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David Adler Lectureship Award Talk: Lattice instabilities and ferroelectricity in complex oxides

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In perovskite oxides, layered perovskites and other complex-structured oxide families, a wide variety of distorted equilibrium structures can be realized, including ferroelectric, antiferroelectric, antiferrodistortive, and mixed-character structures. For an individual material, the equilibrium structure can be understood as being produced by the freezing-in of one or more lattice instabilities of an appropriate high-symmetry reference structure; this concept is central to the long-established soft-mode theory of ferroelectricity. In fact, first-principles phonon-dispersion calculations show that the high-symmetry reference structures of many complex oxides have entire ranges of instabilities that do not contribute to the bulk ground state structure. In this talk, we discuss how the information from first-principles studies of these systems provides guidance for altering the balance of the competition of instabilities of different character through changes in electrical and mechanical boundary conditions characteristic of epitaxial thin films, superlattices, and nanoparticles, leading to the realization of non-bulk phases. For example, it has been shown both theoretically and experimentally that $SrTiO_3$, which has a nonpolar bulk ground state, can be driven ferroelectric by epitaxial strain. To illustrate the further development and application of these ideas, we present results for $CaTiO_3$ and discuss other materials which, while nonpolar in bulk, can be driven in this way through a phase boundary to become ferroelectric. New ferroelectrics thus obtained could have combinations of tunable properties, including switchable polarization, magnetic ordering, and dielectric and piezoelectric response, desirable for current and future technological applications.