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High quality molecular dynamics simulation of carbon nanotubes in DEYU LU, YAN LI, UMBERTO RAVAIOLI, Beckman Institute, University of Illinois at Urbana-Champaign, GIANCARLO CICERO, Istituto Superiore Mario Boella, Italy, GIULIA GALLI, Chemistry department, University of California, Davis, KLAUS SCHULTEN, Beckman Institute, University of Illinois at Urbana-Champaign — Biological applications of carbon nanotubes (CNTs) rely on mechanical, electrical, and chemical interactions between CNTs and biomolecules in water. Efficient computational methods for such nanoscale disordered systems have been developed that take into account the electronic degree of freedom of the CNTs interacting with biological media with thousands of atoms. For this purpose we combined in a molecular dynamics program an empirical CNT model employing a tight-binding CNT Hamiltonian with a classical description of the biological medium (water, ions, protein, DNA). The first application of this new method [1,2] described a potassium ion-CNT complex [3] and revealed a terahertz frequency oscillation of the ion inside a 16 angstrom long CNT segment. At a greatly reduced computational expense, our result showed good agreement with a Car-Parrinello molecular dynamics simulation. [1] D. Lu, Y. Li, U. Ravaioli, and K. Schulten. J. Phys. Chem. B, 109 (2005)11461. [2] D. Lu, Y. Li, S. V. Rotkin, U. Ravaioli, and K. Schulten. Nano Lett., 4 (2004)2383. [3] D. Lu, Y. Li, U. Ravaioli, and K. Schulten. Phys. Rev. Lett., (2005) in press.

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