# Accurate and Efficient Quantum Computation of Molecular Properties

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Quantum computation has recently emerged as a revolutionary numerical scheme for computational quantum chemistry, which plays a crucial role in designing novel materials and drugs. However, current applications of quantum-chemistry calculations on quantum computers are limited to small molecules with a small basis set due to limited quantum resources. During the noisy intermediate-scale quantum (NISQ) era, refined quantum computational approaches to overcome the challenge of limited quantum resources are highly valuable. However, the accuracy of the molecular properties predicted by most 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 excellent agreement with their experimental data [1,2]. We attribute the superb 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]. To demonstrate that our approach can be realized on the NISQ devices [2,3], we present a hybrid quantum-classical machine learning framework that can be trained unsupervisedly to predict molecular vibrational frequencies reliably. We demonstrate with $H_2$, LiH, and PN molecules that our framework exhibits high energy accuracy with the calculated results of vibrational frequencies on NISQ devices in excellent agreement with actual experimental data. Our investigation critically assesses the power of quantum computation of molecular properties and insights into 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 (2025).