Ab Initio Molecular Dynamics on Quantum Computers

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Abstract

Ab initio molecular dynamics (AIMD) is a valuable method for studying the time evolution of molecular systems on potential energy surfaces obtained from accurate electronic structure calculations. In this work, a quantum-computer-based AIMD method is presented. The electronic state energies are calculated on a quantum computer utilizing the variational quantum eigensolver (VQE) method. The energy gradients are computed numerically using the Hellmann-Feynman theorem, finite differences, and a correlated sampling technique. Our method only requires the computation of electron integrals for each degree of freedom on a classical computer, without any additional calculations on a quantum computer. To achieve the same level of accuracy, our gradient calculation method requires three to five orders of magnitude fewer measurements than the brute force methods without correlated sampling. As a proof of concept, AIMD dynamics trajectories are simulated for the H_2 molecule on IBM quantum devices. To the best of our knowledge, it is the first successful attempt to run AIMD for a chemical system on quantum devices. With the increasing quality of quantum hardware and noise mitigation techniques, our method can be used for studying larger molecules.