Technical University of **Leoben**

Science 4 Technology – Poster Exhibition 2026

Department: Physics, Mechanics and Electrical Engineering

Chair: Physics

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Table of contents

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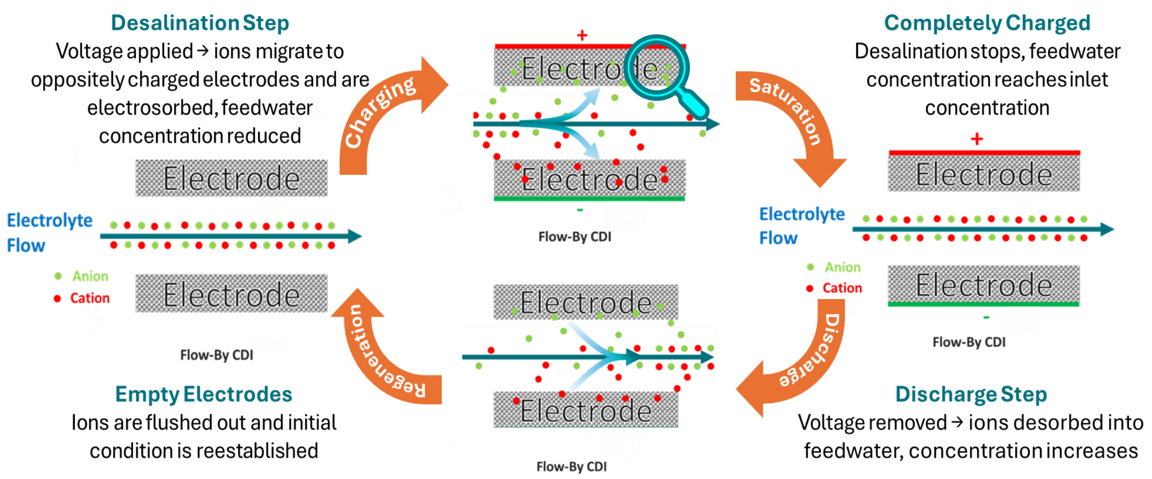
Inside capacitive water deionization

How synchrotron X-ray based techniques help understanding ion diffusion and removal

Fundamental Principle



Desalination Step
Voltage applied → ions migrate to oppositely charged electrodes and are electrosorbed, feedwater concentration reduced

Completely Charged
Desalination stops, feedwater concentration reaches inlet concentration

Empty Electrodes
Ions are flushed out and initial condition is reestablished

Discharge Step
Voltage removed → ions desorbed into feedwater, concentration increases

Key Points:

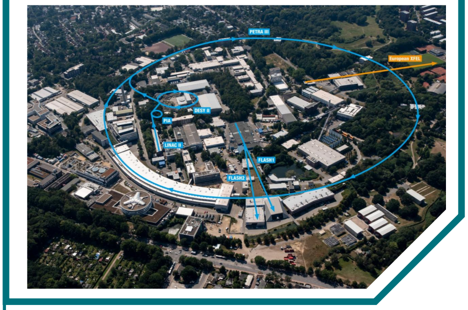
- Discontinuous desalination
- Ions are temporarily adsorbed on the nanoporous carbon surface
- During discharge ions are released back into the electrolyte

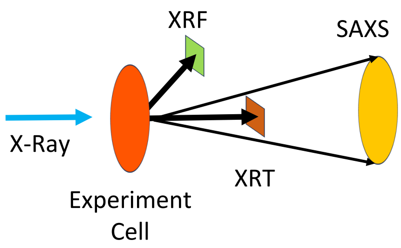
Research Interest:

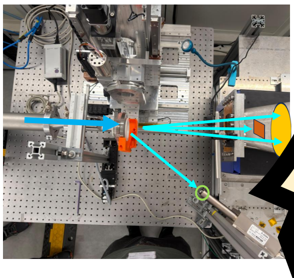
- How does nanopore structure influence adsorption
- How do the ions diffuse and rearrange in the electrode

How to look inside the electrode?

With X-ray imaging it is possible to get information about the ion distribution during charging and discharging! In order to get a high time resolution, we use synchrotron radiation produced by electron accellerators in Hamburg, (DESY) and Trieste (ELETTRA).



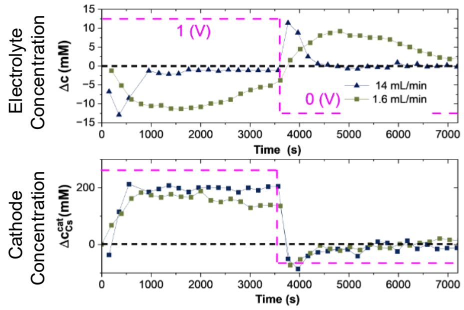




Combination of X-ray techniques, allows separation of pore size-, ion species- and position effects on the electrode.

X-ray Transmission (XRT)

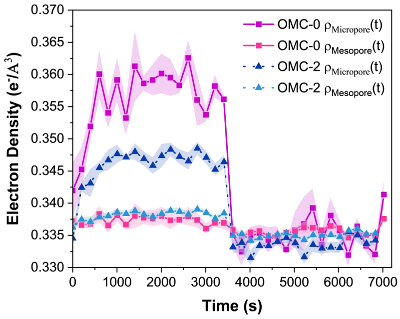
X-ray absorption contrast depends on average ion concentration. Study global concentration changes in feedwater and electrode.



