Organometallic Vanadium-Benzene Sandwich Clusters: Perfect Molecular Spin-Filters

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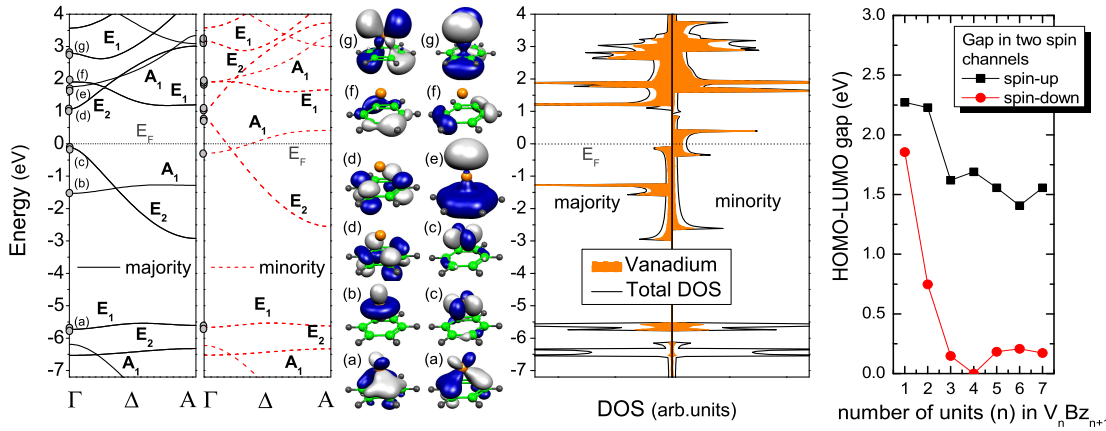
During the last years, molecular magnets have been attracting enormous attention, because they are considered as potential candidates for future applications in high-density information storage and quantum computing. Among such novel systems, we focused on the vanadium-benzene multi-decker sandwich clusters (V_nBz_{n+1}, $Bz=C_6H_6$) consisting of alternating vanadium atoms and benzene rings. The synthesis of the V-Bz clusters was realized up to n=6 during a reaction of laser-vaporized metal atoms with benzene in He atmosphere [1]. Experimental techniques are currently elaborated [2] designed to deposit these molecules from a gas phase onto substrates and to realize novel, two-dimensional composite magnetic materials.

Using density functional theory we have performed theoretical investigations of the electronic properties of a free-standing one-dimensional (1D) organometallic vanadium-benzene wire. We predict that this wire is a *new*, unusual example of a *one-dimensional* half-metallic ferromagnet [3]. It has an integer magnetic moment of $1\mu_B$ per unit cell and a spin-polarized band structure with a finite density of states at the Fermi level for one spin channel and a semiconductor gap for the other (figure below). We found that the half-metallic behaviour is conserved up to 12%, longitudinal elongation of the wire.

We show further more that unusual electronic properties of the infinite 1D wire remain in molecules of finite length (figure, right plot). Because of the HOMO-LUMO gap (~0.2eV) between discrete molecular levels in the minority spin channel is one order of magnitude smaller than the gap in the majority spin channel (~1.5eV), the recently synthesized multidecker vanadium-benzene clusters, when carrying spin-polarized currents, will work as highly effective spin-filters [3]. We confirmed the proposed idea by performing two sets of independent fully *ab initio* transport calculations through the V-Bz clusters connected to Co and Ni fcc (001) electrodes. We have found that the spin-polarization of the electron current approaches 90% that opens a possibility to exploit properties of the considered systems in future *spintronic* devises.



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