Conductivity of a SWNT with a Positive Charge at the Surface

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We study the effect of a positive charge placed in a near proximity of a SWNT surface on its transport properties. In order to introduce such a charge without distorting the band structure of the nanotube we designed an aromatic molecule **1** with a shape suitable for non-covalent binding to the side wall of the SWNT due to van der Waals interactions.

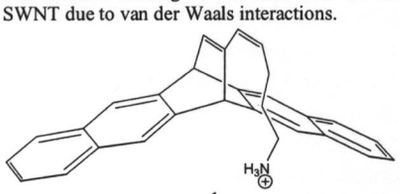

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Figure 1. The structure of **1**. Most of its +1 charge is accumulated at ammonium terminus.

This molecule carries a positively charged ammonium group terminated alkyl chain, sufficiently long for placing the charged terminus near the SWNT surface. The Coulomb forces between the +1 charge of **1**, which is mostly concentrated at the ammonium group, and image charges induced in the SWNT result in a strong attraction. The structure of a complex of **1** with a [10,10] armchair SWNT segment (Figure 2) was optimized using molecular mechanics and dynamics (we used a finite length segment long enough to accommodate the molecule for the geometry optimization because it is not very sensitive to the length of the nanotube).

A higher level of theory calculation of the complex is used to obtain a charge distribution. The distance between the charged terminus of **1** and the nanotube found in this complex (0.35 nm) and the charge distribution are then supplied to the continuum modeling of the nanotube transport properties. The calculation followed the approach to the simulation of nanotube based devices developed by one of us [1]. We introduced a compact model for the nanotube transport calculation. It allows fast calculation of the self-consistent distribution of charge density along the metallic tube placed in the external electric field. In our case, the charge of the molecule **1** is the origin of the external field. We demonstrated in [1] that self-consistent solution of joint Poisson and Boltzmann equations coincides with the full quantum-mechanical result. Therefore, for calculating the transport properties of the SWNT-charged molecule complex we used the drift-diffusion equations.

We demonstrate theoretically that a charge fixed at the SWNT surface by an aromatic molecule may produce changes in the transport properties of the tube.

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[1] Kirill A. Bulashevich, Slava V. Rotkin, "Nanotube Devices: Microscopic Model", (submitted to JETP Letters).

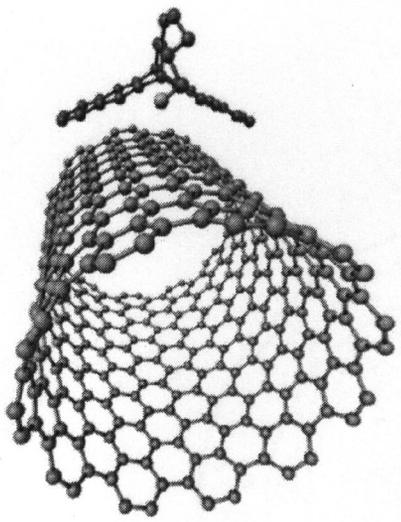

Figure 2. Aromatic molecule **1** bound to the [10,10] SWNT by the van der Waals and Coulomb forces.