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Accurate and efficient modeling for carbon nanotubes in biological applications YAN LI, DEYU LU, KLAUS SCHULTEN, UMBERTO RAVAIOLI, Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL, USA — Carbon nanotubes (CNTs) hold great promise for applications in biomedicine and biotechnology, in particular, as biosensors. For such applications, it is essential to understand the interaction of CNTs and water and/or other biomolecules in the aqueous environment. In this regard, the short-ranged van der Waals interaction together with the Coulomb interaction arising from atomic partial charges and dielectrically induced charges on the CNT play an important role. We have developed an accurate, yet computationally efficient, empirical method to model the electrostatics of finite-length single-walled armchair CNTs. Atomic partial charges are fitted to electrostatic potentials computed at a B3LYP/6-31G* level of density functional theory. The dielectric properties are calculated self-consistently from a third-nearest-neighbor tight-binding Hamiltonian, and are found to be in good agreement with density functional theory results. We demonstrate our description for water transport through a finite-length CNT channel. The atomic partial charges on the edges are found to greatly contribute to the total interaction energy and may influence water entering the CNT, while the polarizability of the CNT significantly lowers the electrostatic energy in the tube center.

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