

Abstract Submitted
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A Density Functional Theory Study of Silicon-Molecule-SWCNTs Nanodevices BRAHIM AKDIM, RUTH PACTER, Wright-Patterson Air Force Research Laboratory, Ohio USA — Electronic devices comprised of oligo(phenylene-ethynylene) and its derivatives, bridged between a silicon slab and a single walled carbon nanotubes (SWCNTs) mat, have been shown to exhibit bistable states, driven by an applied voltage (He et al. Nature Materials 5, 2006). In light of these reports, we present a theoretical study on the switching mechanism of the nitro-oligo(phenylene-ethynylene), via the non-equilibrium Green's function formalism and the density functional theory (DFT) method. We report on the conformational changes of nitro-OPE induced by an applied field, as well as on the interaction at the interface of the SWCNT, emphasizing their effects on the electronic transport of the system (Si—Molecule—SWCNT). DFT properties such as structural parameters, electronic structures, and the density of states near the Fermi level as a function of an applied field, will be outlined. In conjunction with the DFT results, the electron transport obtained via the non-equilibrium Green's function formalism will be discussed.

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