Higher flow, rate improves adsorption but only small concentration gradients in the electrolyte, due to high replenishment [1]

Small angle X-ray Scattering (SAXS)

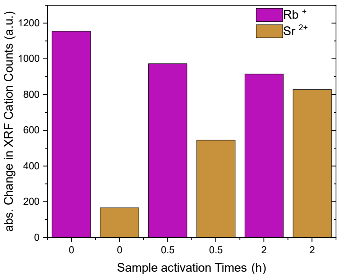
allows to evaluate pore size depended electron density changes over time.



Comparison of similar materials with different micropore size distribution. OMC-0 has smaller pores → higher confinement, higher adsorption

X-ray Fluorescence (XRF)

Ion specific concentration changes



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DESY.
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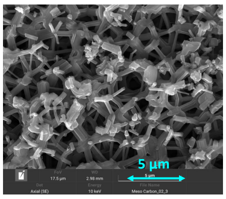
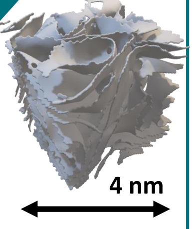
[1] S. Stock et al. Hydrogen densification in carbon nanopore confinement: Insights from small-angle neutron scattering using a hierarchical contrast model, Carbon 221 (2024) 118911. https://doi.org/10.1016/j.carbon.2024.118911.
[2] M.V. Rauscher et al. Beyond global metrics in capacitive water deionization: Position-resolved ion concentration from operando X-ray transmission,. Desalination 623 (2026) 119849. https://doi.org/10.1016/j.desal.2026.119849

Nanopores?



SEM-Image [1]



Atomistic Model [2]

Move mountains

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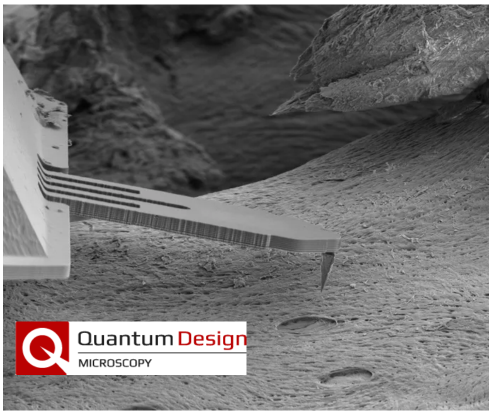
Nanoscale characterization and manipulation

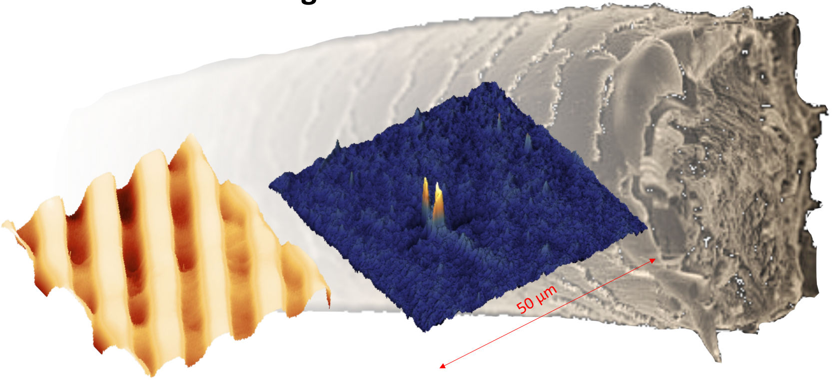
The atomic force microscope as a tool for materials characterization and manipulation

Material and device optimization needs characterization of various parameters on the micrometer and nanometer scale. A universal tool to accomplish this task is atomic force microscopy (AFM), which provides high resolution topography images, but can also track piezoelectric reponse, electric fields, conductivity, friction, adhesion, chemical information, etc. with extremely high resolution.

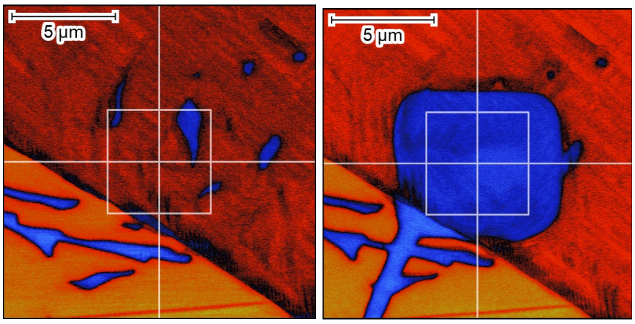


In AFM a fine needle, attached to a silicon cantilever is scanned accross the surface. The forces acting on the tiny tip cause the cantilever to deflect. This deflection is used to evaluate the interaction and to extract properties. (Scanning electron microscopy (SEM) image of an AFM probe scanning a surface (Taken from Quantum Design Microscopy https://www.qd-microscopy.com/afsem/)).

