

Exploring the Structures and Properties of Complex Oxides: New Ideas and Insights from Theory and Simulation

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Perovskite oxides are perhaps the most widely studied and technologically important of all the ABO_3 phases. The remarkable versatility of the perovskite structure (the A and B site can accommodate nearly every element of the periodic table) leads to a huge range of properties, including (but not limited to) ferroelectricity, ferromagnetism and colossal magnetoresistance, piezoelectricity, multiferroicity and metal-insulator transitions. One reason for this is that nearly all cubic perovskites are unstable to energy-lowering structural distortions and hence typically have rich structural phase diagrams. The most common distortions are those that give rise to ferroelectricity (usually an off-centering of the B-site cation) and tilts or rotations of the BO_6 octahedra. We have explored the interaction between these distortions in perovskites using symmetry principles, crystal chemistry arguments and first-principles calculations. Our results revealed some counter-intuitive surprises, including that rotations by themselves do not generally suppress ferroelectricity in perovskites, as is commonly assumed. I will discuss how the knowledge and new insights gained in the course of our investigations can be used to search for and design new functional materials.