

Abstract Submitted  
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**Atomic, electronic and spin-density structure of cobalt/polythiophene/cobalt magnetic tunnel junction** IVAN OLEYNIK, University of South Florida — Electron and spin transport through ferromagnet/organic molecule/ferromagnet junctions depends critically on the properties of the electrical contacts of organic molecules with metallic electrodes. We performed first-principles density functional theory investigation of atomic and electronic structure of cobalt/polythiophene/cobalt magnetic tunnel junction (MTJ). We will present results on geometry and energetics of metal/organic interfaces, distribution of electron charge and spin densities, local atomic charges and spins, and local densities of states on individual atoms. We will discuss the spin-dependent electronic properties of cobalt/polythiophene/cobalt MTJ in connection with its spin-dependent transport characteristics.

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