Interplay of oxygen octahedral rotations and electronic instabilities in strontium ruthenate Ruddlesden-Poppers from first principles

JOHANNES VOSS, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University, Ithaca, NY — The Ruddlesden-Popper ruthenates $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n+1}$ display a broad range of electronic phases including $p$-wave superconductivity, electronic nematicity, and ferromagnetism. Elucidating the role of the number of perovskite blocks, $n$, in the realization of these differently ordered electronic states remains a challenge. Additionally, dramatic experimental advances now enable the atomic scale growth of these complex oxide thin films on a variety of substrates coherently, allowing for the application of tunable epitaxial strain and subsequently the ability to control structural distortions such as oxygen octahedral rotations. Here we investigate from first principles the effect of oxygen octahedral rotations on the electronic structure of $\text{Sr}_2\text{RuO}_4$ and $\text{Sr}_3\text{Ru}_2\text{O}_7$. We discuss possible implications for the physics of the bulk systems and point towards new effects in thin films.

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