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Computing the properties of ferroelectrics and magnetoelectrics in applied electric fields

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The technology for computing properties of insulators in a finite electric field $\mathcal{E}$, based on the coupling of $\mathcal{E}$ to the Berry-phase polarization P, has been available for over a decade and is currently implemented into several standard code packages. I will give an overview of recent developments in the extension of these methods and their applications to studies of ferroelectrics and multiferroics. I will first discuss the extension to allow calculations at fixed electric displacement field D, emphasizing its advantages for calculations on superlattice and ultrathin capacitor geometries. I will also discuss the qualitative differences, as evidenced by their distinct electric equations of state (P *vs.* $\mathcal{E}$, P *vs.* D, or D *vs.* $\mathcal{E}$), for ordinary ferroelectrics, improper ferroelectrics, and "hyperferroelectrics." The latter constitute a new class of proper ferroelectrics that polarize even when the depolarization field is unscreened, i.e., even at fixed displacement field D. I will then turn to magnetoelectric effects, which can be computed by studying the change in magnetization as an electric field is applied. A particularly subtle component is the one that comes from the change of orbital magnetization. This is found to have an isotropic component, the so-called "axion coupling," that takes the form of an integral of a Chern-Simons three-form over the three-dimensional BZ, as well as anisotropic components that can be expressed in a more conventional Kubo-Greenwood form. I will end with some comments on current and future challenges.