Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electronic structure and thermodynamic stability of the $SrTiO_3$ (111) surface[1] NIKHIL SIVADAS, Department of Physics, Carnegie Mellon University, HEMANT DIXIT, VALENTINO COOPER, Material Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, Department of Physics, Carnegie Mellon University — We investigate the electronic structure and thermodynamic stability of the $SrTiO_3$ (111) surface using density functional theory. We observe that, for the Ti-terminated $SrTiO_3$ (111) surface, there is indeed some electronic reconstruction, resulting in the emergence of a metallic surface state. Polar distortions play a crucial role in screening the internal electric field; thereby reducing the amount of charge transferred between the surfaces. Our analysis emphasizes the failure of the simple nominal charge counting argument in thin STO (111) slabs, which ignores the effect of polar distortion. As expected, having a surface oxygen atom at the Ti termination can stabilize the system, eliminating any electronic reconstruction, making the system insulating. An analysis of the surface thermodynamic stability suggests that the Ti terminated (111) surface should be experimentally realizable. This surface may be useful for exploring the behavior of electrons in oxide (111) interfaces and may have implications for modern device applications.

[1]AFOSR Grant No. FA9550-12- 1-0479, U.S. DOE, BES, MSE and the Office of Science Early Career Research Program and NERSC, Office of Science, US DOE under Contract No. DEAC02-05CH11231.

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Date submitted: 14 Nov 2013 Electronic form version 1.4