Two-Dimensional CrFe-Based Half-Metallic Antiferromagnets

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We report that the substitution of Cr ions for half of Fe ions in Fe-based superconductors such as LaFeAsO, SrFeAsF, and FeSe produces quasi-two-dimensional (2D) half-metallic (HM) antiferromagnets (AFMs),[1] or fully compensated half-metallic ferrimagnets, that have no net magnetization, yet 100% spin polarization of the conduction electrons. Using a full-potential augmented plane wave method within density functional theory, we find ordered (striped or checkerboard) structures in the $CrFeAs_2$ and $CrFeSe_2$ 2D planes commonly half-metallic in the normal ground state, where two component magnetic ions in a unit cell have antialigned local moments that cancel exactly because of the integer filling of an insulating channel. With stiff spacer layers such as LaO and SrF, the $CrFeAs_2$ layers show HM-AFM behavior in both striped and checkerboard phases, whereas the spacer-free $CrFeSe_2$ layers become semi-metallic in the striped phase, being degraded by orthorhombic distortion. The checkerboard phase is energetically favored over the striped phase. Despite the absence of inversion symmetry in the checkerboard phase, spin-orbit coupling of spin-polarized conduction electrons shows little effect on the half-metallicity.

[1]Masao Nakao, J. Phys.: Conf. Series **150**, 052182 (2009).