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Interplay of octahedral distortions in electronic and structural phase transitions in ABO_3 perovskites[1] PRASANNA V. BALACHANDRAN, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104 — In this work, we investigate group-subgroup relationships afforded to ABO_3 perovskites from combinations of BO_6 distortions – bond stretching and bond angle rotations – with the objective of identifying new pathways for tuning their properties through electron-lattice interactions. Using nickelate and bismuthate perovskite compounds as a template, we decompose their low-symmetry structures into orthonormal symmetry-breaking lattice modes of the parent cubic space group. Statistical analysis of mode decomposition data uncovers previously unappreciated relationships between microscopic octahedral distortion modes and macroscopic physical properties. Finally, we propose novel crystal engineering strategies to study perovskites near phase boundaries that are otherwise extremely difficult to probe experimentally.

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