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Theoretical study of molecule mediated spin-polarized electron tunneling between magnetic materials HAIYING HE, RAVINDRA PANDEY, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRD-ARL-WM; Aberdeen Proving Ground, MD 21005-5069 — There has been a recent interest in organic molecule-mediated spin-polarized electron transport with a potential application in molecular-scale spintronics. In this presentation, we present the results of a theoretical study on the spin-dependent electron tunneling via a self-assembled monolayer of σ-bonded bicyclo[2.2.2]octane-1,4-dithiol on Ni(111). Comparison with a similar study involving π-conjugated molecules, suggests that the magnitude of the tunnel current and the spin-dependent current are strongly influenced by the nature of chemical bonds in the molecular structure. It gives further understanding of the role of the organic molecules on the spin-polarization of electron transport and provides a basic guideline in choice of molecules in this respect.

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