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Electrostatics of superlattices by first principles XIFAN WU, OSWALDO DIÉGUEZ, 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 mapped the energy E vs. polarization P for these superlattices, and for the parent bulk materials, by extending the $E(P)$ mapping algorithm of Diéguez and Vanderbilt to handle strain relaxation in the c-direction. We then test whether the superlattice results can be understood quantitatively in terms of the $E(P)$ information for the bulk materials and similar information on the interfaces. We reformulate the theory in terms of the electric displacement field D (since this is uniform throughout the superlattice) and the corresponding internal energy $U(D)$, and investigate how to model $U(D)$ in terms of ab-initio derived bulk and interface information. We stress that once the $U(D)$ is obtained for a given superlattice, all the electrostatic properties, both linear and non-linear, can be predicted.

Xifan Wu
Rutgers University

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