Novel Half Metallic Properties observed in Lanthanide Perovskites for Spintronic Applications from First-principles Calculations

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Abstract

Recent researches are focused in search for novel materials essential for spintronic device applications [1-3]. Especially 5d systems are of tremendous interest due to the important role played by spin-orbit coupling (SOC) that generates unconventional properties such as topological insulators and topological superconductors. In general, SOC mixes the spin-up and spin-down bands together, so, the systems with strong SOC may not be suitable as half-metals (HMs). It will be demonstrated that half-metallicity survives for few class of system even under strong SOC.

HMs are a class of materials which are metallic in one spin channel, while insulating in the opposite spin channel due to the asymmetric band structure. HMs can generate spin-polarized currents without any external operation, and thus are very useful for spintronic applications.

Recently, a new material Pr_2MgIrO_6 (PMIO) was synthesized that belongs to the family of double perovskites. PMIO orders antiferromagnetically below T_N (14 K) with a large effective moment [4]. Unlike other perovskites, novel properties are expected due to the presence of Ir and Pr atom in PMIO.

We are exploring the electronic and magnetic properties of both PMIO and Sr-doped PMIO by first-principles density functional theory (DFT). Considering the SOC effect, DFT+*U* calculations are performed using the full-potential WIEN2k code. The ground state magnetic configuration found from our calculation for the parent and Sr-doped (replacement of two Pr by Sr) PMIO are shown in Fig.1. With a Mott-gap of ~0.2 eV opening and large spin magnetization, μ_{eff} = 6 μ_B per unit cell, PMIO is a Mott-Hubbard insulator. PMIO is an interesting material because (i) A site element Pr provides both charge and spin magnetization, as opposed to most of the perovskite materials, and (ii) due to the lattice distortion on IrO_6 octahedra, the spin-up topmost occupied bands lies higher in energy than the spin-down bands which act as a platform for charge transfer when holes are doped. We emphasized that PMIO when doped with holes to the Pr site shows significant change in its electronic and magnetic properties giving rise to novel properties desirable for spintronic applications.

We find that the material $Pr_{(2-x)}Sr_xMgIrO_6$ is HMFiM with μ_{eff} = 3 μ_B and -3 μ_B, at x=0.5 and 1.5 respectively. Upon half-replacement of Pr by Sr atoms (i.e. at x=1) as shown in Fig.1 (b), HMAFM is achieved for which the effective moment compensates to zero with full-spin polarization at the Fermi-level. The interplay between U and SOC plays important role in this material. HMAFM survives even under SOC effect due to the large exchange splitting. To the best of our knowledge, this is the first prediction of HMAFM with sizable SOC.

References:

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Figures

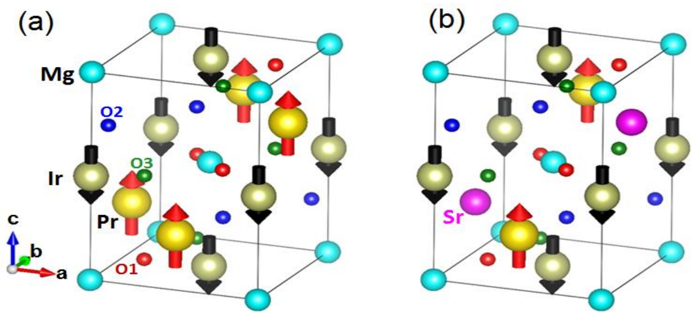

Fig. 1: Ground state crystal and magnetic structures of (a) Pr_2MgIrO_6 and (b) $PrSrMgIrO_6$ with *c* as easy axis. Arrow indicates the spin-direction of Pr (red) and Ir (black) along the easy axis.