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Inverse layer capacitance in perovskite oxide superlattices XIFAN WU, Temple University, MASSIMILIANO STENGEL, ICMAB(CSIC), Barcelona, DAVID VANDERBILT, Rutgers University — Ferroelectricity is one of the most important functionalities that can be tuned in perovskite oxide superlattices. At fixed displacement field D, the overall polar instability can be accessed by the inverse of the capacitance per basal area as $C^{-1} = \partial V/\partial D$, where V is the potential drop across the supercell.[1] Here we propose that C^{-1} can be further rigorously decomposed into contributions from individual AO or BO_2 layers, giving an *layer inverse capacitance* defined as $c_j^{-1} = \epsilon_0^{-1}(h_j + D\partial h_j/\partial D - \partial p_j/\partial D)$, where h_j and p_j are the layer height and Wannier-based layer polarization[2] of layer j, respectively. We compute the c_j^{-1} in several typical multicomponent perovskite superlattices such as $CaTiO_3/BaTiO_3$ and $PbTiO_3/SrTiO_3$, and demonstrate that they satisfy a *locality* principle: their behavior depends mainly on the local chemical environment (i.e., the identities of neighboring layers). Thus, we show that the c_j^{-1} can provide an insightful *local* analysis of the ferroelectric tendency at interfaces in functional oxide superlattices.

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

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