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Nanoscale design routes to polar oxides JOSHUA YOUNG, JAMES RONDINELLI, Drexel University — Many useful material properties, such as ferroelectricity, arise because of inversion symmetry breaking in a material's ground state. Understanding how to purposefully lift spacial parity operations is critical to engineering compounds with 'acentric' properties. Using first-principles density functional calculations, we describe the crystal-chemistry criteria necessary to design artificial nanoscale oxides that display spontaneous polarizations using non-polar metal-oxygen polyhedra. By controlling the flavor of A-site cation ordering in $AA'B_2O_6$ perovskites, we show that spontaneous electric polarizations comparable in magnitude to conventional ferroelectrics are attainable. We conclude by explaining how the criteria can be extended to other material classes to realize polar oxides by design.

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