S3: Energy materials

Ananya Renuka Balakrishna (University of Southern California) & Łukasz Figiel (University of Warwick)

Strong demand for developing alternative sources of energy requires novel materials that enable electro-chemical, thermo-electric, photo-electric, or mechano-electrical conversions, and can sustain extreme in-service conditions (e.g. large volumetric changes, temperatures, or fatigue). Ideally, their design and analysis relies on the fundamental understanding of structure-property relations, and frequently requires development of new experimental, theoretical and computational approaches across all the relevant temporal and length scales.

This session aims to bring together scientific efforts related to the development of theoretical, computational and experimental approaches to structure-property predictions for energy materials. Some topics of interest include:

- Theoretical description of different physico-chemical phenomena (e.g. coupling mechanics with electrochemistry)
- Numerical methods enabling simulations of coupled problems in energy materials (e.g. phase-field methods)
- Multiscale approaches linking atomistic and continuum time and length scales (e.g. computational homogenization)
- Combination of theoretical and computational studies with in-operando experimental techniques (e.g. TEM, XRD, computer tomography)
- Optimization approaches for energy materials (e.g. topology optimization)
- Data-driven approaches for energy materials (e.g. Gaussian processes, or neural networks)

Both organic and inorganic materials, amorphous or crystalline materials, and their combinations are of interest in this session. Special focus will be in sustainable energy materials, such as those involving biodegradable and/or recyclable materials, and their composites. Systems of interest can include batteries, photovoltaic devices, fuel cells, or nuclear materials.