Designing materials with switchable polarizations by artificial structuring

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In this talk, I will start with introducing the general notion of emergent symmetry breaking in condensed matter systems in which the symmetry of the ground-state wavefunction is spontaneously broken with examples exhibiting such symmetry breakings in simple systems. Then, I discuss a particular case in detail regarding the identification of systems with broken inversion symmetry and a new design principle to identify the switchable polar materials by combining charge-ordering and superlattice layering. As the demonstration of the proposed design principle, we use density functional theory to study the effect of artificial structuring on mixed-valence solid-solution $La_{1/3}Sr_{2/3}FeO_3$ (LSFO), a system well-studied experimentally. Our calculations show that A-site (111)-layered LSFO exhibits a ferroelectric charge-ordered phase in which inversion symmetry is broken by changing the registry of the charge order with respect to the superlattice layering. Our calculations reveal that the artificial structuring of LSFO and other mixed-valence oxides with robust charge ordering in the solid solution phase can lead to charge-order-induced ferroelectricity.