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TITLE: Spin-dependent properties of atomic chains

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ABSTRACT:

Half-metallic materials, which possess perfect spin polarization at the Fermi energy, are of interest in view of spintronics (spin-dependent electronics) applications. Using first principles calculations we predict that periodic compound atomic chains composed of carbon and transition metal (TM) atoms have half metallic properties. Finite segments of such chains show interesting magnetic and transport properties. The indirect exchange interaction of the TM atoms through the carbon atomic chain leads to periodic alternations in the magnetic ground state of the molecule. When connected to appropriate metallic electrodes carbon atomic chains capped with TM atoms act as a spin-valve forming a molecular analog of the giant magneto resistance (GMR) effect.

A brief introduction to spintronics and molecular electronics will be made. Analysis of structural, electronic, and magnetic properties of these atomic chains, as well as a simple model of the indirect exchange coupling of the TM atoms through the non-magnetic carbon atomic chain will be presented.