Analog Quantum Simulation of Chemical Dynamics

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Quantum computing offers a promising new paradigm for solving the most difficult open problems in computational quantum chemistry. In this talk, I will introduce an approach for simulating non-adiabatic dynamics using analog quantum simulators, a platform that promises to make quantum computing useful to quantum chemists in the near term and using existing quantum technologies.

Most previous work on applying quantum computing to chemistry has focused on using digital, programmable quantum computers to find energies of ground states. Our approach reduces the quantum resource requirements by an order of magnitude by focusing on dynamics and on using purpose-built analog simulators. For example, we exploit the otherwise-unused motion of trapped ions to represent the motion of the nuclei in a molecule [1]. Our approach enables the simulation of ultrafast chemical dynamics, which is among the most difficult simulation problems in chemistry because it involves the entangled motion of both nuclei and electrons. Our framework can be used to carry out scalable simulations of molecular spectroscopy in the time domain, which we have implemented experimentally, achieving quantitative agreement for the photoelectron spectrum of SO_2 [2]. We have also used our approach to accomplish the first direct observation of destructive nuclear interference caused by wavepacket dynamics around a conical intersection [3].

These theoretical and experimental results a clear path to using near-term quantum devices to carry out chemical-dynamics simulations impossible on current supercomputers.

References:

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[3] Valahu*, Olaya-Agudelo*, MacDonell, Navickas, Rao, Millican, Biercuk, Hempel, Tan, Kassal, “Direct observation of geometric phase in dynamics around a conical intersection”, arXiv:2211.07320 (2022).