

Abstract Submitted  
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**Effect of Epitaxial Strain on the Dynamical Properties of Ferroelectric Perovskites**<sup>1</sup> KEVIN MCCASH, BRAJESH MANI, CHUN-MIN CHANG, INNA PONOMAREVA, Univ of South Florida — The use of ferroelectric perovskites in device applications is in large part determined by the strain induced by their growth on lattice mismatched substrates. The epitaxial strain resulting from such growth has been shown to dramatically alter the soft-mode dynamics of ferroelectrics. Here we take advantage of first-principles-based molecular dynamics simulations to investigate the soft-mode dynamics in epitaxial  $\text{PbTiO}_3$  films. By calculating the complex dielectric response and extracting the soft-mode frequencies we are able to trace the intrinsic dynamics as a function of temperature and strain. Our simulations show that the interplay of applied and spontaneous strain is critical to the soft-mode dynamics and provides insights into some recent experimental findings.

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