DIC株式会社

ibm_kawasaki の活用方法
・原子・分子に関わる様々な量子プロセスを量子計算によってシミュレーションし、量子コンピューターによって拓かれる新しい基礎化学・応用化学の分野を探索する
・IBMの量子コンピュータ実機を用いて様々な分子の計算を実施しエネルギー精度などを検証中

活用実績のご紹介
・分子振動エネルギー準位計算[1]
・直鎖共役ポリエンの軌道エネルギー計算[2]
・そのほか実機を用いた各種計算[3]

[1] E. Lötstedt, K. Yamanouchi, T. Tsuchiya, Y. Tachikawa, *Phys. Rev. A* **103**, 062609 (2021)
[2] R. Yoshida, E. Lötstedt, K. Yamanouchi, "*Quantum computing of Hückel molecular orbitals of π-electron systems*," *J. Chem. Phys.* **156**, 184117 (2022).
[3] E. Lötstedt, K. Yamanouchi, "Comparison of current quantum devices for quantum computing of Heisenberg spin chain dynamics," *Chem. Phys. Lett.* **836**, 140975 (2024).

DIC Corporation

How to use ibm_kawasaki

- Simulating various quantum processes related to atoms and molecules using quantum computing, and exploring new fields of basic and applied chemistry opened up by quantum computers.

・We are currently verifying the energy accuracy of various molecular calculations using IBM's quantum computer.

Introduction of past usage cases

・Molecular vibrational energy level calculations [1]

・Orbital energy calculations for linear conjugated polyenes [2]

-Other calculations using actual equipment [3]

[1] E. Lötstedt, K. Yamanouchi, T. Tsuchiya, Y. Tachikawa, Phys. Rev. A 103, 062609 (2021)
[2] R. Yoshida, E. Lötstedt, K. Yamanouchi, “Quantum computing of Hückel molecular orbitals of π-electron systems,” J. Chem. Phys. 156, 184117 (2022).
[3] E. Lötstedt, K. Yamanouchi, “Comparison of current quantum devices for quantum computing of Heisenberg spin chain dynamics,” Chem. Phys. Lett. 836, 140975 (2024).