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, Dept. of Physics, University of California, Berkeley, and Lawrence Berkeley National Laboratory, XAVIER ANDRADE, ETSF, Centro de Fisica de Materiales, Universidad del Pais Vasco, San Sebastian, Spain, ANGEL RUBIO, ETSF, Centro de Fisica de Materiales, Universidad del Pais Vasco, San Sebastian, Spain, and Fritz-Haber-Institut, STEVEN G. LOUIE, Dept. of Physics, University of California, Berkeley, and Lawrence Berkeley National Laboratory — Chloroform is often used as a solvent when measuring non-linear optical properties of organic molecules. We assess the influence of the solution environment on the molecular properties by calculating directly the non-linear susceptibilities of liquid chloroform at optical frequencies. We use the Sternheimer equation in time-dependent density-functional theory [J. Chem. Phys. 126, 184106 (2007)], on snapshots from ab initio molecular dynamics. We compare the results to those in the gas and solid phases, and to experimental values. We also calculate ab initio local-field factors, used to analyze electric-field-induced second-harmonic generation (EFISH) and hyper-Rayleigh scattering (HRS) experiments.

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