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

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Graphene-based electrodes 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 (CQ) and the electric double layer (CD) capacitance to the total interfacial capacitance (CT) for various carbon electrode systems in ionic liquids (ILs). For instance, our recent study suggests that N doping leads to significant enhancement in CQ as a result of electronic structure modifications while there is virtually no change in CD.