Spin-Lattice Coupling and Third Neighbor Magnetic Interactions in EuTiO₃

TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — An ongoing challenge in materials physics is to identify materials that display a strong coupling between the electrical polarization and magnetism. EuTiO₃ is one such material that has been of much recent interest. This novel material is antiferromagnetic and paraelectric in bulk but becomes simultaneously ferromagnetic and ferroelectric under biaxial strain due to a rather large spin-lattice (phonon) coupling. In this talk we will present the results of our first-principles study on the effect of ferroelectric distortions and octahedral rotations on the magnetic exchange interactions in EuTiO₃. We elucidate the evolution of the octahedral rotation pattern with strain and show how they influence the properties of the multiferroic phase. Going beyond the proposed cation-mediated exchange for EuTiO₃, which has been linked to the large spin-lattice coupling in this material, we uncover the importance of third-neighbor magnetic interactions and illustrate how it is responsible for the “giant” cross-field magnetoelectric effect recently demonstrated.

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