**Screening of water dipoles inside finite-length armchair carbon nanotubes**

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Short single-walled carbon nanotubes (SWNTs) have been proposed as good candidates for artificial nano-scale channels due to their small size and stable structure. Unlike many insulating biological channels in nature, the nanotubes respond to external charges and electric potentials effectively due their delocalized π-electrons. We study the electronic structure and dielectric properties of finite-length armchair SWNTs within a self-consistent π-orbital tight binding (TB) method. By including up to the third nearest neighbor interactions, we have successfully reproduced the periodic oscillation of the finite band gap as a function of the nanotube length and the HOMO/LUMO orbitals predicted by a*b initio* calculations. We also look into the screening ability of SWNTs by applying uniform electric fields along or across the nanotubes. We show that as the length increases, the parallel screening constant $\varepsilon_{||}$ grows almost linearly to infinity while the perpendicular screening constant $\varepsilon_{\perp}$ converges to its bulk value when the nanotube length exceeds ten times the radius. $\varepsilon_{||}$ and $\varepsilon_{\perp}$ are found to have weak and strong dependence on the magnitude of the band gap respectively, which can be explained by the symmetry of the involved subbands.

At a length of several nanometers, the screening constants in both direction are still considerable (~5), which may be important for ion/dipole transport in SWNT-based channels. For example, Fig 1(a) demonstrates that an external dipole $\mu_0$ is fairly well screened by the induced counter dipole on the SWNT surface when positioned near the nanotube center. On the other hand, a parallel dipole is induced when $\mu_0$ is positioned outside the entrance, which may favor the entering of external dipole molecules. We have applied our method to study the polarization of a short SWNT segment filled with a 6-water-wire, with geometry obtained from classic MD simulations. The induced charges on the SWNT surface effectively reduce the total water dipole of 12.23 Debye to a net dipole of 5.24 Debye. The system energy is lowered by 6 $k_BT$ due to the Coulomb interaction between the water wire and its image charges on the nanotube, which may make the filled state energetically more favorable. We expect that with charged particles such as protons, the screening effects will be more significant. Work is in process to study the transport of water molecules in short polarizable SWNTs by combining MD simulation with our efficient self-consistent TB schemes.

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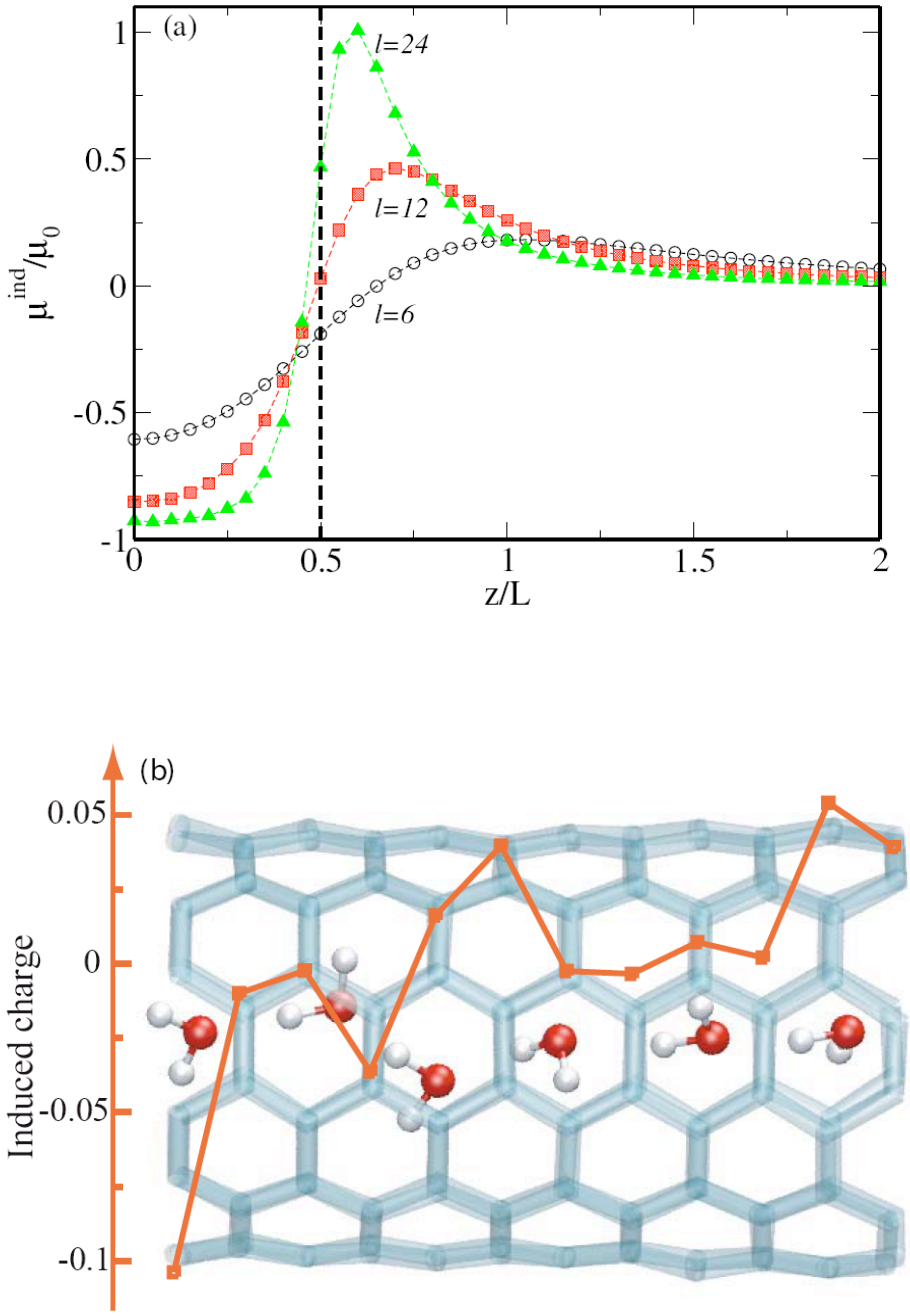


Figure 1: (a) The ratio of the induced dipole $\mu^{ind}$ to an external dipole $\mu_0$ positioned along the axis of a (6, 6) SWNT. The location of $\mu_0$ relative to the nanotube center $z$ is scaled by the nanotube length L with 6, 12, 24 sections respectively. The dashed line indicates the right end of the finite SWNT. (b) The background is a snapshot taken from a MD simulation of a 6-water-wire inside a (6, 6) nanotube segment with 12 sections. The overlaying curve plots the summed induced surface charges (in squares) of each section of the nanotube.

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