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Electrostatics of superlattices by first principles XIFAN WU, Princeton University, OSWALDO DIÉGUEZ, Massachusetts Institute of Technology, MASSIMILIANO STENGEL, U.C. Santa Barbara, KARIN RABE, DAVID VANDERBILT, Rutgers University — A complete theory of epitaxial perovskite superlattices requires an understanding of both epitaxial strain effects and of electrostatic boundary conditions. Here, focusing on the latter issue, we have carried out first-principles calculations of the nonlinear dielectric properties of short-period $BaTiO_3/SrTiO_3$ and $PbTiO_3/SrTiO_3$ superlattices having the in-plane lattice constant of $SrTiO_3$. In particular, we have calculated the layer polarizations p_j as defined using the Wannier-based method of Wu, Diéguez, Rabe and Vanderbilt[1] for each neutral BaO, SrO, PbO, or TiO_2 layer, and modeled p_j as a function of displacement field D (which is uniform throughout the superlattice), the chemical identity of the layer itself, and the chemical identity of its near neighbors. We then test our expectation that the dependence on the identity of neighboring layers should decay rapidly with distance. If we apply a cut-off to the range of this interlayer interaction, we arrive at a model description that allows us to predict $p_j(D)$ for each layer, and thus the overall $P(D)$ (and trivially, also P vs. electric field and related quantities) for a superlattice of arbitrary layer sequence.

[1]X. Wu, O. Diéguez, K. Rabe and D. Vanderbilt, Phys. Rev. Lett. **97**, 107602 (2006).

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