Investigation of Ionic Water Flow Over a Carbon Nanotube: Stick-Slip Mechanism

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Introduction

At early 2001, Kral and Shapiro reported the possibility of generating an electric current by making a liquid flow over some metallic carbon nanotubes [1]. This theory was proved by the experimental production of a CNT-based flow sensor which indicated the generation of an induced voltage in nanotube bundles because of a ionic liquid flow with a number of different velocities [2]. Although Ghosh and his coworkers believe in the main role of pulsating asymmetrical ratchets to explain the transduction mechanism of this sensor [2], there are other suggested models involving phonon wind drag, columbic fields [1], electrokinetic mechanism [3] and a stick-slip flow [4].

The logarithmic dependence of induced voltage on the liquid velocity and also respectively, direct and reversed relation between voltage and liquid's polarity and viscosity are some remarkable properties of the produced sensor, to which is asserted that the stick-slip model has the most conformity. Such a mechanism is based on the alternative adsorption and desorption of ions dissolved in solid-like water layer pinning to nanotube surface.

Molecular Dynamics Simulations

In this work we use molecular dynamics simulations to demonstrate the manner of a ionic flowing water around a carbon nanotube and therefore to investigate the possibility of the stick-slip model. Therefore a metallic (5,5) carbon nanotube immersed in a sodium chloride solution, is computationally simulated by NAMD software [5]. We also use langevin dynamics to appoint a constant temperature in an NVT ensemble.

In spite of some nanoseconds of simulation, we observe that not only sodium ions, contrary to Persson's anticipation [4], don't adsorb on CNT surface, but also such a prinstine nanotube is so much hydrophobic that water molecules don't approach its surface closer than 3.2 A^0, "Fig 1". This space resembles the CNT-liquid interface thickness, while introducing a nanotube into water [1,2]. However, there are some differences with what has been reported for Na^+ (5.5A^o) and Cl^- (5.3A^o) equilibrium distances from CNT surface according to Ghosh et. al *ab initio* studies [6].

We also perform the radial distribution calculations for Na^+ and Cl^-, to evaluate the arrangement over carbon nanotube's surface.

Ab initio Studies

The minimum approaching distance of positive sodium ions to carbon nanotube surface is applied to investigate the interaction of one Na^+ on nanotube density of states, according to density functional theory (DFT). For this purpose we use Siesta code [7] and the pseudopotential approximation. The obtained results indicate some noteworthy changes in the electronic density of states of the nanotube.

Finally it seems that flowing water can force a few of positive ions to approach nanotube surface up to a 3.2 A^o distance, that is a bit similar to what Persson et. al suggest as an arrangement of positive ions on water-CNT interface layer, but there is an obvious contradiction to the theory of ions' periodically adsorption and desorption on nanotube external surface as the transduction mechanism of charge transfer in nanotube due to flowing of water over it.

References:

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Figures:

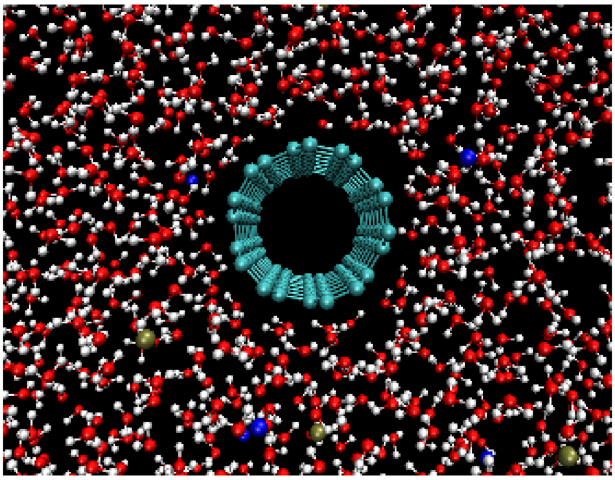

Figure 1. Snapshot of the simulated carbon nanotube immersed in a solution of Na^+ (blue) and Cl^- (green), showing the hydrophobic surface of carbon nanotube.