Multi-scale models and HPC for a better understanding and performance prediction of electrochemical energy storage systems

Progress in the development of novel energy storage systems is hampered by our lack of understanding of the microscopic mechanisms that determine their performance. The key issue is that phenomena on the atomistic scale have consequences on macroscopic length and timescales. In particular, the effects of ionic confinement and diffusion are crucial for device performance, yet experiments that probe properties related to local structure and diffusion are challenging and difficult to interpret without a parallel modelling approach. In this talk, I will focus on carbon-carbon supercapacitors in which the energy is stored by ion adsorption at the electrode surface. In order to understand fundamentally the macroscopic properties of such systems, it is essential to characterise finely the porous materials used and the structural and dynamic properties of the fluid adsorbed. But, in order to screen materials for energy storage applications, it is necessary to develop computationally efficient methods. Here, I will present insights from two different approaches. I will first describe molecular dynamics simulations, conducted using HPC facilities, which provide a microscopic understanding of the charging mechanisms in supercapacitors. I will then show the promising results we obtain with a mesoscopic model we develop, 10,000 times faster than molecular dynamics simulations, for the prediction of electrochemical performance in these systems.