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Physisorption of Nucleic Acid Bases on Boron Nitride Nanotubes: A new class of Hybrid Nano-Bio Materials SAIKAT MUKHOPADHYAY, S. GOWTHAM, Michigan Tech, Houghton, MI, RALPH SCHEICHER, Uppsala University, Uppsala, Sweden, RAVINDRA PANDEY, Michigan Tech, Houghton, MI, SHASHI KARNA, US Army Research Laboratory, APG, MD — We investigate the adsorption of the nucleic acid bases, adenine (A), guanine (G), cytosine (C), thymine (T) and uracil (U) on the outer wall of a high curvature semiconducting single-walled boron nitride nanotube (BNNT) by first principles density functional theory calculations. The calculated binding energy shows the order: G>A≈C≈T≈U implying that the interaction strength of the (high-curvature) BNNT with the nucleobases, G being an exception, is nearly the same. A higher binding energy for the G-BNNT conjugate appears to result from a stronger hybridization of the molecular orbitals of G and BNNT, since the charge transfer involved in the physisorption process is insignificant. A smaller energy gap predicted for the G-BNNT conjugate relative to that of the pristine BNNT may be useful in application of this class of biofunctional materials to the design of the next generation sensing devices.

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