Wannier-based definition of layer polarizations in perovskite superlattices

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In insulators, the method of Marzari and Vanderbilt[1] can be used to generate maximally localized Wannier functions whose centers are related to the electronic polarization. In the case of layered insulators, this approach can be adapted to provide a natural definition of the local polarization associated with each layer, based on the locations of the nuclear charges and one-dimensional Wannier centers comprising each layer. To illustrate the robustness and power of this approach, we present sample calculations of layer polarizations of perovskite superlattices (e.g. bulk $BaTiO_3$, $1SrTiO_3/2BaTiO_3$ supercell), including changes in layer polarizations induced by sublattice displacements (i.e., layer-decomposed Born effective charges). The new method provides a powerful tool for analyzing local dielectric properties in complex layered oxide systems. Immediate applications include modeling of interface effects on total polarization of multicomponent superlattices[2], systematic studies of self-poling effects in superlattices[2], and studies of the coupling of phonons to the interfaces.

[1] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997).

[2] X. Wu, O. Diéguez, K. M. Rabe, and D. Vanderbilt, in preparation.