

Abstract Submitted
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First-principles Raman Spectra of Lead Titanate with Pressure¹

A. SCHAD, P. GANESH, R.E. COHEN, M. AHART — PbTiO_3 displays[1,2] a morphotropic phase boundary (MPB) under pressure at which electromechanical properties are maximal. Previously only complex solid-solutions were thought to exhibit such a boundary. To aid in the experimental study of the MPB region, we compute Raman scattering spectra of different phases of PbTiO_3 with pressure using a DFT based first-principles approach and Density Functional Perturbation Theory (DFPT) [3]. The computed intensities and shifts with pressure agree very well with the experimental data measured on powder samples. Computations further allow comparison of Raman spectra and shifts in energetically competing phases raising the possibility of using calculations for experimental calibration of Raman spectra at any pressure. The results substantiate previous claims of a low-temperature monoclinic phase at the MPB at approximately 10 GPa in PbTiO_3 as well as refute the possibility of an $I4cm$ phase at higher pressures as suggested by other groups [4]. [1] Z. Wu and R. E. Cohen, Phys. Rev. Lett. 95, 037601 (2005), [2] M. Ahart et.al., Nature 451, 545 (2008), [3] P. Hermet et.al., J. Phys.:Condens. Matter 21, 215901 (2009) [4] P.E. Janolin et.al., Phys. Rev. Lett. 101, 237601 (2008).

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