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Spin-Lattice Coupling and Third Neighbor Magnetic Interactions in EuTiO_3 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. EuTiO_3 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 EuTiO_3 . 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 EuTiO_3 , 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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