

Abstract Submitted  
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**Using non-equilibrium Molecular Dynamics to gain insight into the negative capacitance regime in ferroelectrics.**<sup>1</sup> KELLI ANN LYNCH, INNA PONOMAREVA, University of South Florida — The negative capacitance regime has potential for overcoming the Boltzmann tyranny, which limits performance for conventional transistors. Ferroelectrics are of interest for negative capacitance applications due to their potential energy profile. When minimized, the free energy results in an equation of state with an S-shaped dependence of polarization on electric field, whose central region is thermodynamically unstable. Experimental detection of negative capacitance seems to suggest that a ferroelectric can be “tricked” into entering this region. Our investigation aims to provide a clearer understanding of the underlying physical mechanism that drives ferroelectrics into the negative capacitance regime. Technically, we simulated PTO bulk and 39-nm thick film subjected to electric field using classical Molecular Dynamics with the interaction modeled by a first-principles effective Hamiltonian. We will present data for both bulk and film, concluding that the ferroelectric avoids the forbidden region even with high rates of electric field application and epitaxial compressive strain. However, negative capacitance was observed in the dependence of polarization on internal electric field, with the effects of the residual depolarizing field included. Finally, we will conclude that it is possible to tune the negative capacitance regime using the surface charge compensation and amplitude of the applied electric field. The work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under grant DE-SC0005245.

<sup>1</sup>Using Non-Equilibrium Molecular Dynamics to Gain Insight into the Negative Capacitance Regime in Ferroelectrics

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