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Ferroelectric polarization in the magnetic world

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Switchable spontaneous polarization in ferroelectrics is produced by a structural distortion of a high-symmetry reference phase which lowers the symmetry to a polar space group. Under certain conditions, this structural distortion and symmetry breaking can also induce ferromagnetism and other changes, such as a metal-insulator transition, allowing the possibility of electric and magnetic field control. In this talk, I will present first-principles illustrations of specific materials realizations of the rich variety of this behavior in magnetic perovskite oxides, identified using a database of first-principles calculations of the full phonon dispersions of a range of magnetic perovskites, including the d3 compounds SrMnO3and SrCaO3, the d5 compounds BiFeO3, and the series SrMO3 (M= V, Cr, Mn, Fe, Co). First, I will discuss an epitaxial-strain-induced multiferroic phase produced by large spin-phonon coupling in SrMnO3 [1]. Then, I will turn to colossal magnetoresistance based on a ferromagnetic- metal/antiferromagnetic-ferroelectric phase boundary with epitaxial strain in SrCoO3, which exhibits typical ferromagnetic metallic character in room-temperature but with a large spin-phonon coupling by which antiferromagnetic ordering favors a polar distortion. Lastly, I will discuss the identification of perovskite superlattice systems in which the symmetry lowering produced layer-by-layer ordering produces a phase with ferroelectrically-induced weak ferromagnetism. I will present first-principles calculations demonstrating these behaviors in BaMnO3/SrMnO3 superlattices and other systems which could provide robust experimental realizations.

[1] J. H. Lee and K. M. Rabe, "Epitaxial-strain-induced multiferroicity in SrMnO3 from first principles," Phys. Rev. Lett. 104, 207204 (2010)