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Strain and the Metal Insulator Transition in bulk and thin film Ca_2RuO_4[1] QIANG HAN, ANDREW MILLIS, Columbia Univ — The experiments done by J.P.Ruf et.al show that the multi-orbital Mott insulating ground state of bulk Ca2RuO4 can be suppressed (enhanced) in thin films under biaxial compressive (tensile) strain. In this paper, DFT+DMFT, DFT+U methods are used to study the strain dependence of the metal insulator phase transition in bulk and thin-film Ca_2RuO_4. The interplay between bulk strain, substrate pinning of in-plane lattice constants, octahedral distortions and the metal-insulator transition leads to a strain contribution to the energetics of the first order metal-insulator transition which is substantially amplified in films relative to bulk. Comparison to recent data is presented, and generalization of the theory to other transition metal oxides is discussed.

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