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Epitaxial strain-mediated spin-state transitions: can we switch off magnetism? JAMES RONDINELLI, NICOLA SPALDIN, Materials Dept., UC Santa Barbara, MATERIALS RESEARCH LABORATORY COLLABORATION — We use first-principles density functional theory calculations to explore spin-state transitions in epitaxially strained $LaCoO_3$. While high-spin to low-spin state transitions in minerals are common in geophysics, where pressures can reach over 200 GPa, we explore whether heteroepitaxial strain can achieve similar transitions with moderate strain in thin films. $LaCoO_3$ is known to undergo a low-spin (S=0, $t_{2g}^6 e_g^0$) to intermediate-spin (S=1, $t_{2g}^5 e_g^1$) or high-spin (S=2, $t_{2g}^4 e_g^2$) state transition with increasing temperature, and thus makes it a promising candidate material for strain-mediated spin transitions. Here we discuss the physics of the low-spin transition and changes in the electronic structure of $LaCoO_3$, most notably, the metal-insulator transition that accompanies the spin-state transitions with epitaxial strain. As thin film growth techniques continue to reach atomic-level precision, we suggest this is another approach for controlling magnetism in complex oxide heterostructures.

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