Abstract:
Recent developments have allowed first-principles density-functional calculations to be carried out on insulating systems at fixed electric field, fixed electric displacement field, or fixed polarization. This has been particularly important in allowing access to nonlinear bulk dielectric and piezoelectric responses in ferroelectric materials. The methods can also be used to treat ferroelectric superlattices, where it is of great interest to resolve the local polar contributions. These can be shown to be a local function of chemical environment under appropriate circumstances, allowing for realistic modeling of complex superlattice structures based on reference calculations on a database of short-period structures. Finally, local dielectric contributions can also be resolved for ferroelectric insulators in contact with metallic electrodes, allowing access to information about dielectric dead layers or about the minimum thickness for ferroelectric capacitor structures. I shall review recent work from our group that has led to progress in these directions.

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