Role of Quantum Capacitance of Graphene-like Carbon Electrodes in Enhancing Supercapacitor Performance

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Carbon-based nanomaterials such as graphene and nanotubes (CNTs) are a promising class of electrodes for electrochemical double layer capacitors (EDLCs), due to their high accessible surface area, high electrical conductivity, and tunability through functionalization. A series of recent studies have shown that N-doped graphene and CNT-based EDLCs can have improved capacitance, which has been through typically to be associated with the increased double layer capacitance from a high BET surface area or an enhanced electrolyte-electrode interfacial interaction. However, the influence of the electrode's quantum capacitance is relatively unknown.

In this talk, we will present a new computational framework based on density functional theory and classical molecular dynamics to explore the relative contributions of the quantum capacitance of electrode (C_Q) and the electric double layer (C_D) capacitance to the total interfacial capacitance (C_T) for various carbon-electrode systems in ionic liquids (ILs). For instance, our recent study suggests that N doping leads to significant enhancement in C_Q as a result of electronic structure modifications while there is virtually no change in C_D. We will also discuss the impact of the chemical and/or mechanical modifications of graphene-like carbon electrodes on the supercapacitor performance.