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Strain induced magnetization reversal in Ba_2IrO_4 via strong orbital-lattice coupling CHOONG H. KIM, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — We have studied from first principles the structural, electronic, and magnetic properties of the layered-perovskite iridate Ba2IrO4 as a function of epitaxial strain. In contrary to what is usually assumed, we find within density functional theory that the ground state structure displays oxygen octahedra rotations ($\sim 6^\circ$ about the c-axis). This leads to a canting of the nominally antiferromagnetic moments. It turns out that the magnitude and direction of the orbital moment canting, which is in the opposite direction to the spin canting moment, can be controlled with strain. This leads to a situation in which the total magnetization can be tuned and in fact be reversed with strain. Our observations highlight a difficulty with describing magnetism in Ba_2IrO_4 within a simple effective j_{eff}-spin Hamiltonian.

Choong H. Kim
School of Applied and Engineering Physics, Cornell University

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