Ground state structure searching in perovskite superlattices

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Determination the crystal structure is the essential first step in the first-principle calculations of electronic properties. The ground state structure is not always straightforward to measure experimentally in cases of epitaxial superlattices and thin films, mostly because the small thickness. In this work, we propose a novel strategy for first-principle calculations to search for the ground state and low-energy structures in perovskite superlattices. Our approach bases on the assumption that the inner parts of superlattices tend to have similar distortions with their low-energy bulk states. Using 2:2 $PbTiO_3$/$SrTiO_3$ (PTO/STO) superlattice as an example, we first compute the low-energy states structures in pure PTO and STO perovskites, and then construct superlattice by stacking low-energy structures of PTO ans STO, where the atomic positions in interfacial layers are linear superpositions of the two components. Results recover the low-energy structures in previous work. In addition, we find another low-energy structure complementary to previous "ground-state" structure for 0% epitaxial strain, with negligible energy difference, suggesting a "flat" energy surface near the ground-state structure in 2:2 PTO/STO superlattice. The success in the complex PTO/STO system shows the possibility of generalization our approach to other perovskite systems as well as future high-throughput studies.