GRAPHENE-BASED NEW GENERATION SUPERCAPACITORS AS AN ENERGY STORAGE DEVICE

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In this study, a supercapacitor model using first principles calculations based on density functional theory (DFT) has been studied. Bilayer graphene as electrode and nitric acid as electrolyte are used in this graphene-based supercapacitor. Both the combination of electrode and electrolyte are important in order to improve the energy storage capacity of the device. Nitric acid as electrolyte simultaneously generates pores into the graphene due to its active chemical reaction with carbon. Thus, the effect of vacancy defect on electrode was scrutinized. In our calculations, plane wave pseudo-potential method and the local density approximation (LDA) for exchange-correlation potential are used. The different configurations of nitric acid between bilayer graphene (Figure 1) are investigated. The relative position of nitric acid with respect to graphene can be hollow (H), top (T) and bridge (B), where the nitrogen atom of nitric acid is placed at the center of hexagon, on top of the carbon atom and between two carbon atoms, respectively. After structure optimization calculations are completed extensively, electronic structure and quantum capacitance are investigated from density of states (DOS) calculations. It is necessary to include the effect of solution because of the electrolyte in order to obtain realistic modelling of these capacitor devices. We studied to see the effect of the solvent environment on the electronic structure and the quantum capacitance of the graphene based supercapacitor systems using the nonlinear polarizable continuum model.

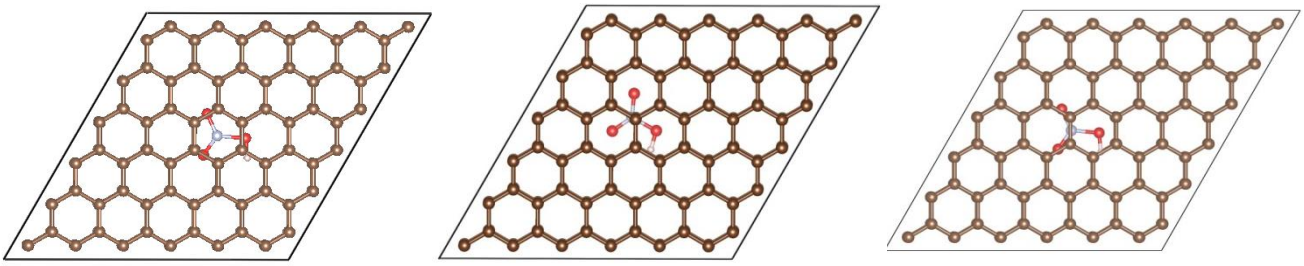

Figure 1. The different configurations of nitric acid between bilayer graphene.