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In pursuit of strongly coupled multiferroic oxides

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The rational design of new materials with emergent properties is a riveting challenge today in materials physics. It begins with understanding a mechanism to control the interplay between diverse microscopic degrees of freedom in order to create targeted macroscopic phenomena and ends with the discovery or design of new material realizations. When combined with first-principles density-functional theory, this approach provides an efficient strategy to survey the vast space of possible materials to target for synthesis. In this talk I will discuss our recently proposed strategies to identify new multiferroics oxides in which magnetism not only coexists with but also is strongly coupled to ferroelectricity. In one case the interplay of spins, optical phonons, and strain leads to a competition between different ordered states producing a colossal magnetoelectric effect. In a second case, a ferroelectric distortion can be designed to induce weak-ferromagnetism facilitating the electric-field control of a switchable magnetization. We also present first-principles density-functional calculations for several potential realizations.