

# Density functional theory-based prediction of the kinetically trapped epitaxial Si/SrTiO<sub>3</sub> interface structure

Alexie M. Kolpak and Sohrab Ismail-Beigi

*Center for Research on Interface Structures and Phenomena, Department of Applied Physics, Yale University  
New Haven, CT, USA*

In this study, we use density functional theory to determine the interface structure of epitaxial SrTiO<sub>3</sub> on silicon. We compute the thermodynamic phase diagram of the system and demonstrate that it is only thermodynamically stable with respect to formation of an interfacial SiO<sub>2</sub> region at unattainably low oxygen partial pressures. Experimentally, however, an atomically abrupt Si/SrTiO<sub>3</sub> interface with no SiO<sub>2</sub> phase can be grown, as demonstrated via scanning transmission electron microscopy (STEM)<sup>1,2,3</sup> and x-ray diffraction (XRD) measurements. This is achieved using controlled layer-by-layer growth procedures<sup>1,2,3</sup> during which SiO<sub>2</sub> formation is presumably kinetically inhibited. Using first-principles to compute the energy barriers for oxygen diffusion in the Si/SrTiO<sub>3</sub> heterostructure, we construct a kinetic model of the growth process which illustrates the mechanism by which the interface structure is kinetically trapped. We show that the observed stability of the interface under both growth and ambient conditions is directly related to the interface chemistry, which gives rise to a large barrier for oxygen diffusion through the interface layer into the silicon substrate. Our understanding of this growth process may lead to the development of procedures for the as-yet unsuccessful growth of other epitaxial perovskites on silicon. Furthermore, our work shows how a combination of first-principles computations, simple kinetic modeling, and experiment can be used to determine non-thermodynamic equilibrium atomic structure in complex heterosystems.

- [1] R.A. McKee, F.J. Walker, and M.F. Chrisholm, *Phys. Rev. Lett.* **81**, 3014 (1998).
- [2] S.B. Mi, *et. al*, *Appl. Phys. Lett.* **93**, 3 (2008).
- [3] M.P. Warusawithana, *et. al*, *Science* **324**, 367 (2009).