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Phonons in $SrTiO_3$ 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 $SrTiO_3$ 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 $SrTiO_3$ 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).

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