Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Ab initio study of the epitaxial BaTiO3/Ge interface MEHMET DOGAN, DIVINE KUMAH, CHARLES AHN, FREDERICK WALKER, SOHRAB ISMAIL-BEIGI, Yale University — 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. An example is provided by the ferroelectric oxide $BaTiO_3$: if it remains ferroelectric on a semiconductor, one may be able to realize non-volatile electronic devices based on the interfacial field effect where the state of the system is encoded in the polarization direction of the oxide. 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 $BaTiO_3$ and Ge. We describe how the structure of the interface depends on the oxygen content of the interface and compare to X-ray diffraction experiments. We show how the polarization of the $BaTiO_3$ thin film changes 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 $BaTiO_3$ both in terms of positional and concentration dependence. We also discuss dynamics of oxygen vacancies by computing the energy barriers for oxygen vacancy diffusion.

Mehmet Dogan
Yale University

Date submitted: 14 Nov 2013 Electronic form version 1.4