Project 3.1 Ionic liquid mixtures for supercapacitor applications: Theory and simulations

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Background:

We are currently witnessing the rapid development of many energy-storage technologies that significantly impact our daily lives. Supercapacitors have emerged as promising electrochemical energy storage devices that provide high power density, excellent cycling stability, and reversibility. However, despite the tremendous research effort, the low energy density and the limited performance at low temperatures remain their main bottlenecks, hindering the widespread application of these ecologically-friendly energy storage systems. So far, the energy storage mechanisms involved at the electrode/electrolyte interface during the charging and discharging processes have not been fully understood. In this international and multidisciplinary project, a selection of different ionic liquid mixtures and nanoporous carbons will be investigated with electrochemical measurements, NMR experiments, and molecular simulations to reach these challenging goals.

Aim:

To scrutinize how the electrochemical performance is correlated with the properties of ionic liquid mixtures and nanoporous carbon electrodes. We will investigate bulk and in-pore ion dynamics with molecular simulations to find an optimal electrolyte/electrode couple boosting power performance that we will assess with electrochemical measurements performed by our partners at Warsaw University and INM (Germany). The overarching goal is to develop useful tools for information-based device design of next-generation high-performance supercapacitors.

Requirements:

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