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\(_n\)O\(_{3n+1}\), 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\(_2\)IrO\(_4\) \((n = 1)\) 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 \((A\text{IrO}_3)_m(A'\text{BO}_3)_{m'}\) with \(A, A' = \text{Ca, Sr}\). [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).