Linking chemistry and phase evolution in metal-O₂/S batteries via in situ Small Angle X-ray Scattering and X-ray Absorption Spectroscopy

The PhD founded by the CERIC-ERIC is embedded into a collaborative project between Heinz Amenitsch TU-Graz, Stefan Freunberger, Institute of Science and Technology, Austria, and Christian Prehal, ETH Zürich.

We are searching for a PhD student interested in a combination of the theoretical and experimental work aimed towards pushing the frontiers in fundamental understanding of next-generation batteries.

Making electrochemical energy storage economically and ecologically sensible on a very large scale requires eliminating the critical elements in current Li-Ion batteries (Co, Ni, Mn). Oxygen and sulphur electrochemistry is in many respects ideal: highly abundant, cheap, light, minor energy input for production and recycling. All this comes with amongst the highest theoretical energy storage of all known options. They are best used in the cathodes (positive electrodes) of metal-O₂ and metal-S batteries with, e.g., Li, Na, Mg, and Al anodes. The latter are the focus of this study.

Structural evolution and chemistry are intimately interlinked in these systems, but their fundamental understanding is critically missing. To this end, we will combine structurally and chemically sensitive methods: *in situ* small and wide angle X-ray scattering (SAXS/WAXS), *in situ* X-ray absorption spectroscopy (XAS), *in situ* RAMAN and UV Resonance Raman at the Inelastic UV Scattering Beamline (IUVS) at the synchrotron radiation facility at ELETTRA, Trieste, Italy.

The PhD requires secondment periods at the partner institutions ETH Zürich and Institute of Science and Technology (IST) Austria to prepare experiments (cell and precursor preparation, electrochemical characterization, etc.)

Required qualifications: Master- or Diploma degree in Physics, Chemistry, or Material Science

Additional desired criteria:

- background in physical and inorganic chemistry
- experience in X-ray techniques
- experience in scientific computing
- willingness to work in an international environment in Italy and Austria.

The PHD is associated with a temporary position for three years at the Institute of Inorganic Chemistry, Graz University of Technology. The yearly salary is 33.414, 83 € (pre-tax) according to the rules of the FWF (based on an employment of 32 working hours per week working on the project.

Desired starting date: 1. March 2022 (The position is open until a suitable candidate is found). Contact address: amenitsch@tugraz.at