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Band gap engineering *via* electrostatic chemical strain in cation ordered LaSrAlO₄¹ PRASANNA V. BALACHANDRAN, JAMES M. RONDINELLI, Drexel University, Philadelphia, PA, USA — In this work, we employ density functional theory to examine a novel design route that employs A-site cation ordering to engineer the band gaps of (A,A')BO₄ Ruddlesden-Popper (RP) oxides. Using LaSrAlO₄ as a model material, we show that the band gap is highly sensitive to the A-site cation ordering ranging from 3-4.5 eV. When the [AlO₂]⁻¹ layers are interleaved between two chemically equivalent [LaO]¹⁺ or [SrO]⁰⁺ layers, we obtain the smallest band gap with a reduction of ~1 eV determined from the Heyd, Scuseria, and Ernzerhof (HSE) hybrid exchange-correlation functional. We relate the observed band gap reduction to the local bond distortions arising from electrostatic chemical strain induced changes to the O 2*p* and La 5*d* states in the valence and conduction bands, respectively.

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