Competing (anti-)ferrodistortive and ferroelectric instabilities in SrTiO$_3$ and layered La$_2$Ti$_2$O$_7$ ULRICH ASCHAUER, NICOLA SPALDIN, Materials Theory, ETH Zürich — We present first-principles calculations on the competition between antiferrodistortive (AFD) and ferroelectric 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$_2$Ti$_2$O$_7$, where conventional ferroelectricity is suppressed by ferrodistortive modes, these modes however still leading to improper ferroelectricity due to the layered structure.

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