Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Competing (anti-)ferrodistortive and ferroelectric instabilities in $SrTiO_3$ and layered $La_2Ti_2O_7$ ULRICH ASCHAUER, NICOLA SPALDIN, Materials Theory, ETH Zürich — We present first-principles calculations on the competition between antiferrodistortive (AFD) and ferroelectic instabilities in oxides. High temperature cubic $SrTiO_3$ is well known to undergo an AFD transformation at around 105 K. Further reducing the temperature shows a softening of the ferroelectric polar phonons, however the material remains incipient-ferroelectric with an overall paraelectric behavior. This behavior is believed to be linked to a suppression of the polar instability by the AFD one, the mechanism still being debated. Our calculations show that freezing in the AFD indeed reduces the polar instability. At the theoretical equilibrium angle, the material however still retains a polar instability with a double-well depth of $\sim$0.2 meV per $SrTiO_3$ unit, inline with the material being incipient-ferroelectric. A change in polar eigenvectors with increasing AFD rotation together with a decomposition of forces into long- and short-range components allows us to propose an underlying mechanism. We will further discuss a similar suppression mechanism observed in layered $La_2Ti_2O_7$, where conventional ferroelectricity is suppressed by ferrodistortive modes, these modes however still leading to improper ferroelectricity due to the layered structure.

Ulrich Aschauer
Materials Theory, ETH Zürich

Date submitted: 05 Dec 2011 Electronic form version 1.4