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Magnetic instability in heavily n-doped Fe-based full Heusler compounds: Origin and impact on thermoelectric properties

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Fe_2YZ full Heusler compounds, on which first principles on density functional theory (DFT) simulations predict very large thermoelectric power factor (PF), are promising candidates for thermoelectric applications. The building blocks of their interesting thermoelectric properties are the carriers belonging to the Fe-eg orbitals that can be opportunely engineered to maximize PF. These anti-bonding states are represented by a flat band (mainly composed of Fe dx^2-y^2 character) along the ΓX direction of the Brillouin Zone, related to the highly directional Fe-Fe bond, becoming dispersive along the other directions. This band satisfies the "flat-and-dispersive" requirements proposed by Mahan and Sofo and leads to one-dimensional transport strongly enhancing the PF. However, due to its strongly localized nature, explicit n-doping may induce a Stoner instability driving the system to a half-metallic phase. The present study, performed through DFT using both hybrid functional and GGA+U methods on $Fe_2YZ_{1-x}A_x$ (Y = Ti, V, Nb, Ta, Z=Al, Si, Sn, Ga and A=Si, P, Sb, Ge) n-doped systems, shows that the appearance of such a magnetic phase is strictly linked to the Fe-eg and Y-site eg orbital hybridization and that it possesses a pure electronic origin, independent on the dopant species. Although the Stoner instability can provide half-metallicity with coupled thermomagnetic responses, the PF is typically reduced in the half-metallic phase due to a reduction of the number of carriers available at the Fermi level. In certain cases, however, the values of the PF are still large (for $Fe_2TaGa_{1-x}Ge_x$ or $Fe_2TiSi_{1-x}P_x$ PF is between 9 and 15 10^{-3} W K^{-2} m^{-1} at 600 K, for example) which stays promising for thermoelectric applications. Going further, we elucidate the possibility to exploit the broader nature of 4d and 5d orbitals at the bottom of the conduction band to overcome the magnetic phase appearance in the doping range of interest.

Biography

Fabio Ricci did his PhD on both simulations and experimental measurements on magnetic properties of materials (diluted magnetic semiconductors and soft magnetic materials) by means of the magneto-optical Kerr effect. Subsequently, he worked on theoretical simulations on Fe-based superconductors, principally iron-chalcogenides. He developed and implemented in the ABINIT code the formalism for the non-collinear magnetism in the density functional perturbation theory and, at the same time, started to work on the theoretical engineering of thermoelectric properties of the Fe-based full-Heusler compounds.

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