

Abstract Submitted
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Understanding the A-Cation Order Dependent Band Gap Variation in Ruddlesden-Popper Oxides¹ YONGJIN SHIN, JAMES RONDINELLI, Northwestern Univ — Many atomically layered oxide superlattice are constructed from three-dimensionally connected bulk perovskites. Here we examine the electronic structure of quasi-two-dimensional Ruddlesden-Popper (RP) oxides, focusing on (LaSr)AlO₄ and changes induced by A cation order. The partial connectivity of perovskite layers enables the structure to distort without tilting or further symmetry reduction. It also provides opportunities to tune the Coulomb interactions between adjacent atomic AO layers that produce internal electric fields. Indeed, an aluminate RP superlattice was recently predicted to show massive band gap variations, up to 200%, depending on the A cation ordering using first-principles electronic structure calculations. Here we extend this concept to a greater number cation ordered variants, showing that longer period arrangements of the monoxide planes lead to greater control over the band gap and even its full collapse, i.e., metal-insulator transition, using density functional theory calculations. We conclude by summarizing our findings into a set of working principles for band gap control in layered oxides without chemical doping or changes in cation stoichiometry.

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