

Solvophobic Effect on Capacitance of Carbon/Organic Electrolyte Double Layers

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Electrochemical interfaces of carbon electrodes and organic electrolytes are important in energy storage applications such as supercapacitors. The differential capacitance of the electrochemical interfaces is an important performance metric of supercapacitor devices, and its voltage dependence reflects important physical properties of the interfaces. However, for carbon electrodes and ionic liquid based electrolytes these difference capacitance profiles are not fully understood. In the past two years, we utilized constant voltage molecular dynamics simulations to investigate the relationship between capacitance and interfacial structure of supercapacitor systems composed of model carbon electrodes combined with several ionic liquids as well as their mixtures with organic solvents. In this talk, I will report differential capacitance profiles of ionic liquids mixed with organic solvents, at perfectly flat graphene electrodes. Our results show that both pure and 10% mole fraction ionic liquid electrolytes exhibit camel shaped capacitance profiles with two peaks on either side of a minimum centered at the potential of zero charge. This profile shape results from electric field induced rearrangement of ion structure within the inner layer closest to the electrode interface. I will also present the influence of electrode nanostructures on the double layer structure and differential capacitance of ionic liquids. The nanostructured electrode can promote nonpolar interactions between nonpolar functional groups of like-charged ions. This nonpolar association facilitates separation between cations and anions at the electrode interface, increases the amount of net charge within the electrolyte double layer, and leads to significantly enhanced capacitance of the nanostructured electrode.