Investigating Local Structure of Complex Oxides

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The perovskite solid solutions $A(B_xB'_{1-x})O_3$ are multicomponent oxides with great industrial importance, and they offer a series of fundamental challenges. The local displacements of the atoms in each unit cell and the ordering of the B and B′ cations can exhibit varying degrees of order, leading to structures which defy simple description. In addition, these systems can exhibit structural defects, including chemical inhomogeneity, ferroelectric domains, oxygen vacancies, and grain boundaries.

The observed overall symmetry provides important clues concerning the underlying structure, but symmetry masks many of the important structural features. Experimental techniques, including X-ray and neutron scattering and surface probes, provide additional insights into the structure. However, in many cases this information is insufficient to elucidate all the salient structural features.

I will present our first-principles investigations into the structure of PZT, $Pb(Zr_xTi_{1-x})O_3$. Using density functional theory calculations, we will compare symmetry-constrained and unconstrained structures, and examine the effects of lattice strain and unit cell size on the computed structures. The predicted low-energy structures will be placed in the context of known experimental evidence, and the discrepancies will be discussed.

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