Please do not schedule for Monday or Friday.

Abstract Submitted
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Lack of ferroelectricity in $PbTiO_3$ at high pressures[1] R.E. COHEN[2], MUHTAR AHART, Extreme Materials Initiative, GL, Carnegie Institution, RUSSELL J. HEMLEY, Dept. Civil Environment Engineering, George Washington Univ. and LLNL — The classic ferroelectric $PbTiO_3$ continues to surprise. It was believed that ferroelectrics would become paraelectric under pressure, and this was observed in Raman experiments on $PbTiO_3$. [1] We predicted a morphotropic phase transition under pressure [2] and verified it experimentally. [3] At higher pressures it become paraelectric, but DFT [4, 5] predicted higher pressure ferroelectricity, and this seemed confirmed by experiments. [6] New Second Harmonic Generation (SHG) measurements on $PbTiO_3$ to 100 GPa and down to 10 K find no evidence for ferroelectricity above 20 GPa. Our DFT computations show centrosymmetric I4mcm as most stable from 20-90 GPa; I4mcm is the ground state of $SrTiO_3$, and the rotations quench the polar instability. We predict a polar I4cm structure above 90 GPa, but the double well depth is very small. [1] J. Sanjurjo et al., PRB 28, 7260 (1983). [2] Z. Wu and R. Cohen, PRL, 037601 95 (2005). [3] M. Ahart et al., Nature 451, 545 (2008). [4] I. A. Kornev and L. Bellaiche, Phase Transitions 80, 385 (2007). [5] I. A. Kornev et al., PRL 95 196804 (2005). [6] P. E. Janolin et al., PRL 101 237601 (2008).

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