Project 3.2 Physical insights into charging mechanisms and performance optimisation of nanoporous supercapacitors

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Background:

The ever-growing global energy demand requires developing novel energy-storage technologies to increase energy production from renewable sources and the transition from hydrocarbon-based fuel to electrical drive. Supercapacitors with nanoporous electrodes have emerged as a critical energy-storage technology, offering high power densities and remarkable cyclability. However, they provide only moderate energy densities compared with conventional batteries. Neat ionic liquids as electrolytes allow high operating voltages (even more than 4 V), boosting energy storage, but the reduced ion mobility lowers the power density. Increasing the energy storage without compromising the power density would make these ecologically friendly energy storage systems more broadly applicable.

Aim:

We will develop a multiscale framework to investigate how energy storage and power density correlate with electrode properties. We will scrutinise the in-pore ion dynamics with molecular simulations and develop continuous models to find an optimal charging protocol, boost power performance, and assess it with electrochemical measurements. The acquired knowledge will translate into a working toolkit for the intelligent design and optimisation of next-generation highperformance supercapacitors.

Requirements:

- MSc in physics or related disciplines,
- experience in simulations and HPC,
- knowledge of python,
- enthusiasm and interest in multidisciplinary research.