Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Scale-bridging simulations of surfaces and defects in BaTiO3[1]
ANDREA GRECO, PAUL TANGNEY, Imperial College of London, JOHN FREELAND, Argonne National Laboratory, ARASH MOSTOFI, Imperial College of London — BaTiO3 (BTO) is a ferroelectric perovskite oxide that is of particular interest in thin-film form for its technological application in tunable nanoelectronic devices. The dielectric properties of BTO thin films depend on many different factors, among which the presence of oxygen vacancies is believed to be one of the most important. Oxygen vacancies, however, are difficult to characterize directly in experiments and usually even their concentration is unknown. On the one hand, first-principles simulations based on density-functional theory (DFT) are invaluable for providing insight into the role of defects in materials and, in principle, could be used for the study of oxygen vacancies in BTO thin films. On the other hand, the large length and time-scales associated with structures and processes in realistic surfaces are well beyond the scope of DFT calculations. To overcome some of these limitations we use DFT in conjunction with a computationally efficient classical interatomic force field that has been fitted to DFT energies, forces and stresses in bulk BTO. We assess the transferability of this potential to defects and surfaces. We then use it to study the prevalence of oxygen vacancies and their structures, both in bulk BTO and near BTO surfaces.

[1]Support from the CDT in Theory and Simulation of Materials (Imperial College of London) and Argonne National Laboratory is thankfully acknowledged.

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Date submitted: 14 Nov 2013 Electronic form version 1.4