Measuring Electric Fields

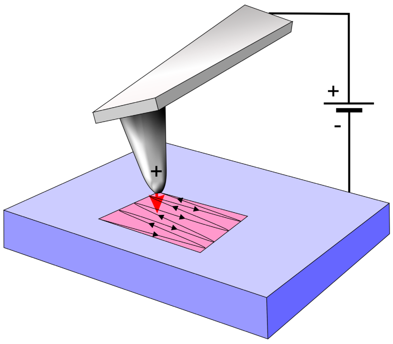


Images of a periodically poled $LiNbO_3$ ferroelectric sample. While in the topography (right) the poled regions are invisible, the electric field can be visualized using the AFM in electrostatic force microscopy mode (left). In the background a human hair is shown for comparison to illustrate the small size of those features.

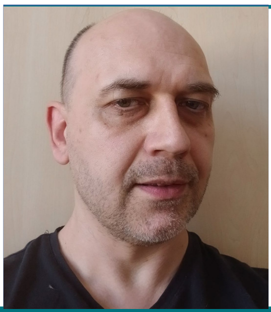


A ferroelectric $BaTiO_3$ surface before (left) and after (right) local polarization with an AFM tip. The newly formed domain is clearly visible in the image obtained in the piezo-reponse force microscopy mode of the AFM. (Taken from P. Münzer‘s Master‘s Thesis, MUL 2023).

Manipulation with a tip



The AFM can be used to modify surfaces either mechanically or electrically. Here, an AFM tip with an applied voltage is moved across the surface. The high field under the tip can locally deposit charge or polarize ferroelectric material.



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Reserach Focus/Collaborations

Electrical, mechanical and chemical nanochracterization and manipulation.

Ferroelectrics, 2D materials, SiC, hBN

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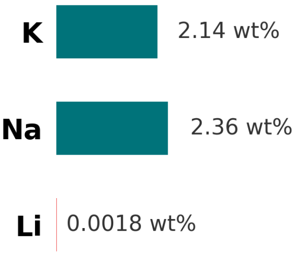
PARIS LODRON UNIVERSITÄT SALZBURG
JAGIELLONIAN UNIVERSITY IN KRAKÓW

Move mountains

From Forest to Battery

Utilizing hard carbons from wood as anodes in batteries and investigating storage processes



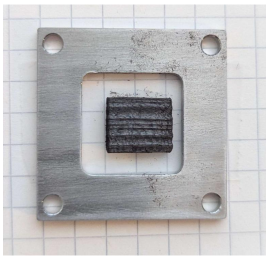
Elemental abundances of Na, K, and Li in the Earth's crust. Na and K are given in wt%, while Li is shown in ppm. Na and K are approximately 1000 times more abundant than Li. Data adapted from Wedepohl (1995).

As the global need for batteries increases, the interest in alternatives to Li-ion batteries (LIBs) grows. Na and K are more abundant and cheaper and Na-Ion/K-Ion battery systems (SIBs and PIBs) are of particular interest. With wood as a precursor for anodes, a regional and green material is under investigation.

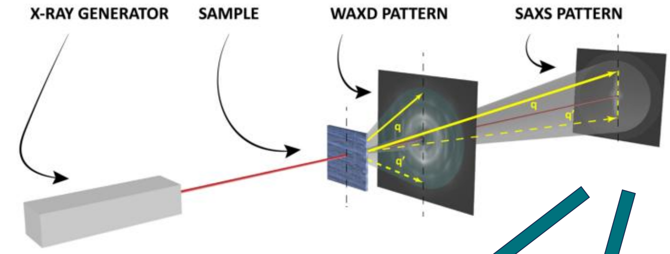
While LIBs require graphite as anode material, SIBs and PIBs need the more open structure of hard carbons. Pyrolysing wood samples in two steps under N_2 atmosphere to temperatures between 280-500°C and afterwards to 1100-1500°C reveals hard carbon structures with different nanopore architecture. Tuning nanostructure determines how well Na or K ions will be stored.

Small- and Wide-Angle X-ray Scattering (SAXS/WAXS) are used to characterize the carbon material. Electrochemical tests in battery SIB and PIB half cells will show the performance of the wood derived electrodes. Future operando SAXS/WAXS at synchrotron facilities will reveal ion movement in real time during charge/discharge

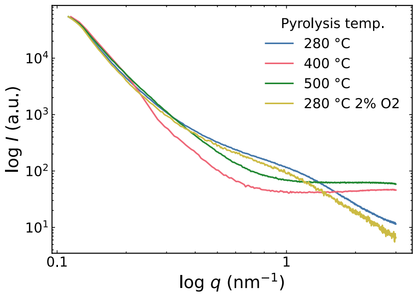
Image generated with AI assistance (Nano Banana 2).

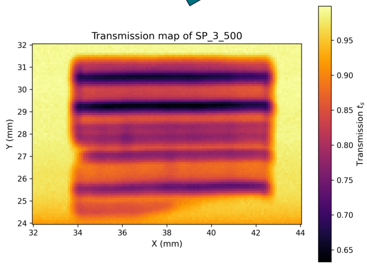


Pre-pyrolyzed wood sample at 500°C.

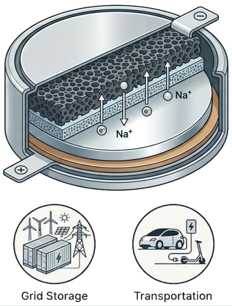


Sketch of the SAXS/WAXS setup, reproduced from [2].





1D SAXS profiles show the structural change at higher temperatures. The right figure shows an X-ray transmission image of the sample, highlighting the annual rings. The battery illustration shows a later application of these samples.



