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Molecular insights into electrical energy storage in supercapacitors with ionic liquid mixtures as electrolytes

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Ionic liquids (ILs), used as electrolytes in supercapacitor, are attracting more and more attention in energy storage community. In many of their applications, the use of ionic liquids is related to their mixtures with different solvents. In this talk, our work on supercapacitors with IL mixtures as electrolytes will be discussed in two classifications: one shows the effect on supercapacitors by adding beneficial solvents and the other presents the influence by the remaining solvent taken as impurity in electrolytes.

To address the issue that the use of ILs, in particular dicationic ILs (DILs) electrolytes in supercapacitors is impeded by their slow dynamics, organic solvents were added into DIL electrolytes to improve ion transport and then enhance the power density of supercapacitors. In this work, we investigated the influences of organic solvents on the conductivity of DILs and their electrical double layer (EDL) of DILs-based supercapacitors, and found that the conductivity of DILs electrolyte was greatly increased in the presence of organic solvents, and the capacitive performance of supercapacitors became more stable without compromising their energy density under pure IL electrolytes.

Complete removal of water from ionic liquids is nearly impossible, and such impurity water may bring significant effects on IL-based supercapacitors since the electrolysis of water possibly arises due to the potential applied on IL supercapacitors larger than water decomposition voltage ($\sim 1.23\text{V}$). In this talk, we will show for the first time the work on the adsorption of water on electrode surfaces in contact with humid ILs. The results revealed that the enrichment of water near electrodes as the surface charge density increases is likely a universal phenomenon in EDLs formed by ILs with ions larger than water molecules. The type of ions affects water accumulation, due to the difference of the ion volume/shape and the “subtleties” of water ion interaction, but it will not change the concave shape of the water accumulation versus surface charge curve, although the symmetry of the curve does depend on the type of ions.

Keywords: Ionic liquid; Electrical double layer; Organic solven; Water impurity; Molecular dynamics