

We are currently witnessing exponential growth in the development of energy-storage technologies with a significant impact on our daily lives. This development is visible in a wide range of industrial sectors ranging from portable electronics and health monitoring systems to large-scale applications, including environmentally-friendly electric vehicles. These applications require fast energy delivery on a minute or even second timescale and a long operational lifespan. Supercapacitors have emerged as promising electrochemical energy storage devices, satisfying the mentioned requirements due to their high power density, excellent cyclability and reversibility. The supercapacitor market already involves numerous commercial applications, including saving braking energy in cars, electric-drive buses built on supercapacitors, etc. However, the low energy density and energy-power trade-off of supercapacitors hinder the wide-spread application of these ecologically-friendly energy storage systems.

Despite the tremendous research effort, the energy storage mechanisms and the charging dynamics in supercapacitor electrodes with complex nanoporous networks have not yet been fully understood. Numerical modelling plays a pivotal role in acquiring these new insights necessary for developing next-generation supercapacitors. Still, currently available computational resources worldwide limit simulations to simple models and electrodes of nanoscale sizes. We will create a computational and experimental framework employing multiscale models to bridge nanoscale simulations with realistic micrometre-sized supercapacitor electrodes. Energy storage and power density will be correlated with the electrode structure using a multi-disciplinary approach based on electrochemistry, nano and mesoscale modelling, and X-ray and gas sorption measurements. The knowledge and tools acquired in this project will open up new horizons to design and optimise high-performance supercapacitors in the near future.