Leveraging near-term quantum computers with unitarily downfolded Hamiltonians

Renke Huang, Francesco A. Evangelista

Department of Chemistry and Emerson Center for Scientific Computation, Emory University, Atlanta, GA 30322

Simulating strongly correlated molecules and materials is one promising application for quantum computers. However, the resource requirements of quantum algorithms for molecular simulations are not amenable for current quantum devices. To address this, we utilize a quantum-classical hybrid strategy that combines an active space computation using the variational quantum eigensolver (VQE)[1,2] to treat static correlation and a downfolding of Hamiltonian based on the multireference driven similarity renormalization group (MR-DSRG)[3,4] to treat dynamical correlation. We compute the potential energy curves of H_2 in the cc-pV5Z basis, atomization energy of H_4, and the adiabatic singlet-triplet splitting of *para*-benzyne diradical. We benchmark the results on both the simulator and IBMQ quantum devices.

---

[1] A. Peruzzo, J. McClean, *et al. Nat. Commun.* **5**, 4213 (2014).

[2] A. Kandala, A. Mezzacapo, *et al. Nature* **549**, 242 (2017).

[3] C. Li and F.A. Evangelista, *J. Chem. Phys.* **144**, 164114 (2016).

[4] C. Li and F.A. Evangelista, *J. Chem. Phys.* **155**, 114111 (2021).