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Nonlinear Optical Response of Polar Semiconductors in the Terahertz Range ERIC ROMAN, University of California, Berkeley, JONATHAN YATES, University of California, Berkeley and Lawrence Berkeley National Laboratory, MAREK VEITHEN, Université de Liège, DAVID VANDERBILT, Rutgers University, IVO SOUZA, University of California, Berkeley and Lawrence Berkeley National Laboratory — We compute the recently measured [1] infrared dispersion of the second-order nonlinear susceptibility $\chi^{(2)}$ in zincblende semiconductors from first principles. At infrared frequencies, but above the elastic resonance of the medium, the total $\chi^{(2)}$ depends not only on the purely electronic response $\chi^{(2)}_{\infty}$, but also on three additional parameters: C_1, C_2, and C_3. They relate to the TO Raman tensor, second-order dipole moment, and lattice anharmonicity, respectively. We apply small, finite electric fields and finite ionic displacements along [111], and extract the desired parameters from the forces induced on the atoms and the change in macroscopic polarization. By analyzing the resulting displacements of the Wannier-function centers, we make contact with bond-polarizability models and assess the influence of the cation d-electrons.

[1]T. Dekorsy, V. A. Yakovlev, W. Seidel, M. Helm, and F. Keilmann, Phys. Rev. Lett. **90**, 055508 (2003)

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