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Epitaxial strain effects from first principles CLAUDE EDERER, NICOLA SPALDIN, Materials Department, University of California, Santa Barbara — Epitaxial strain can substantially enhance the spontaneous polarizations and Curie temperatures of ferroelectric thin films compared to the corresponding bulk materials. In this work we use first principles calculations to calculate the effect of epitaxial strain on the spontaneous polarization of the ferroelectrics $BaTiO_3$, $PbTiO_3$, and $LiNbO_3$, and the multiferroic material $BiFeO_3$. We show that the epitaxial strain dependence of the polarization varies considerably for the different systems, and in some cases is in fact very small. We discuss possible reasons for this different behavior, and show that the effect of epitaxial strain can easily be understood in terms of the piezoelectric and elastic constants of the unstrained materials. Our results provide a computational tool for the quantitative prediction of strain behavior in ferroelectric thin films.

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