Wannier-Based Definition of Layer Polarizations in Perovskite Superlattices

Xifan Wu,[1] Oswaldo Dieguez,[2] Karin M. Rabe,[3] and David Vanderbilt[3]

[1] *Department of Chemistry, Princeton University, Princeton, New Jersey NJ 08544, USA*
[2] *Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139-4307, USA*
[3] *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA*

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. Here, we use this approach to compute and analyze layer polarizations of ferroelectric perovskite superlattices, including changes in layer polarizations induced by sublattice displacements (i.e., layer-decomposed Born effective charges) and local symmetry breaking at the interfaces. The method provides a powerful tool for analyzing the polarization-related properties of complex layered oxide systems.

[1] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12 847 (1997).