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.

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Date submitted: 14 Nov 2013

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