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Understanding, enhancing and fine-tuning polar properties in multicomponent perovskite superlattices[1]

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Modern epitaxial thin-film techniques make it possible to synthesize artificial multicomponent perovskite-oxide superlattices (SLs) with interfaces that are atomically flat and compositionally abrupt. The behavior of such systems is dominated by strong interactions between individual SL layers, high levels of epitaxial strain and symmetry lowering relative to the bulk. All of these factors can be manipulated in order to enhance or custom-tailor the useful polar properties — such as polarization and piezoelectric response — for a wide variety of technological applications. First-principles computational techniques are a tool of choice to help us understand how the strain, symmetry and composition of these complex systems influence their polar properties. However, the prohibitive computational costs associated with such simulations, growing rapidly as the period of the SL increases, make it impossible to answer some broader, more interesting questions: in particular, how could the SL layer arrangement be optimized to obtain the best possible polar properties? Here we show how first-principles calculations combined with a simple model for SL polarization and a genetic-algorithm optimization allow us to find answers to the questions mentioned above and, among other things, to predictively identify the most polar perovskite-oxide SLs that can be grown on currently available substrates. This flexible modeling procedure can be applied to a wide variety of layered perovskite-oxide nanostructures, providing guidance for experimental development of nanoelectromechanical devices with substantially improved polar properties.

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