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

Nicole A. Benedek

Materials Science and Engineering Program, The University of Texas at Austin

Austin, Texas, USA

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.