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DNA-CNT Interaction - A Density Functional Approach RALPH SCHEICHER, S. GOWTHAM, RAJEEV AHUJA, Fysiska Institutionen, Uppsala Universitet, Sweden, RAVINDRA PANDEY, Michigan Technological University, USA — Standing at the intersection of the biological regime and the nanomaterials world, DNA-coated carbon nanotubes (CNT) possess features which can make them attractive for a range of applications, e.g., as highly specific nanosensors [1], or as a method to efficiently separate CNTs according to their structure [2]. It is therefore certainly worthwhile to obtain a detailed understanding of the binding between the bases in DNA and the surface of CNTs, preferably from first principles. To this end, we have studied the interaction between single-stranded DNA and single-walled CNTs (SWCNTs) using density functional theory. More specifically, we were interested in assessing the differences in the interaction of the four different bases in DNA, and how important the underlying structure of the CNT is for the orientation of the bases relative to the tube axis. We will report our results on the binding energy, the charge density, and the respective distortion in the electronic structure of the constituents of this hybrid system, depending on the geometrical properties of the CNT and the relative positioning of the DNA.

[1] C. Staii *et al.*, *Nano Letters* **5**, 1774-1778 (2005)
[2] M. Zheng *et al.*, *Science* **302**, 1545-1548 (2003)

Ralph Scheicher
Michigan Technological University

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