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***Ab Initio* Quantum Simulations of Liquid Water**[1] JOHN GERGELY, DAVID CEPERLEY, University of Illinois Urbana - Champaign, FRANCOIS GYGI, University of California Davis — Some recent efforts at simulating liquid water have employed "*ab initio*" molecular dynamics (AIMD) methods with forces from a version of density functional theory (DFT)[2] and, in some cases, imaginary-time path integrals (PI) to study quantum effects of the protons. Although AIMD methods have met with many successes, errors introduced by the approximations and choices of simulation parameters are not fully understood. We report on path integral Monte Carlo (PIMC) studies of liquid water using DFT energies that provide quantitative benchmarks for PI-AIMD work. Specifically, we present convergence studies of the path integrals and address whether the Trotter number can be reduced by improving the form of the (approximate) action. Also, we assess 1) whether typical AIMD simulations are sufficiently converged in simulation time, i.e., if there is reason to suspect that nonergodic behavior in PI-AIMD methods leads to poor convergence, and 2) the relative efficiency of the methods.

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[2]E. Schwegler, J.C. Grossman, F. Gygi, G. Galli, J. Chem. Phys **121**, 5400 (2004).

John Gergely
University of Illinois Urbana - Champaign

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