

## *Ab initio* study of the BaTiO<sub>3</sub>/Ge interface

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Growing thin films of crystalline metal oxides on silicon or germanium has been of great research interest for decades because of the possible applications of such systems in electronic devices. Being ferroelectric in the bulk, BaTiO<sub>3</sub> on a semiconductor points to a chance to realize e.g. non-volatile transistors. In such a system, the state is encoded in the ferroelectric polarization direction of the oxide, which directly modifies the transport properties of the semiconductor under it.

Thanks to recent advances in epitaxial growth methods, one can explore such interfaces in parallel with the experiment. Here, we use density functional theory to study the interface between BaTiO<sub>3</sub> and Ge. We describe how the structure of the interface depends on the oxygen content of the interface and compare to X-ray diffraction results for fabricated interfaces. We show how the polarization of the BaTiO<sub>3</sub> thin film changes when compared to the bulk. We analyze the electronic structure of the interface and illustrate how valence and conductance bands are aligned. We explore the energetics of oxygen vacancies in BaTiO<sub>3</sub> both in terms of positional and concentration dependence and try to explain the results with simple lattice models of vacancy-vacancy interactions.