

Atomistic simulation of the interaction of electrolyte with graphite nanostructures in advanced supercapacitors.

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Carbon supercapacitors represent a promising energy storage devices based on liquid electrolyte ion adsorption on the surface of highly porous carbon [1]. The presence of a developed surface with a pore size down to nanometers provides more contact surface area per unit mass. Optimization of this kind of technology requires detailed understanding of the physics of the electrical double layer formation, its behavior during supercapacitor charging and discharging, information on the mechanisms of diffusion of the electrolyte in nanopores.

The level of development of methods of classical and quantum molecular dynamics and the use of parallel high performance computing allow one to build realistic models of such processes. The most precise characteristics of electrolyte solutions can be calculated with the use of ab initio molecular dynamics in the framework of DFT [2]. Such an approach allows studying the interaction of the ion subsystem of the electrolyte with the surface of carbon material. Including of carbon in the model gives the opportunity to consider the peculiarities of adsorption of electrolyte components at the phase boundary. In particular it suggests a strong adsorption of alkali metal ions on the surface of carbon material. It is found that the carbon material electron-hole plasma determines the capacity of the system. The ratio of the ion subsystem capacity and full system capacity has the order of $C_3/C \sim U/\Delta U_3 > 4$ where U is the full potential drop superimposed on the system. The maximum capacity of the carbon electrode of pure defect-free graphite is estimated $C_{\max} \sim 22\text{F/cm}^3$.

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2. *Modern Methods and Algorithms of Quantum Chemistry* / ed. By J. Grotendorst - Julich: John von Neumann Institute for Computing, 2000. - pp. 301-449