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Engineering polar perovskites from centric polyhedra building blocks JAMES RONDINELLI, Drexel University, CRAIG FENNIE, Cornell University — Increasing demands for electric field-tunable electromagnetic (EM) materials has renewed interests in ferroelectricity and its coupling to EM properties in perovskite oxides. Using density functional computations combined with group theoretical methods, we detail the crystal-chemistry criteria that enable the rational design of new perovskite oxides displaying octahedral rotation-induced ferroelectricity—electric polarizations (P) without second-order Jahn-Teller cations from $B\mathrm{O}_6$ building blocks. We show that interleaving two bulk perovskites to form an ordered and layered arrangement of A-site cations [chemical composition $(A, A')B_2\mathrm{O}_6$] produces a new trilinear free energy term coupling $B\mathrm{O}_6$ rotations to P. This symmetry rule combined with an energetic condition, describing the lattice dynamical properties of the bulk materials, enables the routine design of synthetic ferroelectric perovskites. We illustrate these guidelines and achieve sizeable electric polarizations in layered gallate and aluminate perovskites, i.e. bulk materials with no tendencies to ferroelectricity. Finally, we argue that this strategy could be exploited for the design of ferroelectricity in a variety of crystal classes exhibiting flexible cation–anion polyhedral frameworks.

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