References:
[1] Wedepohl, K. H. (1995). *The composition of the continental crust*. **Geochimica et Cosmochimica Acta, 59**(7), 1217–1232. https://doi.org/10.1016/0016-7037(95)00038-2
[2] Herreria Gil, H. (2025). *Effects of partial oxidation on the microstructure of wood derived carbons* (Master's thesis). Technical University of Leoben, Chair of Physics.

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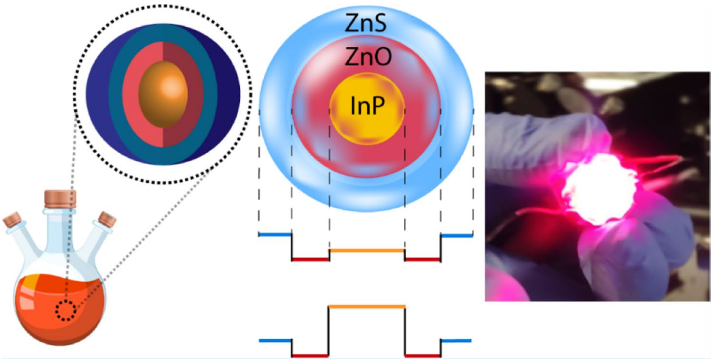
Research Focus:

- Na- and K-ion battery anode materials
- Biobased hard carbon from wood precursors
- Nanostructure characterization via SAXS/WAXS
- Ion storage mechanism during charge/discharge
- Operando synchrotron experiments

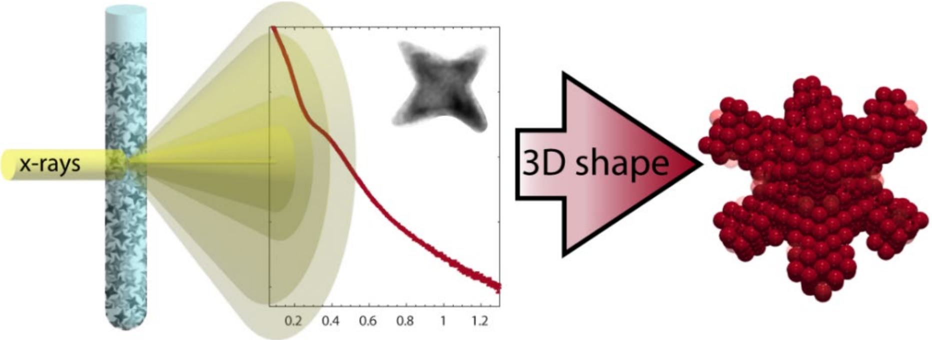
X-ray Investigations of Nanocrystals & Supercrystals

Revealing the relation between structure and functionality of colloidal nanoparticles using x-ray techniques at laboratory- and synchrotron-sources.

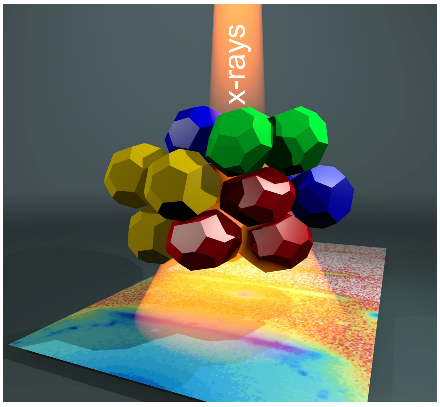


Nowadays nanometer (= one-billionth of a meter) sized crystalline particles can be fabricated by wet chemical synthesis methods. These ***nanocrystals*** (NCs) consists of metallic or semiconducting compounds that can form so called quantum dots (QDs). These dots are used as brilliant colourful light emitters, e.g. in todays TV screens (QD-LEDs). The significance of colloidal QDs is underlined by the awarding of the 2023 Nobel Prize for Chemistry for this research topic.

We investigate the NCs' internal crystal structure, as well as their size and shape in atomic resolution to understand and thus to tune their optical, electronic or magnetic properties. The such gained knowledge allows, e.g., to replace toxic materials like CdSe with the more environmentally friendly InP, but keeping the optical performance the same.



Furthermore, we can use these NCs as building blocks for assembling ***supercrystals*** that are artificial solids with novel functionalities. During these self-assembly their structure is probed in real-time by x-ray scattering techniques:



Many x-ray experiments have to be performed at ***synchrotron*** sources, which are large scale research facilities. There, electrons are accelerated close to the speed of light emitting very brilliant ***x-ray beams***. From the synchrotron facilities in Europe, we use mainly three: The synchrotrons **ELETTRA** in Trieste (Italy), **ESRF** in Grenoble (France) and **DESY** in Hamburg (Germany) allows to probe changes in structure & shape with sub-second time resolution.

