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Molecular Dynamics Investigation of Ionic Flow and Separation by Carbon Nanotube Electrodes SOUMIK BANERJEE, Virginia Polytechnic Institute and State University, SOHAIL MURAD, University of Illinois at Chicago, ISHWAR PURI, Virginia Polytechnic Institute and State University, ENGINEERING SCIENCE AND MECHANICS TEAM — We report on molecular simulation studies of the ionic flow in the presence of charged carbon nanotubes. Our domain contains three species; viz. positively charged sodium ions, negatively charged chlorine ions and neutral water; and a pair of single-walled carbon nanotube electrodes. One of the nanotube is positively charged and the other is negatively charged. The system of 1024 atoms is initially allowed to equilibrate from an FCC crystal structure for the solution. The nanotubes are tethered and the carbon atoms are assumed to vibrate as in a One-Dimensional Harmonic Oscillator (ODHO) about their mean positions. The sodium ions travel towards the negatively charged carbon nanotube and the chlorine ions likewise flow towards the positively charged nanotube. The simulation uses a Lennard-Jones soft sphere potential model and coulombic potential for interaction between the charges. In addition to the ion transport mechanism, the hydrophobic character of carbon nanotubes is clearly evident from the simulated flow.

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