Simulating Quantum Chemical Dynamics on Quantum Computers

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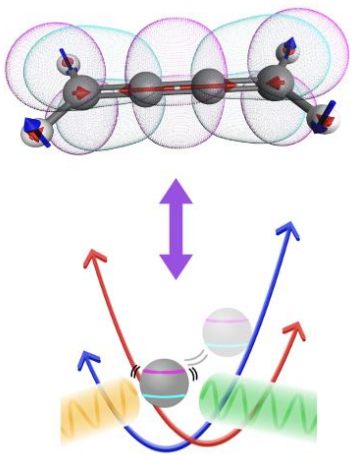
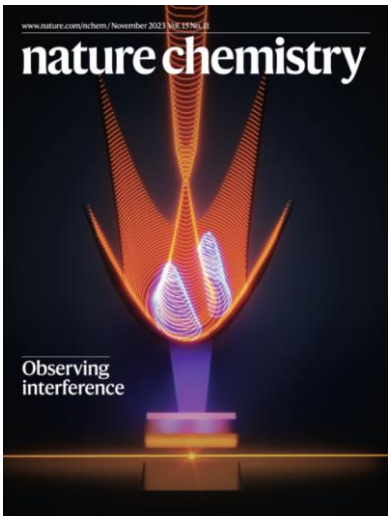
Computational resources required for the most accurate quantum-chemical calculations grow rapidly with molecule size because of the difficulty of representing the full quantum-mechanical motion of electrons and nuclei. Quantum computers could solve this problem, allowing chemical simulations that are exponentially faster than what is possible currently.

I will present my group's recent results that bring forward useful quantum computing for chemistry through orders-of-magnitude reductions in required quantum resources [1]. We have developed a new approach for performing fully non-adiabatic simulations of chemical dynamics using trapped-ion quantum computers by exploiting the motion of the trapped ions to represent the motion of the nuclei. Our experimental demonstrations have led to the first simulations of chemical reactions on a quantum computer [5], the best quantum simulation of spectroscopy to date [2], and the first direct observation of geometric-phase interference in dynamics around a conical intersection in any system [3]. These demonstrations pave the way for near-term demonstrations of quantum advantage with existing technology.



Our work indicates that quantum chemistry on quantum computers will be fundamentally different from chemistry on conventional computers. On quantum computers, full quantum dynamics simulations will be easier than calculating single-point energies and simulating open quantum systems (such as reactions in solution) could be easier than simulating molecules in vacuum [4]. This indicates a complementarity between problems best solved classically and those better left to quantum computers.



References

[1] MacDonell et al., *Chemical Science* **12**, 9794 (2021).
[2] MacDonell et al., *Chemical Science* **14**, 9439 (2023).
[3] Valahu et al., *Nature Chemistry* **15**, 1503 (2023).
[4] Olaya-Agudelo et al., arXiv:2407.17819 (2024).
[5] Navickas et al., arXiv:2409.04044 (2024).