Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Detection of bio-molecules of different polarities by Boron Nitride Nanotoube SAIKAT MUKHOPADHYAY, Michigan Technological University, RALPH SCHEICHER, Department of Physics and Astronomy, Uppsala University, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, U.S. Army Research Laboratory, Weapons and Materials Research Directorate, DEPARTMENT OF PHYSICS, MICHIGAN TECHNOLOGICAL UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, UPPSALA UNIVERSITY COLLABORATION, U.S. ARMY RESEARCH LABORATORY, WEAPONS AND MATERIALS RESEARCH DIRECTORATE COLLABORATION — The effect of molecular polarity on the interaction between a boron nitride nanotube (BNNT) and amino acids is investigated with density functional theory. Three representative amino acids, namely, tryptophane (Trp), a nonpolar aromatic amino acid, and asparatic acid (Asp) and argenine (Arg), both polar amino acids are considered for their interactions with BNNT. The polar molecules, Asp and Arg, exhibit relatively stronger binding with the tubular surface of BNNT. The binding between the polar amino acid molecules and BNNT is accompanied by a charge transfer, suggesting that stabilization of the bioconjugated complex is mainly governed by electrostatic interactions. The results show modulation of the BNNT band gap by Trp. Interestingly, no change in band gap of BNNT is seen for the polar molecules Asp and Arg. The predicted higher sensitivity of BNNTs compared to carbon nanotubes (CNTs) toward amino acid polarity suggests BNNTs to be a better substrate for protein immobilization than CNTs.

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Date submitted: 09 Nov 2011 Electronic form version 1.4