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Spin state disproportionation and ferromagnetism in strained LaCoO3: Ab-initio study SEO HOSUNG, ALEXANDER DEMKOV, Department of Physics, The University of Texas at Austin — Strain engineering of artificial oxide heterostructures opens up routes for the creation of novel electronic phases that do not exist in the bulk. To fully exploit the functionalities of the oxide, understanding its electronic and structural response to epitaxial strain is crucial. One example is the recent demonstration of biaxial tensile strain stabilizing an insulating ferromagnetic ground state in normally non-magnetic LaCoO3. However, theoretical understanding is incomplete. In this talk, using the LSDA+U method we discuss the origin of strain induced transition to insulating ferromagnetic ground state in LaCoO3. We show that beyond biaxial tensile strain of 2.5% local magnetic moments, originating from high spin state of Co3+, emerge in low spin Co3+ matrix. We further show that these local moments are ferromagnetically coupled via superexchange interaction. In contrast, we find that compressive strain by itself is not able to stabilize a magnetic state, that agrees with recent experiment. Ferromagnetism found in tensile-strained LaCoO3 is tightly coupled to the material's orbital and structural response to applied strain. We discuss how LaCoO3 accommodates tensile strain via spin state disproportionation, resulting in an unusual sublattice structure.

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