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**The electronic structure of epitaxially strained iridate thin films and superlattices from first principles** JOHANNES VOSS, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, NY — Within the Ruddlesden-Popper iridates $Sr_{n+1}Ir_nO_{3n+1}$, strong spin-orbit interactions lead to the formation of a half-filled, narrow $J_{\text{eff}} = 1/2$ band and filled $J_{\text{eff}} = 3/2$ bands. This places the iridates in the vicinity of a Mott transition, which is sensitive to perturbations in crystal structure, despite relatively weak on-site Coulomb interactions [1]. For example, $Sr_2IrO_4$ ($n = 1$) is an antiferromagnetic Mott insulator that displays an almost rigid coupling between spin canting and $IrO_6$ octahedron rotations [2], while epitaxially stabilized $SrIrO_3$ ($n = \infty$) is a correlated metal. In this talk, we will discuss from first-principles within the LDA+SO+$U$ approach the possibility to engineer the electronic structure of $SrIrO_3$ and $CaIrO_3$ thin films using epitaxial strain and by creating superlattices of the form $(AIrO_3)_m(A'BO_3)_{m'}$ with $A$, $A'$ = Ca, Sr. [1] S.J. Moon, H. Jin, K.W. Kim, W.S. Choi, Y.S. Lee, J. Yu, G. Cao, A. Sumi, H. Funakubo, C. Bernhard, and T.W. Noh, PRL 101, 226402 (2008). [2] B.J. Kim, H. Jin, S.J. Moon, J.-Y. Kim, B.-G. Park, C.S. Leem, J. Yu, T.W. Noh, C. Kim, S.-J. Oh, J.-H. Park, V. Durairaj, G. Cao, and E. Rotenberg, PRL 101, 076402 (2008).

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