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Theoretical study of Ge/$BaTiO_3$ Interfaces KURT FREDRICKSON, ALEXANDER DEMKOV — It has been shown (McKee *et al.,* Phys. Rev. Lett. **81,** 3014 (1998), and R. McKee, *et al.*, *Science* **293**,468 (2001)) that perovskite oxides $SrTiO_3$ and $BaTiO_3$ (BTO) can be grown epitaxially on Si and Ge, respectively. It would be interesting to achieve the reverse, i.e. to grow for example, Ge on BTO. It is not clear, however, whether one can achieve wetting of BTO by Ge. Theoretically, the energy of the Ge (001) surface is estimated to be anywhere between 591 and 1700 erg/cm^2 and the surface energy of BTO is in the range of 1083-1496 erg/cm^2 depending on termination and environment. The missing piece of information is the energy of the Ge/BTO interface. We examine five possible Ge/BTO interface structures and calculate their energies using density functional theory to determine which one has the lowest energy, and whether wetting can be achieved.

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