

Molecular Modeling of Supercapacitor Systems

Peter T. Cummings[†]

Department of Chemical and Biomolecular Engineering, Vanderbilt University, USA

(peter.cummings@vanderbilt.edu[†])

Supercapacitors, also known as ultracapacitors or electric double layer (EDL) capacitors, are energy storage devices that store electrical energy in the form of charges adsorbed to the electrodes, which are typically micro- or meso-porous conducting materials to maximize the electrode surface area. The goal of supercapacitor research is to bridge the energy storage gap with batteries, while retaining high power density. This requires fundamental understanding of the properties of the EDL, the nanoscale layering of ions interacting with an electrode. We use molecular dynamics simulations to study the properties of electrolytes and electrodes, from which we obtain structural, transport, and electrochemical properties. We review some of our key work in this area, supported by collaborations with experiments and materials synthesis performed at Oak Ridge National Laboratory, Drexel University, and other institutions that belong to the Fluid Interface Reactions Structure and Transport (FIRST) Center, a U.S. Department of Energy-funded Energy Frontier Research Center [<https://web.ornl.gov/sci/first/>].