Abstract Submitted
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Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study[1] DAVID A. STRUBBE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, XAVIER ANDRADE, ANGEL RUBIO, European Theoretical Spectroscopy Facility, Universidad del Pais Vasco and Centro Mixto CSIC-UPV/EHU, San Sebastian, Spain, STEVE G. LOUIE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — Chloroform is often used as a solvent and reference when measuring non-linear optical properties of organic molecules. We calculate directly the non-linear susceptibilities of liquid chloroform at optical frequencies, using molecular dynamics and the Sternheimer equation in time-dependent density-functional theory [X. Andrade et al., J. Chem. Phys. 126, 184106 (2007)]. We compare the results to those of chloroform in the gas and solid phases, and experimental values, and make an ab initio calculation of the local-field factors which are needed to extract molecular properties from liquid calculations and experimental measurements.

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