The Flow Behavior of Organic Liquids Inside Carbon Nanotube

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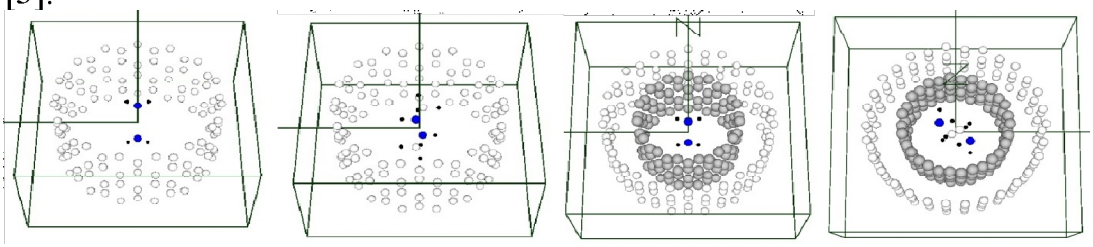
Research efforts over the past 20 years have been focused on the electrical, optical, and mechanical properties of the carbon nanotubes. Although several early experiments had shown the ability to open up carbon nanotubes (CNTs) to serve as nanoscale containers, it is in the past 5-10 years that experimental molecular transport through CNTs, or the interstice between vertically oriented CNTs, has become a subject of intense interest. This interest has been generated by the discovery of the fascinating mass-transport properties of this nanoscale material. For example, the transport rate of water is almost four to five orders of magnitude higher than that of other porous materials of comparable size, and is very close to that of biological membrane channels, such as aquaporin [1].

The aim of this work is to understand the flow behavior of liquids (water and methanol) in nanometrically bounded spaces with a cylindrical geometry, in particular, inside carbon nanotube (SWCNT) with clean walls and covered inside atoms Au (fig.1). Au nanoparticles have been actively studied because of the discovery of quantum size effects and the significant change in physical properties at the nanoscale. In particular, a dewetting event generally starts from the deposition of Au thin films on poorly wetting substrates [2].

We performed calculations of the (diffusion) migration energetic barriers of the water (methanol) molecules inside the zigzag (15,0) nanotube within the framework of the methods of the electron density functional and the ab initio pseudopotential. All calculations have been made with the proprietary source code [3].



a b c d

Fig. 1. The supercell of the model superstructure for the flow of water or methanol inside nanotube with clean walls (a, b) and inside covered by the gold atoms (c, d).

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2. Lee S.-H. et al. Dewetting behavior of electron-beam-deposited Au thin films on various substrates: graphenes, quartz, and SiO_2 wafers // Appl. Phys. A . – 2015. – V. 118. – P.389–396.
3. Balabai R.M. Electronic properties of functionalized graphene nanoribbons // *Ukr. J. Phys.* – 2013. – V. **58**, № 4. – P.389-397.