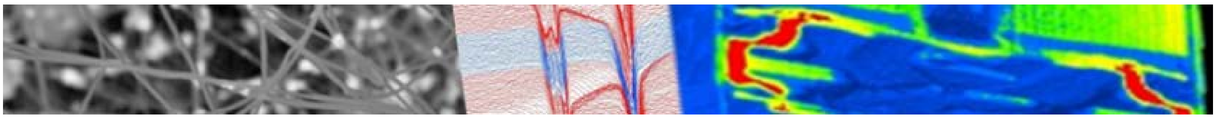
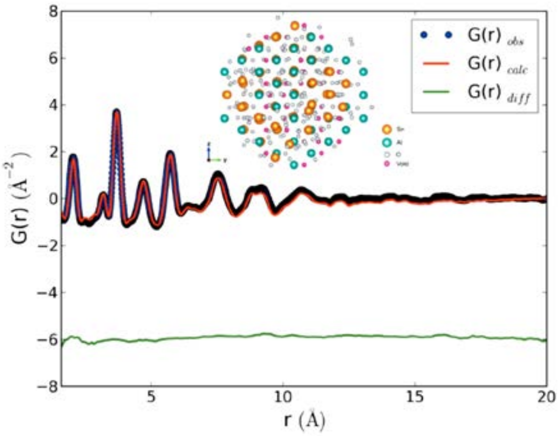


Bachelor or master thesis

Nanocrystalline battery anode materials

Starting date June 2016 and later

$Al_xSn_{1-x}O_{2-x/2}$ and its parent material SnO_2 are interesting compounds which might be used as negative electrode for batteries because of the high Li-capacity compared to conventionally used graphite. It suffers from irreversible Li_2O formation during the first charge cycle and large changes in size during the following cycles, leading to amorphization of the particles, contact loss and low cycling stability.



In this work the influence of the Al content and annealing temperature on the structure and electrochemical behavior during Li and Na intercalation shall be investigated.

- A considerable amount of nanosized material with specific Al content shall be synthesized by a co-precipitation method.
- Phase purity and crystallite size will be determined via temperature dependent X-ray diffraction, XRD. One aspect is the crystallite growth at a given temperature (time dependent kinetic study) and maximum crystallite size in dependence of the annealing temperature. In parallel thermogravimetry TG will indicate oxygen loss or phase transitions.
- For all relevant samples the electrochemical behavior such as initial capacity loss, reversible capacity and reversibility will be determined via galvanostatic cycling.
- For relevant samples the structural behavior during Li (Na) de-/intercalation will be investigated via in-situ XRD at laboratory and synchrotron sources
- MAS NMR and Moessbauer-spectroscopy will be performed on promising candidates to investigate local structure in the as-prepared and lithiated state (Al, Sn, Li NMR, Sn-Moessbauer)
- Pair distribution function, PDF, and total scattering experiments will be performed on promising candidates in different lithiated states to investigate local structure of the nanomaterial and compared to NMR results

In the future, the most promising material could be cycled in full cells versus standard positive electrode materials or prepared by electrospinning to reduce structural degradation and improve conductivity.

The candidate should have a background in one of the fields: inorganic chemistry, materials science or physics with a focus/basic knowledge on one of the following aspects: inorganic preparation methods, solid state physics, crystallography, diffraction and spectroscopy.

The project outlined above covers several master or bachelor theses and the work program will be finally agreed with the candidate.

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References:

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