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Spin Polarized Electron Transport in a Magnetically Coupled Molecular Wire L. SENAPATI, J. SCHRIER, K. B. WHALEY, Department of Chemistry and Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720-1460, USA — Nanostructured materials present new opportunities for spintronics and for coherent applications such as quantum information processing. In order to make progress in these areas, new materials that are optimized for spin transfer are required. We will present theoretical studies of electronic structure and transport in magnetically coupled bridging molecules that reveal how coherent spin transport between nanostructures may be enhanced by suitable molecular design. We will present a study on a bridge consisting of two molecules coupled by a vanadium atom and sandwiched by two magnetic contacts (Ni) at both ends. Our first-principles density functional calculations suggest that by controlling the spin of the vanadium atom, one can control the spin polarized transport through the magnetically coupled molecules. The ground state of the magnetically coupled molecular bridge when sandwiched between similar magnetic cluster contacts at both ends (e.g. magnetic clusters such as Ni), prefers anti-parallel to parallel spin configurations. Control of the vanadium spin could be implemented by magnetic STM tips. The large difference in resistance between the two spin configuration states of such a system could be used to make GMR like devices.

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