Effect of Anion on the Quantum Capacitance of Graphene Cathode in Lithium Ion Capacitor: A DFT Study

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Graphene is widely employed as cathode because it can provide excellent capacitance, as well as constructing an effective conducting network [1, 2]. However, the detail understandings of electrode/electrolyte interface in graphene-based LIC is still limited.

Based on our previous results, graphene with single vacant defect or pyridinic and pyrrolic doped N atom show much higher quantum capacitance (QC) than the pristine one [3]. However, when it comes to the real LIC system, reactions may occur between the electrolyte and those reactive atoms in graphene cathode. Therefore, the presence of electrolyte will disturb the density of states (DOS) of graphene-based cathode, and hence the QC and the energy storage ability will vary accordingly. In this work, the interaction between the anion in the electrolyte and graphene cathode with high QC is investigated using First Principle calculation. The results suggest that the defect states of graphene cathode can enhance the adsorption energy towards anion, and hence the QC and electrical double layer (EDL) structure is different with that of pristine graphene cathode. Furthermore, this interaction also decrease the stability of the anion in electrolyte. The results from this work would help to further develop high energy graphene-based LIC and shed some light on its capacity fading mechanisms.

Reference:

[1] Chen, et al., Energ Environ Sci, 6(2013), 1623.

[2] Yu, et al., Nano Energy, 15(2015), 43.

[3] Su, et al., Catalysts 8(2018,) 444