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Magnetism in 1D Cobalt-Cyclopentadienyl Sandwich Molecular Wire[1] HANNES ALLMAIER, Technical Univ. Graz, AT, C. MORARI, Univ. Catholique Louvain, DICE, Elect, BE, L. CHIONCEL, E. ARRIGONI, Technical Univ. Graz, AT, F. BEIUSEANU, Univ. of Oradea, RO, A. LICHTENSTEIN, Univ. of Hamburg, DE, M. KATSNELSON, Univ. of Nijmegen, NL — A challenge for technological applications at the nanometer scale is to find magnetic materials with reduced dimensionality. Recent theoretical studies have predicted ferromagnetic and half-metallic behavior for the 1D-organometallic benzen vanadium wire. Here we discuss a variety of magnetic orderings such as anti-ferromagnetic and ferrimagnetic half-metallicity in the cobaltocen Co2(C5H5)2 nanowire. We performed DFT-calculations to optimize its geometry and used the NMTO downfolding technique to construct the real-space low energy Hamiltonian. To describe electronic correlations beyond the mean-field, we used the developed Variational Cluster Approach. Our preliminary results show that non-quasiparticle states appear in the half-metallic gap, which reduce considerably the spin polarization of such a wire. Ab-initio electron transport calculations are in progress to establish the role of cobaltocen nanowire as part of a future spin filter.

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