Designing materials with switchable polarizations by artificial structuring

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In this talk, I first introduce the 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. Then, a case regarding the broken inversion symmetry is discussed with a new design principle to fabricate an artificial polar material by combining charge-ordering and superlattice layering. As the demonstration of the proposed design principle, I discuss the artificial structuring of the experimentally reported mixed-valence solid-solution $La_{1/3}Sr_{2/3}FeO_3$ (LSFO). Our density functional theory calculations show that A-site (111)-layered LSFO exhibits a ferroelectric charge-ordered phase in which the inversion symmetry breaking is induced 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.