Abstract Submitted
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Quantum Monte Carlo studies of solvated systems KATHLEEN SCHWARZ, Cornell University, Department of Chemistry, KENDRA LETCHWORTH WEAVER, T.A. ARIAS, Cornell University, Department of Physics, RICHARD G. HENNIG, Cornell University, Department of Materials Science and Engineering — Solvation qualitatively alters the energetics of diverse processes from protein folding to reactions on catalytic surfaces. An explicit description of the solvent in quantum-mechanical calculations requires both a large number of electrons and exploration of a large number of configurations in the phase space of the solvent. These problems can be circumvented by including the effects of solvent through a rigorous classical density-functional description of the liquid environment, thereby yielding free energies and thermodynamic averages directly, while eliminating the need for explicit consideration of the solvent electrons. We have implemented and tested this approach within the CASINO Quantum Monte Carlo code. Our method is suitable for calculations in any basis within CASINO, including b-spline and plane wave trial wavefunctions, and is equally applicable to molecules, surfaces, and crystals. For our preliminary test calculations, we use a simplified description of the solvent in terms of an isodensity continuum dielectric solvation approach, though the method is fully compatible with more reliable descriptions of the solvent we shall employ in the future.

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