

SWITCHING BEHAVIOR IN SILICON-MOLECULE-SWCNTS DEVICES: A DENSITY FUNCTIONAL THEORY STUDY

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Most recently, a new testbed for exploring the electrical properties of single molecules has been developed [1], in order to eliminate the possibility of metal nanofilament formation and to ensure that molecular effects are measured, whereby Si and single-wall carbon nanotubes (SWCNTs) are used as electrodes for the molecular monolayer, demonstrated, for example, for molecules such as those based on oligo(phenylene-ethynylene) in a Si-OPE/NO₂-SWCNT device configuration. Interestingly, the use of such structures with π -conjugated organic molecules resulted in a hysteresis loop with current-voltage measurements that are useful for a memory device [1]. Devices without π -conjugated molecules ((Si-H) surface only), or with alkyl-bearing molecules produced no hysteresis, indicating that the observed memory effects is molecular relevant.

In this work, we present a density functional theory study of the OPE derivative either physisorbed or chemisorbed (**a**, **b** in Fig. 1) at a SWCNT, and covalently bonded at the Si slab, as well as of an alkyl derivative (**c**, cf. Fig. 1), with respect to conformational changes, taking place under an applied field. Structural parameters, electronic structure, and charge transfer as a function of an applied field will be discussed in detail.

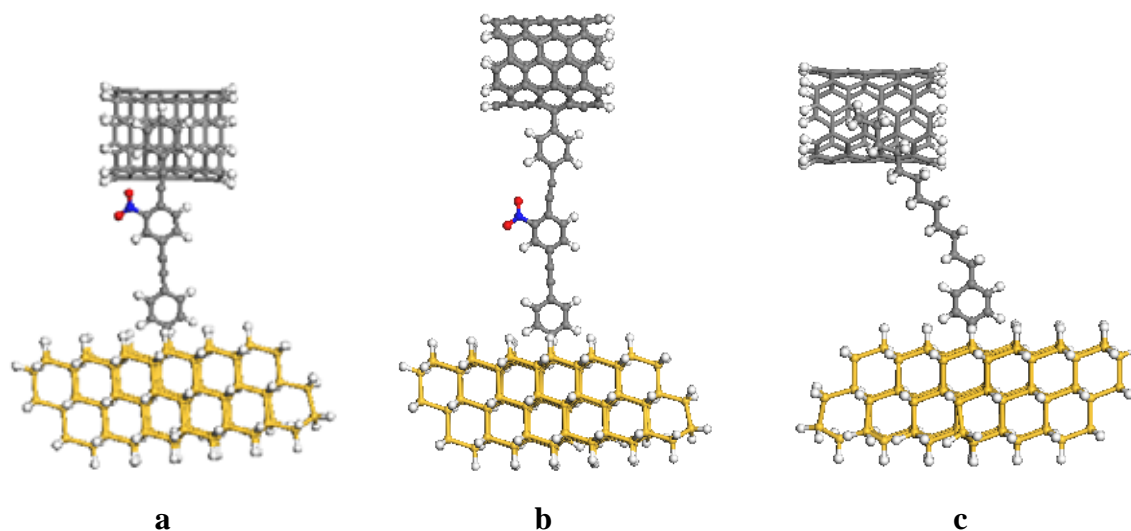


Figure 1: Models representing a physisorption (a) and a chemisorption (b) in the Si—OPE/NO₂—CNT complex, and a physisorption of alkyl derivative (c).

References:

- 1 He, J., Flatt, A. K., Stephenson, J. J., Condell, D. Doyle, J. M. Tour, Nature Materials 5, 63 (2006).