Systematic benchmarking of molecular solvation free energies using effective field coupled-cluster theory

Jason N. Byrd,[1, a)] Robert W. Molt, Jr.,[1] Beverly A. Sanders,[2] and Rodney J. Bartlett[1]

[1)] *Quantum Theory Project, University of Florida, Gainesville, FL 32611*

[2)] *Department of Computer Science and Engineering, University of Florida, Gainesville, FL 32611*

Molecular embedding methods are powerful techniques for overcoming scalability limitations in electronic structure theory by dividing large molecular systems into individual units that are small enough to be treated using standard techniques. We have developed a massively parallel, linear-scaling coupled-cluster based fragment effective field method, molecular cluster perturbation theory (MCPT), that provides a systematically convergent description of the electronic wavefunction. We will present a systematic computational benchmarking study of small organic molecule solvation free energies obtained from MCPT using various perturbation corrections using experimental and large-scale ab initio reference values. The molecular solvent systems presented here are carefully chosen so as to provide a robust test set for the fragment electronic structure community.

[a)] Electronic mail: byrdja@chem.ufl.edu