Abstract:
Despite ever-improving computing efficiency, energy use by information technology applications such as artificial intelligence is growing rapidly. In order to address this energy challenge and develop the next generation of microelectronics, a rethinking of how computing is performed is needed. One pathway towards highly efficient computing is to introduce novel materials that can be operated at voltages much lower than those in use today. In this context, ferroelectric oxides are one family of materials of interest. A ferroelectric material exhibits a spontaneous electrical polarization which can be reversed in direction by applying an electric field, thus the two polarization directions encode two states and can be applied in logic and memory devices. In this talk, I will discuss how theory combined with computer modeling of the quantum mechanical properties of materials can be used to understand key properties of ferroelectric oxides, such as the amount of energy needed to reverse the polarization (the ‘switching energy’). In particular, I will present some of my research group’s recent work on the switching energy and atomic-scale mechanism of polarization reversal in a family of layered perovskite oxide ferroelectrics. I also will discuss how novel functionalities can arise when ferroelectricity is combined with other ordered states (such as magnetism) in materials, and comment on future open research questions in this field.