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Research Focus:

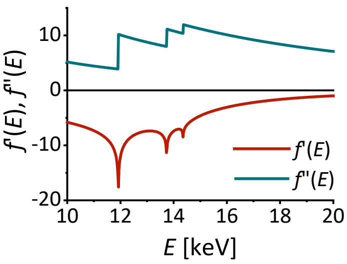
in-situ **&** ***ex-situ*** studies at synchrotrons: (A)SAXS/WAXS & XAS
SAXS & XRD in the lab combined with TEM

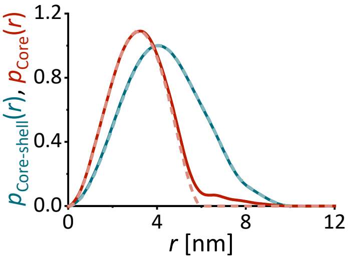
ASAXS Evaluation of Crystalline Nanoparticles

Separation of Anomalous Scattering Data based on Crystal Lattice

The Technique

Scattering power of atoms energy dependent close to absorption edge. These resonance effects are described by the factors f' and f''. Measuring at several energies allows to separate contribution of resonant atom from overall particle [1].

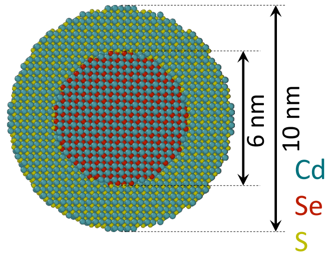


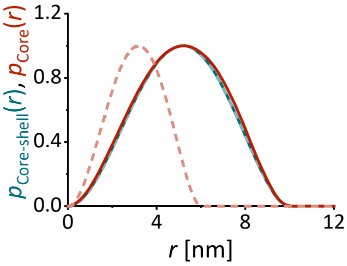


Example: Nanodiamond (radius 5 nm) with gold core (resonant - radius 3 nm). Scattering data transformd into real space. Dashed: Theoretical

The Problem

If several heavier elements are present, their f' and f'' change slightly also far from absorption edges. This can cover up effects of the resonant elements and prevent separation.

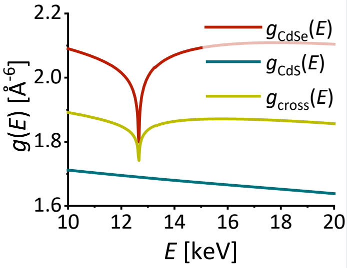




Example: CdSe core (radius 3 nm) with CdS shell (radius 5 nm). Measurements close to Se-edge. Slight changes of f' and f'' of Cd 'drown' effects by Se. Dashed: Theoretical. Real space analogues shown.

The Solution

Known unit cells allow to compute energy dependent scattering power of a material. If two materials A and B form a particle, this leads to scattering factors $g_A(E)$, $g_B(E)$, and a cross term $g_{AB}(E)$. The energy dependent scattering curves $I(q,E)$ can then be linked by equation

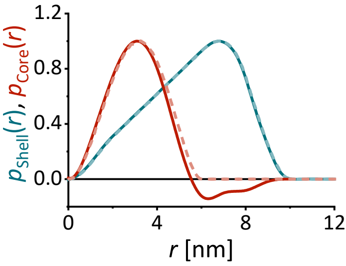


$$\begin{pmatrix} I(q,E_1) \\ \vdots \\ I(q,E_n) \end{pmatrix} = \begin{pmatrix} g_A(E_1) & g_B(E_1) & g_{AB}(E_1) \\ \vdots & \vdots & \vdots \\ g_A(E_n) & g_B(E_n) & g_{AB}(E_n) \end{pmatrix} \begin{pmatrix} P_A(q) \\ P_B(q) \\ F_A(q)F_B(q) \end{pmatrix}$$

to the scattering curves $P_A(q)$ and $P_B(q)$ of material A and B only and a cross term $F_A(q)F_B(q)$, describing the relative positions of the materials. Solving this equation gives $P_A(q)$, $P_B(q)$, and $F_A(q)F_B(q)$.

Example

The system shown in "The Problem" was evaluated again. The information on the core (red curve) is obtained much better. Note: The bluish curve now corresponds to the shell only, not the overall structure like previously.



References

[1] Sztucki, M.; Di Cola, E. & Narayanan, T. *The European Physical Journal Special Topics*, **208**, 2012, 319-331

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Research foci:

Nanostructured materials
Therory of small angle scattering (SAS)
Evaluation techniques for SAS
Physics in Antiquity

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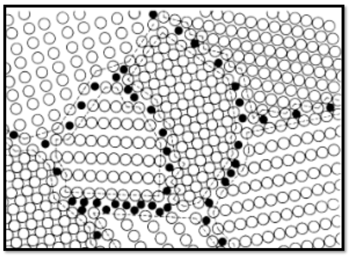
Nanostructured Titanium Alloys

Processing and Properties

Introduction and Motivation

Nanocrystalline materials, defined by grain sizes below 100 nm, exhibit promising mechanical properties, including significantly enhanced hardness and strength compared to conventional alloys at similar weight. However, these materials suffer from limited thermal stability, with grain growth initiating at relatively low temperatures. Therefore, improving thermal stability is essential to extend their usability to higher temperatures.

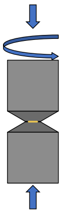


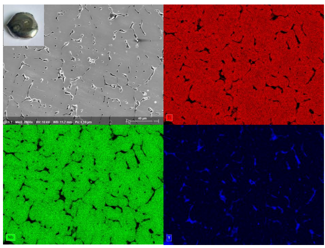
Schematic structure of a nanocrystalline alloy with segregation at the grain boundary (black atoms).

The presence of an additional species at the grain boundary can stabilize the structure by either slowing (kinetically) or completely inhibiting (thermodynamically) grain growth.

