Variational Quantum Chemistry Programs in JAQALPAQ

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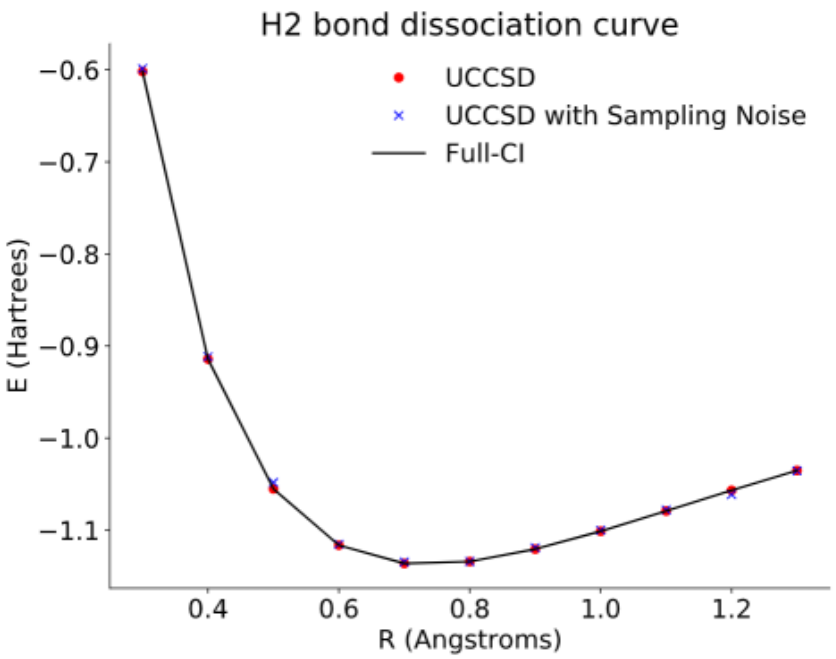

Dissociation curve of H_2: The black line is the theoretical ground state energy. The red and blue points show the simulated optimized energies with and without noise due to finite sampling.

Maupin, Oliver G., Baczewski, A. D., Love, P. J., & Landahl, A. J. (2021). *Entropy* 23.6 (2021): 657.

Work was performed at Tufts University.

Scientific Achievement

Simulated previous quantum chemistry experiments using JAQAL (Just Another Quantum Assembly Language), matching expected results.

Significance and Impact

Lays the groundwork for QSCOUT (Quantum Scientific Computing Open User Testbed) users to conduct their own quantum experiments, and tests the capabilities of the JAQAL language.

Research Details

- Previous experiments calculated the dissociation curves of small diatomic molecules
- Variational Quantum Eigensolver algorithm allows for accurate calculations on small systems like QSCOUT
- Simulated energies using UCCSD (Unitary Coupled-Cluster for Singles and Doubles) match exact full-CI energies with and without sampling

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