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***Ab initio* study of adenine and thymine adsorption on carbon nanotubes.** YAROSLAV SHTOGUN, LILIA WOODS, Department of Physics, University of South Florida, GALYNA DOVBESHKO, Institute of Physics of National Academy of Sciences of Ukraine — The adsorption properties of the DNA bases, adenine and thymine, on the surface of single walled metallic and semi-conducting carbon nanotubes are calculated from first principle density functional theory calculations using the VASP code (Vienna Ab initio Simulation Package). Calculations for the adsorption of the charged adenine and thymine molecules are also presented. The equilibrium positions and their energies are determined. The adsorption process is analyzed in terms of the electronic structure of the various configurations. The effects of charging of the DNA bases in the adsorption on the nanotubes are also determined. The results for the density of states, band structure and charge transfer analysis are used to establish a model of the interaction of these biological molecules with carbon nanotubes.

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