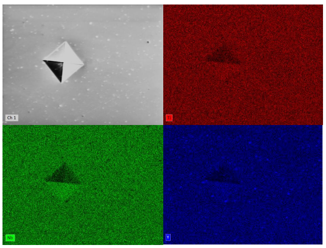
Experimental Methods

Samples are prepared by arc melting, followed by severe plastic deformation using a high-pressure torsion (HPT) machine. This deformation enables the dissolution of elements with otherwise immiscible compositions through mechanical alloying, resulting in a homogeneous nanocrystalline structure.





Microstructure and elemental mapping of TiNbY alloy after casting.

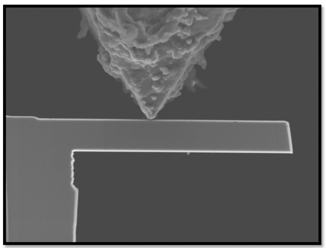


Microstructure and elemental mapping of TiNbY alloy after severe plastic deformation.

Micromechanical Testing

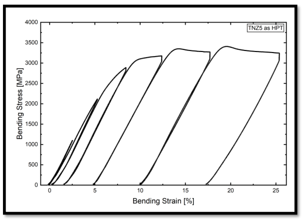
Focused ion beam (FIB) techniques are employed to fabricate and shape microcantilevers for mechanical testing at the microscale. This approach enables precise site-specific preparation of samples with well-defined geometries, allowing the investigation of various mechanical properties, such as strength, Young's modulus and internal friction.

Overview over microcantilevers on a sample of nanocrystalline Ti-Nb-Zr alloy.

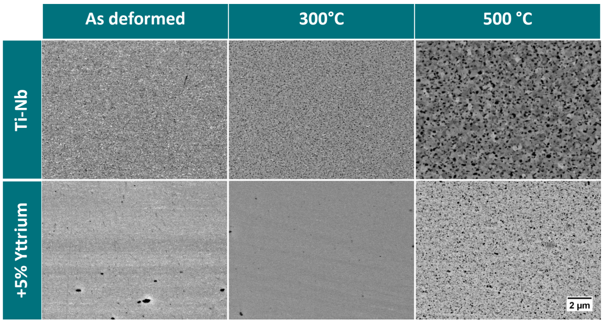


Detail of a microcantilever with the tip of the nanoindenter during testing.

The nanocrystalline Ti-Nb-Zr alloy shows a high yield strength along with strain hardening to a strength of approximately 3000 MPa. The combination of high yield strength with low Young's modulus is desirable for orthopedic implants.



Thermal Stability



The deformed samples are annealed at different temperatures to evaluate their resistance to grain growth. To correlate microstructure, electrical resistivity, and hardness, all measurements are performed on the same sample. For resistivity measurements, a miniaturized four-point probe was developed using 3D-printed components and tungsten wire.

Summary

Combining arc melting with severe plastic deformation enables the production of a homogeneous nanocrystalline structure with tunable nanoscale properties. Micromechanical testing is used to assess strength, elastic properties, and internal friction, revealing the microstructural evolution of a low-modulus titanium alloy after various treatments.

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Project leader: Dr Markus Alfreider

FWF Österreichischer Wissenschaftsfonds

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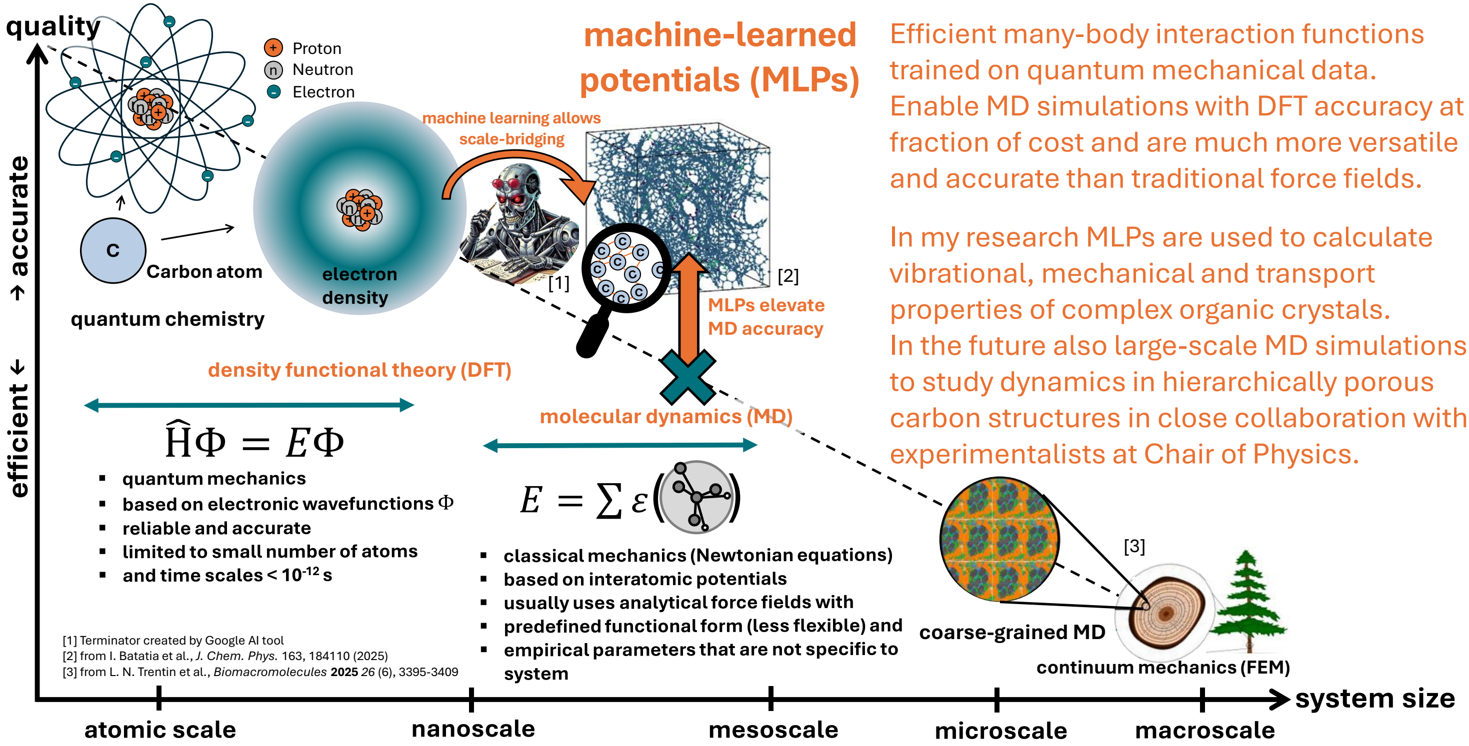
Move mountains

