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Formulation of predictive models for use in first principles design of non-centrosymmetric perovskite oxides JOSHUA YOUNG, JAMES RONDINELLI, Drexel University — Because many useful electronic properties such as ferroelectricity arise solely due to the lack of inversion in a material's crystal structure, predictive microscopic models describing how to deterministically remove this symmetry operation can allow for the rapid identification and design of new polar compounds. By understanding how structural distortions influence the connectivity between oxygen polyhedra in solid state oxides, we elucidate a series of geometric design rules necessary to develop polar materials. We then apply these criteria to the family of ABO_3 perovskite oxides by systematically investigating how distortions of the corner-connected BO_6 polyhedral network influence the A-site environments, resulting in a detailed description of the octahedral rotation patterns and A- and B-site cation ordering arrangements capable of producing centrosymmetric, polar, and enantiomorphic structures. Using this as a guide, we then show how such a method allows for the targeted design of new non-centrosymmetric oxides. We conclude by using these rules in combination with density functional theory calculations to predict a series of rhombohedral $(A,A')B_2O_6$ perovskites displaying electric polarizations in their ground state.

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