

Abstract Submitted
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Size-dependent alternation of magnetoresistive properties in atomic chains¹ R. TUGRUL SENGER, ENGIN DURGUN, HALDUN SEVINCLI, Bilkent University, HATEM MEHREZ, SALIM CIRACI, Bilkent University — Spin-polarized electronic and transport properties of carbon atomic chains are investigated when they are capped with transition-metal (TM) atoms like Cr or Co, using density functional theory. The magnetic ground state of the TM-C_n-TM chains alternates between the ferromagnetic (F) and antiferromagnetic (AF) spin configurations as a function of n . The desirable AF state is obtained for only even- n chains with Cr; conversely only odd- n chains with Co have AF ground states. We present a simple model that can successfully simulate these variations, and the induced magnetic moments on the carbon atoms. Depending on the relative strengths of the spin-dependent couplings and the on-site energies of the TM atoms there induces long-range spin polarizations on the carbon atoms which mediate the exchange interaction. When connected to appropriate electrodes these atomic chains display a strong spin-valve effect. Analysis of electronic and magnetic properties of these atomic chains, and the indirect exchange coupling of the TM atoms through carbon chain will be presented. ¹E. Durgun *et al.*, J. Chem. Phys. **125**, 121102 (2006). ²E. Durgun *et al.*, Phys. Rev. B **74** (*in press*).

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