

Colloquium Notice

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Accurate and Efficient Quantum Computations of Molecular Properties

During the noisy intermediate-scale quantum (NISQ) era, quantum computational approaches refined to overcome the challenge of limited quantum resources are highly valuable. However, the accuracy of the molecular properties predicted by most of the quantum computations nowadays is still far off (not within chemical accuracy) compared to their corresponding experimental data. Here, we propose a promising qubit-efficient quantum computational approach to calculate the harmonic vibrational frequencies of a large set of neutral closed-shell diatomic molecules with results in great agreement with their experimental data [1,2]. We attribute the great performance of the proposed method to three factors: (i) a better description of the Hamiltonian by introducing the Daubechies wavelets molecular orbitals, (ii) incorporating the electron correlation effect into the molecular orbitals via the exchange functional, (iii) a suitable selection of active space based on an energy criterion of a first-order pair energy in the theory of independent electron pair approximation. Remarkably, our proposed approach significantly reduces the number of qubits required for the 43 diatomic molecules from 20 to 60 with the use of the traditional cc-pVDZ basis set and the frozen core approximation to only 2 to 12, but with similar accuracy for the obtained results [2]. This verifies that the harmonic vibrational frequencies of molecules could be calculated accurately by quantum computation in the NISQ era [2,3]. Our benchmark investigation provides a critical assessment on the power of quantum computation of molecular properties and insights on further improvements.

References:

- 1]. C.-L. Hong, T. Tsai, J.-P. Chou et al., P.-J. Chen, P.-K. Tsai, Y.-C. Chen, E.-J. Kuo, D. Srolovitz, A. Hu, Y.-C. Cheng, and H.-S. Goan*, "Accurate and efficient quantum computations of molecular properties using Daubechies wavelet molecular orbitals: a benchmark study against experimental data", PRX Quantum **3**, 020360 (2022).
- 2]. S.-K. Chou, J.-P. Chou, A. Hu, Y.-C. Cheng*, and H.-S. Goan*, "Accurate Harmonic Vibrational Frequencies for Diatomic Molecules via Quantum Computing", Physical Review Research **5**, 043216 (2023)
- 3]. C.-T. Chu, S.-K. Chou, and H.-S. Goan*, "Demonstration of quantum computation of molecular properties in agreement with experimental data on NISQ devices," in preparation (2024).

Monday
November 11, 2024
Starts at 12:15 PM
Coffee at 12:00 PM
Physics Conference Room, SB B326
This talk is accessible via [Zoom](#) or use
meeting ID 829 2687 2594 and **passcode 866995** to join

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