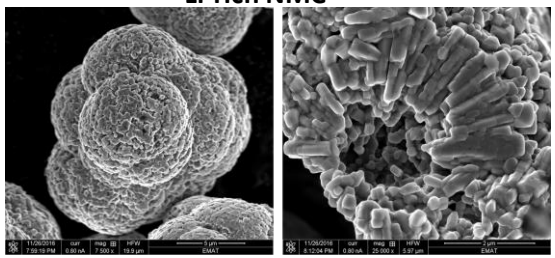


Polymer shell strength tests

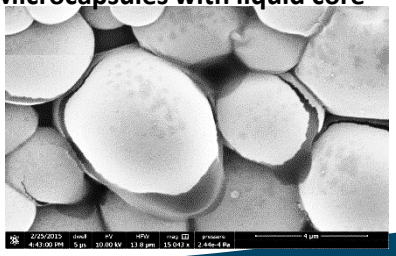


- (FIB-)SEM imaging & slicing of battery materials, polymer capsules, metal alloys,…

Li-rich NMC



Microcapsules with liquid core



Condensed Matter Theory

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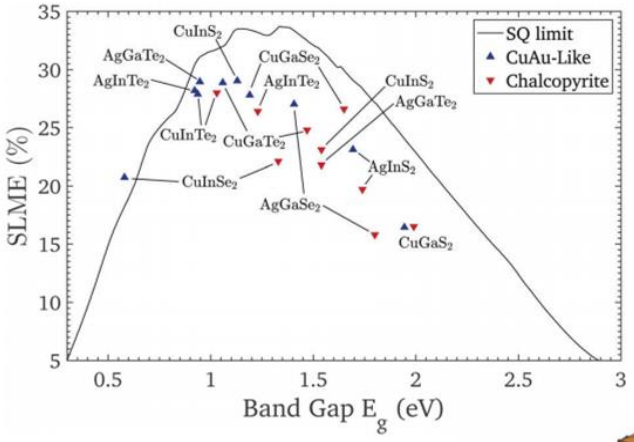
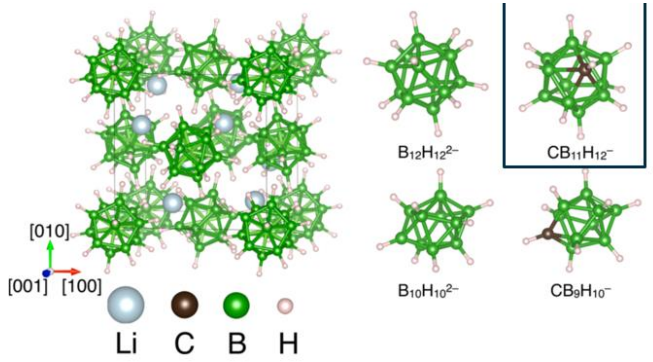
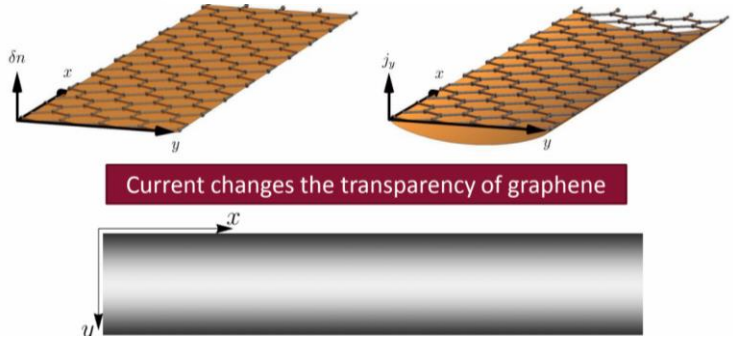
- High-throughput computational screening of materials
- Ab initio modelling of nanostructures and two-dimensional crystals
- Modelling electronic properties of (nano)materials

Spectroscopic efficiency of of different PV material phases



Investigation of ionic conductivity in solid state electrolytes





Condensed Matter Theory & PLASMANT

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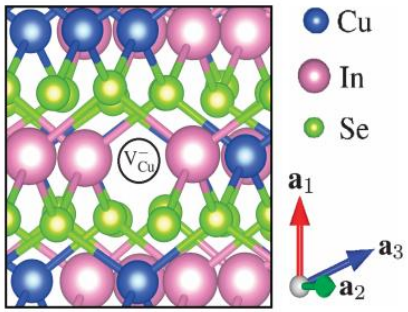
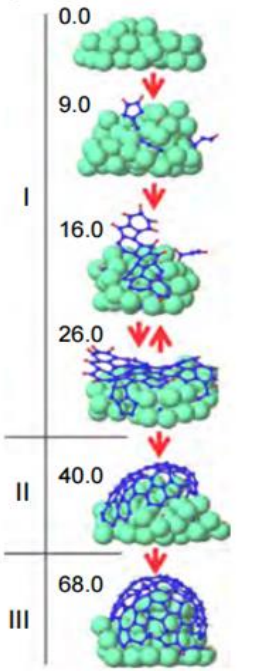
- Modelling of defects & impurities
- Reactive molecular dynamics (with laser and plasma interactions)
- Calculations for reaction barrier

Point defects in semiconductors



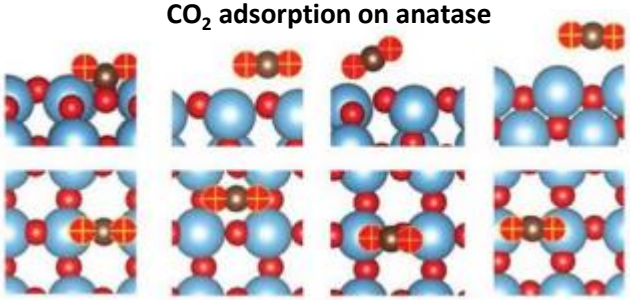
Growth stages of CNT



⇨ Materials: 2D-materials, photovoltaics, nano-catalysts, superconductors, semiconductors, nanoparticles

⇨ Applications: opto-electronics, micro-electronics, energy materials, plasma based technology

CO_2 adsorption on anatase



Summary of interests

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Characterization

- Determining (atomic) structure of nanomaterials using **3D reconstruction techniques**
- Imaging **soft matter** interactions and soft/hard matter interfaces
- Electronic structure mapping and identification of **magnetic materials**
- Transformation, mirostructures and defects for (printed) **metals and alloys**
- **In situ characterization** of advanced energy materials

Modelling

- Simulations of **2D materials** (graphene, etc.) in prototype devices for opto-electronics applications.
- Simulations of thin-film **magnetic materials** for spintronic applications
- Advanced modelling of **single photon emitters** in quantum dots, nanowires, defects in 2D materials.
- Advanced multiscale simulations of superconducting **single-photon detectors**.