Atomistic Modeling of Carbon-Based Materials:

Machine-Learned Potentials are revolutionizing computational material science with quantum mechanical accuracy for large and complex structures.



machine-learned potentials (MLPs)

Efficient many-body interaction functions trained on quantum mechanical data. Enable MD simulations with DFT accuracy at fraction of cost and are much more versatile and accurate than traditional force fields.

In my research MLPs are used to calculate vibrational, mechanical and transport properties of complex organic crystals. In the future also large-scale MD simulations to study dynamics in hierarchically porous carbon structures in close collaboration with experimentalists at Chair of Physics.

density functional theory (DFT)

$$\hat{H}\Phi = E\Phi$$

- **quantum mechanics**
- **based on electronic wavefunctions Φ**
- **reliable and accurate**
- **limited to small number of atoms**
- **and time scales < 10^{-12} s**

molecular dynamics (MD)

$$E = \sum \varepsilon(\quad)$$

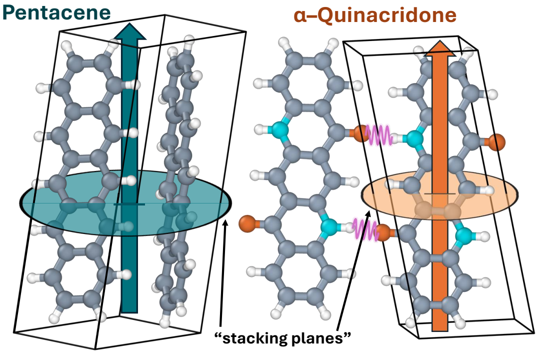
- **classical mechanics (Newtonian equations)**
- **based on interatomic potentials**
- **usually uses analytical force fields with**
- **predefined functional form (less flexible) and**
- **empirical parameters that are not specific to system**

[1] Terminator created by Google AI tool
[2] from I. Batatia et al., *J. Chem. Phys.* 163, 184110 (2025)
[3] from L. N. Trentin et al., *Biomacromolecules* **2025** *26* (6), 3395-3409

In materials science, modeling approaches differ in accuracy and efficiency, covering system sizes from the atomic scale to macroscopic structures. Machine learning brings quantum-mechanical insight to atomistic simulations at near-mesoscale sizes.

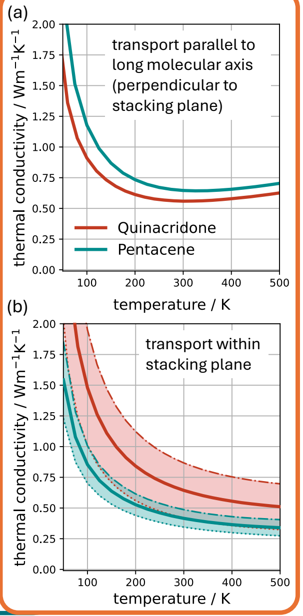
Structure modification of pentacene

Pentacene is the most studied crystalline organic semiconductor. A common strategy to tune its properties is heteroatom substitution. Introducing **nitrogen** and **oxygen** yields **Quinacridone**, which forms directed **hydrogen bonds** and promotes favorable self-assembly, enhancing stability and crystallinity. However, this substitution also affects electronic transport [1]. Here, we investigate its impact on heat transport by comparing the thermal conductivity [2] parallel and perpendicular to the stacking planes.
While the out-of-plane conductivity remains unchanged (a), hydrogen bonding significantly increases the conductivity within the planes (b).

