

Abstract Submitted
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Electronic and optical properties of $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$ from first-principles: the effect of epitaxial strain and composition JAWAD ALSAEI, PAUL TANGNEY, ARASH MOSTOFI, Imperial College London — Ferroelectrics such as $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$ (BST) solid solutions are very good candidates for tunable dielectric devices. BST in thin film form is of particular interest for its application to the manufacture of smaller device components and the potential to tailor its electronic properties both via composition x and epitaxial strain. In this work, we use first-principles calculations to study the effect of composition and epitaxial strain on the band gap and optical properties of BST. Our simulations enable us to disentangle the effects of cell volume, cell shape and atomic relaxation on the electronic structure. Our results demonstrate the potential to exploit structure-property and composition-property relationships in thin-film BST and help to improve our fundamental scientific understanding of this technologically important class of materials.

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