

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Interface properties of nickel/organics/nickel magnetic tunnel junctions** WESLEY FABELLA, University of South Florida, IVAN OLEYNIK, University of South Florida — In recent years, substantial experimental efforts were directed towards developing a new class of spintronic devices based on organic polymers, oligomers and small molecules. In particular, recent experiments indicate efficient spin injection and spin transport in ferromagnet/organic systems. However, the electron and spin transport through metal-molecule-metal junctions depends crucially on the properties of ferromagnet/organics interfaces. We performed first-principles density functional theory (DFT) calculations of nickel/organic-molecule/nickel magnetic tunnel junctions. Organic systems include both saturated alkane and unsaturated thiophene molecules. The choice of the system was made based on available experimental information. The atomic structures of metal/molecule interfaces were built and the geometries of molecule/metal interfaces were determined by optimizing the interfacial work of separation. We will discuss the electronic properties of molecule/electrode junctions including distribution of charge densities, local charges, local magnetic moments and local densities of states on individual atoms. The spin-dependent interfacial properties will be discussed in relation to spin-dependent transport in organics-based MTJs.

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Date submitted: 30 Nov 2005

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