

Quantum computing of Hückel molecular orbitals of π -electron molecules

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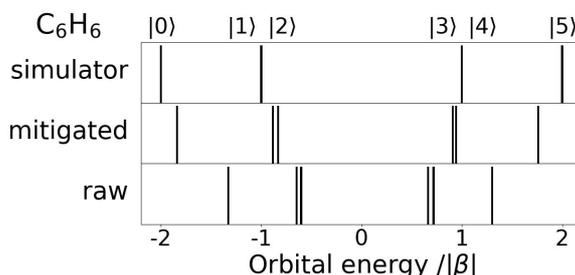
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Describing the electronic structure of molecules composed of many electrons with high accuracy is one of the central themes in modern quantum chemistry. Recent advances in quantum computation technologies have shown us a promising route towards an ideal theoretical computation of electronic structures of large-size molecules in a full configuration-interaction level in the future.

In the present study, in order to demonstrate an applicability of quantum computing to fundamental electronic structure problems of molecules, we calculate orbital energies of π -electron molecules by the Hückel molecular orbital (HMO) method. We describe the Hückel Hamiltonian matrix in terms of quantum gates and the orbital energies using quantum circuits composed of the quantum gates. When constructing the Hamiltonian written in terms of the Pauli matrices, we assign the respective basis functions to qubits according to a direct mapping. For example, for C_2H_4 , we use 2 qubits to represent two basis functions, $|01\rangle$ and $|10\rangle$, where $|q_1q_0\rangle$ represents that the zero-th qubit is q_0 and the first qubit is q_1 . For a molecule with N carbon atoms, we use N qubits and represent the i -th basis function as a set of qubits in which only the i -th qubit is 1 and the rest are 0.

We have run the program constructed by the quantum circuits to calculate the orbital energies of fundamental π -electron molecules (C_2H_4 , C_3H_4 , C_4H_4 , C_4H_6 , and C_6H_6) using a superconducting-qubit type quantum computer, *ibm_kawasaki* [1] with a post-selection error mitigation method. In the error mitigation, we have discarded all the unphysical quantum states after the measurements. We have demonstrated that the orbital energy of HMOs can be obtained with sufficiently high accuracy for all the five fundamental π -bonding systems after the error mitigation as shown in Fig. 1 for C_6H_6 .

Fig. 1 The HMO energies of benzene (C_6H_6) relative to the value of the Coulomb integral (α) represented by the absolute values resonance integral (β). The i -th excited orbital is denoted as $|i\rangle$, “raw” represents the orbital energies calculated on the *ibm_kawasaki* machine, “mitigated” represents those obtained after the error mitigation, and “simulator” represents those calculated by the state-vector simulator.



Reference:

1) IBM Quantum, “*ibm_kawasaki* falcon r5.11,” (2021).