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Dynamical Properties of PbTiO3 Under Pressure, Stress and Strain[1] KEVIN MCCASH, INNA PONOMAREVA, University of South Florida
— Ferroelectric perovskites have been in the focus of attention for many years owing to their remarkable properties and variety of applications. Of notable importance is the manner in which external stimuli alter the properties and dynamics of such materials. Here we take advantage of first principles based molecular dynamics simulations to probe the dynamics of $PbTiO_3$ at finite temperature and under the application of pressure, stress and strain. Our simulations show that the complex dielectric response and soft-mode dynamics of $PbTiO_3$ can be tuned by the application of pressure, stress and strain over a range of values available in a laboratory setting. This tunability can lead to the use of $PbTiO_3$ and other polar perovskite oxides in novel applications.

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