MAR06-2005-001533

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Spin-lattice coupling from first principles

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The hexagonal manganites are a class of multiferroic materials that are simultaneously ferroelectric and antiferromagnetic, in which many physically interesting and potentially technologically relevant manifestations of spin-lattice coupling have been observed. Chromium spinels such as $ZnCr_2O_4$ and $CdCr_2S_4$ are antiferromagnetic and ferromagnetic insulators respectively, each displaying a differrent manifestation of a spin-lattice effect. In $ZnCr_2O_4$ a large magnetically induced phonon anisotropy has been observed while mode-dependant phonon anomalies have been measured in $CdCr_2S_4$. With the continuing advances in theoretical algorithms such as the LSDA+U method and in computational power it is now possible to study structurally and magnetically complex solids such as these using density-functional first-principles methods. Here, I describe a first-principles approach to study the influence of magnetic order on the phonons and dielectric properties of $YMnO_3$, $ZnCr_2O_4$, and $CdCr_2S_4$, our ongoing investigation of the coupling between the magnetic order and polarization in hexagonal manganites, and the search for ferroelectric behaviour in the simple ferromagnet $CdCr_2S_4$.