Electrode – Electrolyte Interface Analysis by Molecular Dynamics Simulation

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The research for renewable energy generation methods requires the development of novel, sustainable energy storage methods. Supercapacitors are much promising for future energy storage applications, owing to their high energy density and rapid charge-discharge time. supercapacitors are widely used in the following ways: firstly, the largest proportion of commercial supercapacitors are used in consumer electronics, in which they mainly serve as backup sources for memories, system boards, clocks and microcomputers; secondly, supercapacitors are used as the main power source, such as fail-safe positioning devices and starter applications. The performance of supercapacitors can be improved by using high surface area electrode materials, which could increase the energy density of the device. In this regard, nanomaterials are much advantageous owing to their high surface to volume ratio.

In this study, graphene and titanium dioxide nanotube arrays are studied as a supercapacitor electrode material, using molecular dynamic simulation. This study focuses on mathematical modeling of electrode-electrolyte interface, to study the charge storage mechanism of the electrode when in contact with the electrolyte. Firstly, the molecular dynamic simulation (MD simulation) method was used to study graphene-electrolyte system using a planar electrode model. There, the formation of electric double layer with different charge levels are studied. secondly, molecular dynamics simulations have been conducted to study the interaction between anatase TiO2 (100) surface and water. The effect of surface orientation of the TiO_2 surface on the interface properties was studied.

Keywords: molecular dynamic simulation (MD simulation)