MOLECULAR DYNAMICS SIMULATION OF ELECTRIC DOUBLE LAYER CAPACITANCE OF GRAPHENE ELECTRODES

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Graphene has been identified as a promising material for electric double layer capacitors (EDLCs) owing to its large surface area and high conductivity. This study aims to develop a computation model to study the double layer formation of graphene electrodes when it is in contact with an electrolyte. Classical molecular dynamic simulation method was selected as a promising method to study the electrode-electrolyte interactions of electric double layer capacitors. This simulation study was performed to understand the electric double layer capacitance of graphene electrodes and acetonitrile electrolyte. The computational analysis has been performed using the molecular dynamics tool (LAMMPS). In this study, to understand the EDL performance on capacitance, number density profile, and charge density profile, data was obtained. The simulations show that electrolyte (acetonitrile) is formed into a highly ordered structure near the surface in graphene-based systems, which leads to electric double layer formation. According to capacitance values that have been calculated, the presence of defects in graphene reduces the electric double layer capacitance.

Keywords: Graphene, Molecular dynamic simulations, EDLC