Abstract Submitted
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Green's function analysis of path integral Monte Carlo molecular simulations[1] DAEJIN SHIN, Arizona State University, JOHN SHUMWAY, Arizona State University — We demonstrate the direct determination of molecular properties from path integral Monte Carlo simulations. By sampling Matsubura Green's functions, we have calculated several linear response properties of the hydrogen molecule (H_2) directly from quantum Monte Carlo. We show that the vibration frequency of H_2 as calculated directly from the phonon temperature Green's function is in very good agreement with the calculated Born-Oppenheimer potential energy surface. We have also obtained the polarizability from the polarization correlation function, and we are looking at Raman spectra. For the high-accuracy simulations needed in chemical physics, we have developed new, fast and accurate techniques for the tabulation of Coulomb density matrices. This work motivates future path integral Monte Carlo simulations on larger molecules and could also be immediately useful in simulations of hydrogen storage materials.

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Daejin Shin
Arizona State University

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