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Determination of ground-state structure of perovskite super- lattices from first principles YUANJUN ZHOU, KARIN RABE, Department of Physics & Astronomy, Rutgers University — We propose an efficient method to find the ground state structure (GSS) of superlattices. It is based on the assumption that in the GSS of the superlattice, structures of the constituent layers will closely resemble a low-energy state of the pure compound at the relevant epitaxial strain. This method is especially suitable for high-throughput first-principles studies for the design of functional superlattices since the information about the low-energy states for a relatively small set of pure compounds, generated in a preprocessing step and stored in a database, can be used for the structure determination of a large space of constituent and layer thickness combinations. The method is demonstrated by application to the 2:2 PbTiO3/SrTiO3 superlattice. For tensile and compressive epitaxial strain, we find the GSS consistent with previous studies. For 0% epitaxial strain, however, our method identifies two degenerate distinct ground-state structure candidates, only one of which was previously identified; further investigation confirms a complex energy landscape for this phase. Results for the SrMO3/SrTiO3 series of superlattices, where M = V, Cr, Co and Fe, will also be presented.

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