Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Electronic and structural reconstruction in titanate heterostructures from first principles ANDREW T. MULDER, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Recent advances in transition metal oxide heterostructures have opened new routes to create materials with novel functionalities and properties. One direction has been to combine a Mott insulating perovskite with an electronic d^1 configuration, such as $LaTiO_3$, with a band insulating d^0 perovskite, such as $SrTiO_3$. An exciting recent development is the demonstration of interfacial conductivity in $GdTiO_3/SrTiO_3$ heterostructures that display a complex structural motif of octahedral rotations and ferromagnetic properties similar to bulk $GdTiO_3$. In this talk we present our first principles investigation of the interplay of structural, electronic, magnetic, and orbital degrees of freedom for a wide range of d^1/d^0 titanate heterostructures. We find evidence for both rotation driven ferroelectricity and a symmetry breaking electronic reconstruction with a concomitant structural distortion at the interface. We argue that these materials represent an ideal platform to realize novel functionalities such as the electric field control of electronic and magnetic properties.

Andrew T. Mulder
School of Applied and Engineering Physics, Cornell University

Date submitted: 14 Nov 2013 Electronic form version 1.4