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Path Integral Monte Carlo Study of the Electrical Polarizability of Dimerized Hydrogen Chains MARK SANGER, JOHN SHUMWAY, Arizona State University — Density functional theory is a powerful technique for obtaining ab initio properties of molecules. However, the commonly used techniques have well known weaknesses, especially when computing polarizabilites or band gaps. We have developed a new Quantum Monte Carlo(QMC) technique for calculating static polarizability of molecules using current-current correlation functions in imaginary-time path integrals. The method is applicable to isolated molecules as well as periodic structures. We present the successfull results obtained from simulating the polarizability of dimerized chains of hydrogen atoms at T=300K for both open and periodic boundary conditions. We find excellent agreement with high accuracy quantum chemistry estimates, with a very modest order(N^3) scaling with system size and easy accommodation of periodic boundary conditions.

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