Phonons in SrTiO\textsubscript{3} under finite electric fields

IVAN NAUMOV, HUAXIANG FU, Physics Department, University of Arkansas, Fayetteville, Arkansas 72701, USA — It has been nearly 40 years since Worlock and Fleury discovered by means of Raman scattering that under finite electric fields the transverse-optic (TO) phonons in SrTiO\textsubscript{3} exhibit a striking increase in frequency—by more than 400\% of its zero-field value—when a very small field of 12 kV/cm is applied [1]. Despite its obvious importance, this giant field-induced shift of phonon frequency has not thus far been independently investigated via the density-functional theory (DFT). Here, we propose an approach within the DFT theory to determine the phonon structure of infinite solids under finite electric fields. We applied this approach to SrTiO\textsubscript{3} and found a giant shift in TO frequencies, in accordance with the observations [1]. Our calculations further predict other unusual properties that occur under finite electric fields, that is, an anomalous piezoelectric response and large dielectric tunability. (This work was supported by ONR). [1] J.M. Worlock and P.A. Fleury, Phys. Rev. Lett. 19, 1176 (1967).