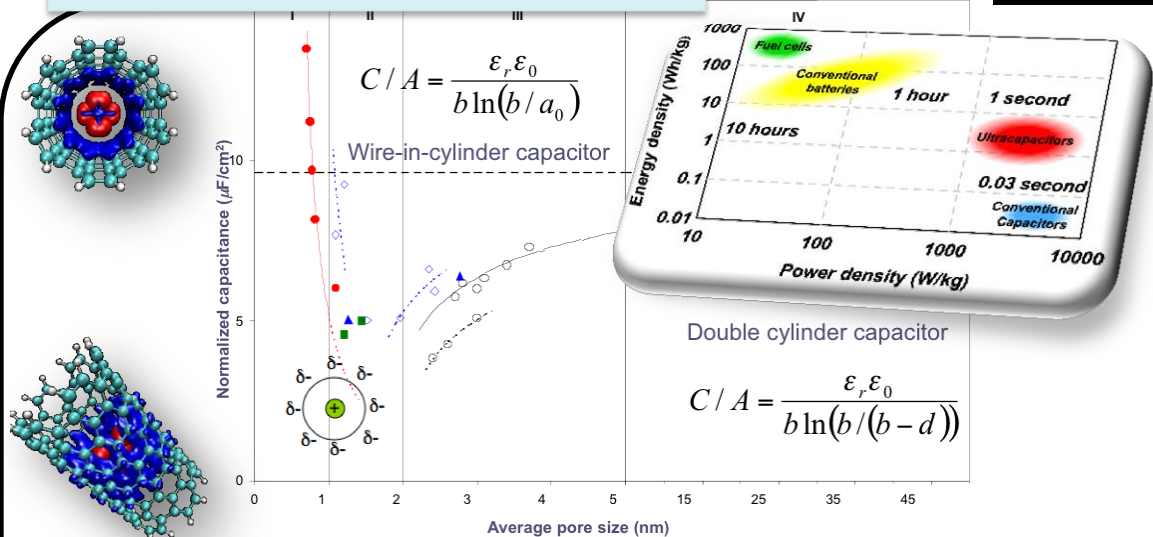


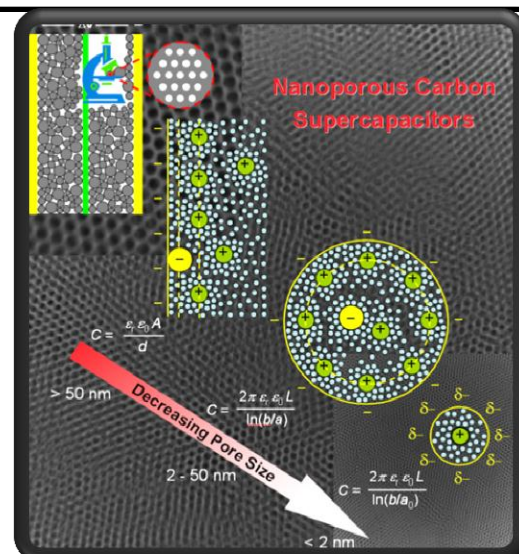
Electrical Energy Storage Modeling

“Fundamental Studies of the Ion Transport and Adsorption Phenomena in Electrochemical Capacitors,”

Some Achievements



Understanding anomalous capacitance increase at the nanoscale regime: density functional theory and large scale computations (*Angewandte Chemie Int. Ed.* 47, 520 2008)



Universal Model for Nanoporous Carbon Supercapacitors. (*Chem.: A Eur. J.* 14, 6614 2008)

1. Multiscale modeling of the electrolyte dynamics inside and outside the pore: from continuum modeling to quantum-level theory.
2. Effect of pseudo-capacitance (fast redox reactions): large-scale quantum chemistry calculations and scale spanning methods.
3. The capacitance can be evaluated from first-principles (with minimum input)