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Novel Functionalities in Switchable Polar Materials from First Principles[1]

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First-principles methods have proved over recent years to be an increasingly powerful tool for the design and discovery of new materials with functional behavior driven by applied electric fields and stress. Systems of particular interest are piezoelectrics, ferroelectrics, antiferroelectrics, and materials with electric-field- or stress-controlled magnetic, optical, transport and topological properties. In this talk, I will present examples illustrating several current research directions, including (1) identification of new functional materials characterized by symmetry-inequivalent competing low-energy states, including antiferroelectrics, double ferroelectrics, and "fraternal-twin" ferroelectrics, and (2) investigation of the rich physics of ferroelectrics with free carriers, including leaky ferroelectrics, doped ferroelectrics, and electric-field-switchable polar metals. Interaction with experimental groups through the continued development of "virtual instrument" tools that connect first-principles results to experimental measurements will be discussed.

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