Materials Science and Technology Division
Materials Theory Group

" Revealing new phases from old oxides via spin-lattice coupling"

Jun Hee Lee
Princeton University

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Abstract

Competitive interactions between spins, superexchange (*J*) vs. Dzyaloshinskii-Moriya (*D*), are also strongly coupled to various lattice distortions in complex oxides [1]. First, I will talk about how to induce drastic phase transitions by altering *J*, the major magnetic interaction, via its coupling to lattice distortions such as ferroelectric [2,3] or Jahn-Teller [4]. Second, although *D* is weak compared to *J*, it is correlated to inversion symmetry breaking. Through symmetry analysis, I will discuss how to design non-zero net magnetic moments switchable by electric-field in oxide superlattices such as $BiFeO_3/LaFeO_3$ via the coupling of *D* to antiferrodistortive rotation, the most ubiquitous distortion in oxides. Overall, I will highlight the importance of microscopic understanding of the coupling of *J* and *D* to various lattice distortions to reveal hidden phases and maximize functional properties in magnetic oxides.

[1] *"Large spin-phonon coupling and magnetically induced phonon anisotropy in $SrMO_3$ perovskites (M=V,Cr,Mn,Fe,Co)"*, J. H. Lee and K. Rabe, PRB **84**, 104440 (2011).
[2] "*Epitaxial-Strain-Induced Multiferroicity in $SrMnO_3$ from First Principles*", J. H. Lee and K. Rabe, PRL **104**, 207204 (2010).
[3] "*Coupled Magnetic-Ferroelectric Metal-Insulator Transition in Epitaxially Strained $SrCoO_3$ from first principles*", J. H. Lee and K. Rabe, PRL **107**, 067601 (2011).
[4] "*Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially-strained orthorhombic $LaMnO_3$*", J. H. Lee *et al.*, (In preparation).

Host: Randy Fishman (574-5786, fishmanrs@ornl.gov)