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Nonlinear Optical Response of Polar Semiconductors in the Terahertz Range ERIC ROMAN, JONATHAN YATES, University of California, Berkeley, MAREK VEITHEN, Université de Liège, DAVID VANDERBILT, Rutgers University, IVO SOUZA, University of California, Berkeley — Using the Berry-phase finite-field method, we compute from first-principles the recently measured[1] infrared (IR) dispersion of the nonlinear susceptibility $\chi^{(2)}$ in III-V zincblende semiconductors. At far-IR (terahertz) frequencies, in addition to the purely electronic response $\chi^{(2)}_{\infty}$, the total $\chi^{(2)}$ depends on three other parameters, C_1, C_2, and C_3, describing the contributions from ionic motion. They relate to the TO Raman polarizability and the second-order displacement-induced dielectric polarization and forces, respectively. Contrary to a widely-accepted model,[2] but in agreement with the recent experiments on GaAs,[1] we find that the contribution from mechanical anharmonicity dominates over electrical anharmonicity. By using Richardson extrapolation to evaluate the Berry's phase in k-space by finite differences, we are able to improve the convergence of the nonlinear susceptibility from the usual[3] $\mathcal{O}[(\Delta k)^2]$ to $\mathcal{O}[(\Delta k)^4]$, dramatically reducing the computational cost.

[1]T. Dekorsy, V. A. Yakovlev, W. Seidel, M. Helm, and F. Keilmann, Phys. Rev. Lett. **90**, 055508 (2003).
[2]C. Flytzanis, Phys. Rev. B **6**, 1264 (1972).
[3]P. Umari and A. Pasquarello, Phys. Rev. B **68**, 085114 (2003).

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