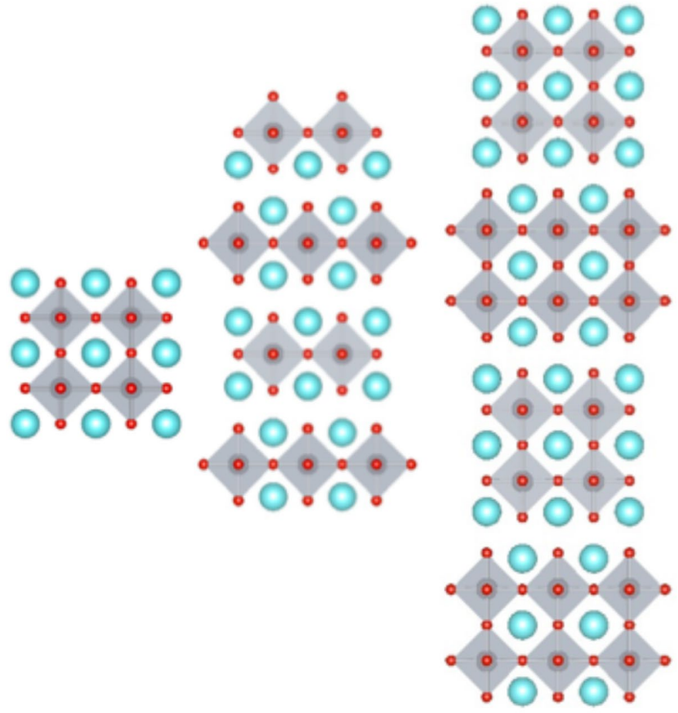
Physics Colloquium

Dr. Elizabeth Nowadnick, University of California Merced

Ferroelectricity and piezoelectricity in perovskite oxides: perspectives from theory and computation

ABSTRACT

Ferroelectric and piezoelectric materials display many fascinating properties related to their phase transitions and electrical polarization, and find applications in areas such as capacitor dielectrics, ultrasound, and computer logic and memory devices. Many ferroelectric and piezoelectric materials are members of the ABO_3 perovskite family of materials. The versatile structural motifs and lattice distortions in perovskite oxides facilitate highly tunable local atomic environments, which can be tuned to realize a range of electronic, magnetic, and other properties. In this talk, I will discuss how theory and first-principles computations can be used to understand and design novel ferroelectric/piezoelectric properties in perovskites. As a first example, I will discuss ferroelectric oxides hosting dilute concentrations of magnetic dopants as a platform for electric field control of single spins, which is desirable for information processing applications. Here, the local crystal field of a magnetic dopant, via spin-orbit coupling, determines the dopant's magnetic anisotropy energy, and hence its preferred spin orientation. As a second example, I will show how some Ruddlesden-Popper phases, where perovskite layers interleave with other structural units, can host a novel form of piezoelectricity where the material expands or contracts in all directions under an applied electric field. I will briefly comment on future research directions arising from these results.



Perovskite and layered perovskite crystal structures

3:00-4:00 p.m., Friday, September 19th, 2025

In-person in McLane Hall 162