Quantum computing of heteroatom-containing conjugated systems with error mitigation methods

(*Department of Chemistry, School of Science, The University of Tokyo*) ○Ryuhei Yoshida, Erik Lötstedt, Kaoru Yamanouchi

Keywords: Quantum computing, Quantum error mitigation, Zero-noise extrapolation, Heteroatom-containing conjugated systems, Hückel MO

Quantum computers are now available for scientists. In molecular science, an application of quantum computing to quantum chemistry problems has attracted much attention. Last year, our group developed a quantum algorithm for the implementation of the Hückel molecular orbital (HMO) theory and computed electronic energies of HMOs of π-bonding molecular species using *ibm_kawasaki* [1], a superconducting-qubit type quantum computer [2]. We showed that the orbital energies can be calculated with good precision by adopting a quantum error mitigation method. In the present study, we have further developed the quantum algorithm so that we can calculate the HMO energies of heteroatom-containing π-conjugated systems.

In the calculation, we assign each basis function to a qubit using a direct mapping and minimize the number of quantum gates in quantum circuits. For a molecule having N carbon and hetero atoms, we use N qubits and represent the ith basis function as a set of qubits in which only the ith qubit is 1 and the rest are 0. We have run the quantum circuits using *ibm_kawasaki* with two error mitigation methods, that is, the spurious-state elimination and the zero-noise extrapolation (ZNE). We have calculated the HMO energies of pyridine on *ibm_kawasaki* with no error mitigation, with the spurious-state elimination, and with both the spurious-state elimination and ZNE and compared these results with those obtained using a classical computer with the Hückel Hamiltonian (simulator). As shown in Fig. 1, the orbital energies are in good agreement when both the spurious-state elimination and the ZNE are adopted.

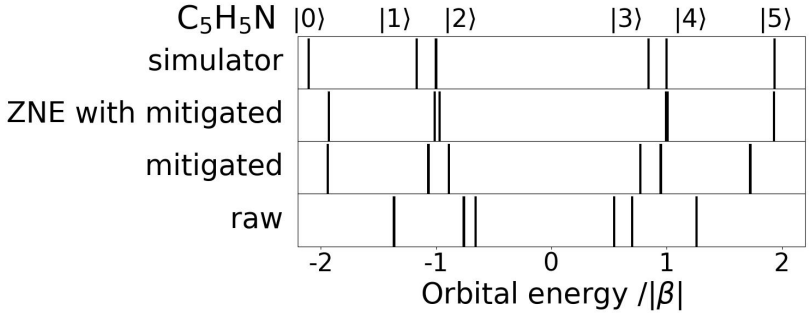

Fig. 1 The orbital energies of pyridine (C_5H_5N) represented by the resonance integral (β). The Coulomb integral (α) is set to be 0. The ith excited orbital is denoted as $|i\rangle$.

References

(1) R. Yoshida, E. Lötstedt, K. Yamanouchi, *J. Chem. Phys* **156**, 184117 (2022)
(2) IBM Quantum, "*ibm_kawasaki* falcon r5.11," (2022).