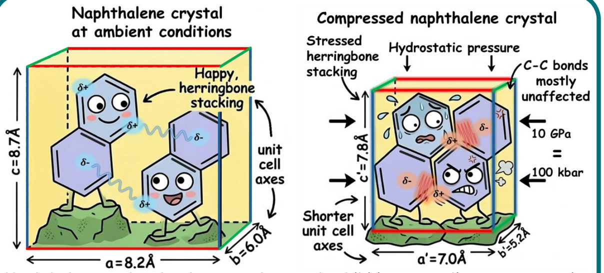


[1] C. Winkler et al., *Chemistry of Materials* **2019** *31* (17), 7054-7069
[2] Lukas Legenstein et al., *npj Comput Mater* **11**, 29 (2025)

Thermal transport

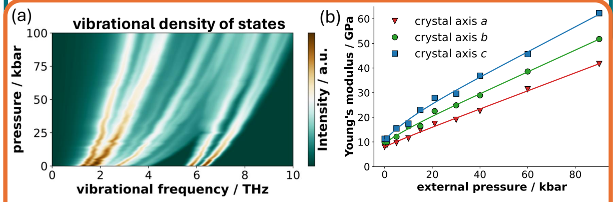


Crystal structure changes under pressure



Naphthalene molecules form a soft crystal exhibiting a non-linear compression under hydrostatic pressure. Drastic changes to the crystals properties follow.

Vibrational and mechanical properties



Simulations of soft molecular crystals under pressure using MLPs: Compression strengthens intermolecular bonds, raising frequency of associated vibrations. (a) This mechanism makes the crystals stiffer, i.e. more resistive to deformation. (b)

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Research focus:

- Heat transport in crystalline organic semiconductors
- Thermo-mechanical properties of molecular crystals
- Reactive MD simulations for "realistic" carbon structures

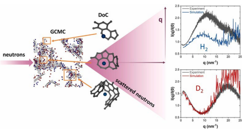
FWF Project No. P 33903
TU Graz
Vienna Scientific Cluster
TU Wien
Columbia Engineering

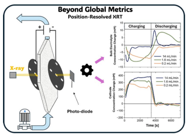
Physics, Nanoelectronics, Energy and more

Science at the Chair of Physics

Research at the **Chair of Physics** focusses on the physics of **functional nanomaterials** for applications in **micro- and nanoelectronics** and **energy storage**. Examples of actual core research topics include nanoporous materials, nanoparticles, surface nanostructures, and two-dimensional (2D) materials. Key competences are the **fabrication** (nanoporous carbons, 2D heterostacks, organic nanocrystals) and **advanced experimental characterization** (small-angle scattering, scanning probe microscopy, gas sorption, electrical) of **nanostructured materials.** Members of the Chair regularly conduct in-situ and operando experiments at international **large-scale research facilities** for **synchrotron radiation** and **neutrons**.

Synchrotron & Neutrons for Energy Materials (SyNergy_Mat) Paris Lab





- Colloidal Nanoparticles
- Nanoporous Carbon
- Supercapacitors
- Water Desalination
- Hydrogen Storage

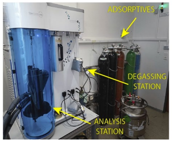
SAXS Lab

X-ray & neutron scattering

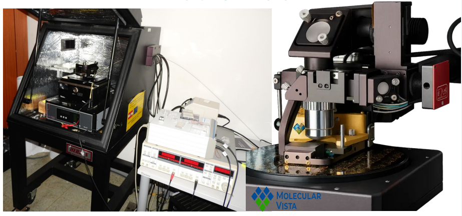

P62 Beamline @ DESY Hamburg


D16 instrument @ ILL Grenoble

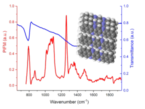
Gas Sorption Lab

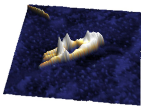


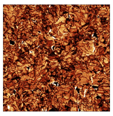
Scanning Probe Microscopy (SPM) Kratzer Lab

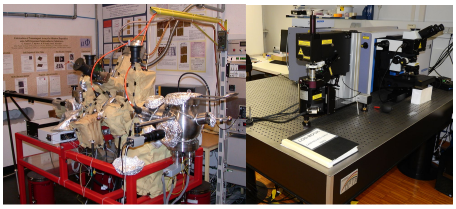


6 SPMs for characterization and manipulation on the nanometer scale

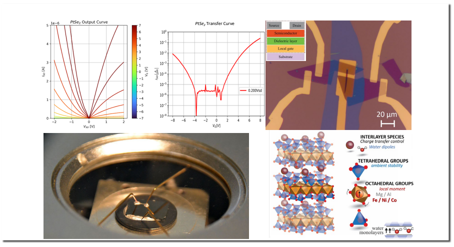




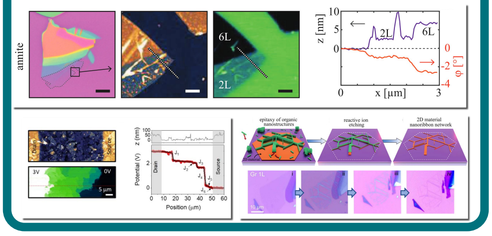




2D Materials (2D_Mat) Matkovic Lab



- 2D materials-based electronics
- Interfacial band engineering
- 2D semiconductor growth
- Van der Waals heterostructures



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Senior
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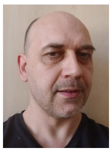
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Johannes
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Heinz
Pirker


Bernhard
Mürzl


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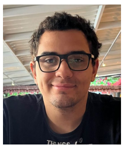
Simon
Leitner


Luis Felipe
Almeida


PhD candidates

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