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Molecular Spintronics: Theory of Spin-Dependent Electron Transport Between Iron Nano-Contacts Bridged by Organic Molecules and Fe Atomic Chains* HUGH DALGLEISH, GEORGE KIRCZENOW, Department of Physics, Simon Fraser University, Burnaby, BC, Canada, V5A 1S6 — Recent experiments [1] have lent support to theoretical predictions [2] that organic molecules connecting nickel nano-contacts may exhibit magneto-resistance and spin-valve effects. Here we present predictions of spintronic phenomena in another class of ferromagnetic nano-systems: Fe nano-contacts bridged by single conducting or insulating molecules or chains of Fe atoms. Models are constructed based on semi-empirical considerations, the known electronic structure of bulk Fe and ab initio density functional calculations. Using Lippmann-Schwinger and Green's function techniques, and Landauer theory, significant magneto-resistance is predicted in these systems. Under appropriate conditions, novel device characteristics such as negative magneto-resistance are also predicted to emerge.

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1 J. R. Petta et al., Phys. Rev. Lett. 93, 136601 (2004).
2 E. G. Emberly and G. Kirczenow, Chem. Phys. 281, 311 (2002); R. Pati, et al., Phys. Rev. B 68, 100407 (2003).

Hugh Dalgleish
Simon Fraser University

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