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Organometallic Spintronics: Dicobaltocene Switch RUI LUI, SAN-HUANG KE, WEITAO YANG, HAROLD BARANGER, Duke University — We propose a spintronic switch formed from a single molecule containing two cobaltocene complexes. Spin-dependent transport has been investigated, using first-principles density functional theory and the non-equilibrium Green function method. By switching the dicobaltocene system between singlet and triplet states, our calculations reveal that the spin antiparallel configuration blocks electron transport in the vicinity of the Fermi energy, while the spin parallel configuration enables much higher current through the lead-molecule-lead junction. We find that the energy difference between the ground state (antiparallel) and the excited state (parallel) is a function of the length of insulating spacer separating the two spins residing in the cobaltocenes; this implies that the switching functionality can be realized by applying a moderate magnetic field. This work was supported in part by the NSF (DMR-0103003).

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