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Interaction of Nucleobases with Semiconducting Nanotubes and Nanocages: Does the Solvent Matter? ZHOUFEI WANG, Department of Physics, South China Agricultural University, Guangzhou, China, WILLIAM SLOUGH, HAIYING HE, RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, MI 49931, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM, Aberdeen Proving Ground, MD 21005-5069 — The tremendous advancement in nanotechnology has brought great promise in the area of bio-applications. Nanoscale materials and structures have attracted a lot of interest for their potential applications in biosensing, biorecognition, luminescent probes for DNA, biomedical labeling, drug delivery etc. Gaining fundamental understanding of the interaction of bio-systems with nanomaterials is critical in putting all these applications into full play. Despite the fact that most of these interactions appear in aqueous environment, the solvent effect has often been neglected in previous computational studies. In this talk, we will report our comparison study of nucleobases interacting with BN nanotubes and chalcogenide nanocages with/without considering the aqueous solution, based on first-principles calculations. The results reveal a significant effect from the water solution, which may largely reduce the interaction energy due to the polarization of the dielectric solvent medium.

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