Molecular Modeling of Liquid-Solid Interfaces in Carbon Supercapacitors

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ABSTRACT

The use of electricity generated from renewable but intermittent energy sources (e.g., solar and wind) requires concepts for efficient energy storage. Electrical energy storage devices are a rising star on the horizon of energy storage technologies and among them, electrical double layer capacitors (EDLCs), also called supercapacitors, have attracted considerable attention in the electrical energy community. Supercapacitors store electrical energy via ion electrosorption directly in the EDLs at the liquid-solid (electrolyte-electrode) interface, suggesting that EDLs play a dominant role in the underlying energy storage mechanism and the resulting device performance.

To date, carbons are the most widely used electrode materials in supercapacitors, due to their high specific surface area, good electrical conductivity, chemical stability in a variety of electrolytes, and relatively low cost. To improve the energy density and the transport properties of the charge carriers in supercapacitors, carbons have been developed in diverse forms such as activated carbons, carbide-derived carbons, carbon nanotubes (CNTs), onion-like carbons (OLCs), graphene, and so on. From the view points of modeling, based on the geometry of pores of carbon electrodes and the way electrolyte molecules interact with the electrode surface, in this talk, supercapacitors are classified into three categories:

(1) the term “endohedral supercapacitor” is used to denote supercapacitors with porous carbon electrodes showing a zero or negative surface-curved pores where ions can enter inside (i.e., the charge stored in the pore, e.g., ions inside CNTs),

(2) the term “exohedral supercapacitor” is for supercapactiors in which ions reside on the outer surface of carbon particles (i.e., the charge stored on the positively curved surfaces, e.g., ions on outside surfaces of OLCs and end-capped CNTs),

(3) the term “planar supercapacitor” is for supercapacitors with zero/negligible curvature of electrode (e.g., flat graphene sheets).

With the help of modeling via molecular dynamics (MD), we investigated the interfaces between the electrolytes and the “planar”, “exohedral”, and “endohedral” electrodes to understand the energy storage mechanism of supercapacitors that rely on the EDLs established at liquid-solid interfaces. The contents of this talk would include:

(1) MD modeling of EDLs in room-temperature ionic liquids (RTILs) at open surfaces (e.g., planar, cylindrical, spherical, with defects, etc.) and the integration with experiments (e.g., atomic force microscopy, AFM), which would focus on the EDL microstructure and its influence from ion size, ion type, applied potential, electrode curvature, etc.

(2) MD modeling of porous carbon supercapacitors to find the energy storage mechanism, and some of them are compared with small angle X-ray scattering (SAXS) and neutron spin echo (NSE), which would embody the pore size effects on capacitance, the ion dynamics under porous confinement, and pore expansion during charging.

(3) The influence of water impurity on EDLs, which would show for the first time the work on the adsorption of water on electrode surfaces in contact with humid ILs.

(4) The preliminary investigation of a new type of RTILs used as electrolytes in carbon supercapacitors (that is the study of dicationic ILs in bulk and at liquid-solid interfaces).

BIOGRAPHY

Prof Guang Feng received his B.S. and M.S. degrees from Huazhong University of Science and Technology (HUST) in 2002 and 2005, respectively. In 2010 he received his Ph.D. degree from Clemson University and then joined Vanderbilt University and The Fluid Interface Reactions, Structures and Transport (FIRST) Energy Frontier Research Center supported by US-DOE as a postdoctoral and then a research assistant professor. In 2013 he became a professor in HUST through 2013 "Hubei Provincial 100-Talents Program". He has published 3 book chapters (by Wiley-VCH, Springer and CRC/Taylor & Francis, respectively) and 47 papers in peer-reviewed journals including Nano Letters, Advanced Energy Materials, ACS Nano, Nano Energy, etc. His current research is mainly focused on study of micro-/nano-scale interface and transport phenomena in applications of energy storage, capacitive deionization for desalination and water treatment, and carbon capture and utilization. More information is available at http://itp.energy.hust.edu.cn.