Abstract for an Invited Paper
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Polarization, electric fields, and dielectric response in insulators
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I will give a review of developments that have occurred over the last decade leading to powerful new tools for the computation of electric polarization and related dielectric properties of insulating materials in the context of density-functional theory. These include the Berry-phase theory of electric polarization and methods for the explicit treatment of applied electric fields. I will also show how the determination of maximally localized Wannier functions provides a local, real-space probe of dielectric response. Finally, I will mention some of the systematic improvements in the implementation of density-functional perturbation theory in packages such as ABINIT or PWSCF that now allow for sophisticated calculations of the coupling between structural, electric, and elastic degrees of freedom in complex dielectric, piezoelectric, and ferroelectric materials.