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Trapped-ion quantum simulations for condensed-phase chemical dynamics: seeking a quantum advantage

Mingyu Kang (Duke University)

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ABSTRACT

Simulating the quantum dynamics of molecules in the condensed phase represents a longstanding challenge in chemistry. Trapped-ion quantum systems may serve as a platform for the analog-quantum simulation of chemical dynamics that is beyond the reach of current classical-digital simulation. To identify a "quantum advantage" for these simulations, performance analysis of both classical-digital algorithms and analog-quantum simulation on noisy hardware is needed. In this Perspective, we make this comparison for the simulation of model molecular Hamiltonians that describe intrinsically quantum models for molecules that possess linear vibronic coupling, comparing the accuracy and computational cost. We describe several simple Hamiltonians that are commonly used to model molecular systems, which can be simulated with existing or emerging trapped-ion hardware. These Hamiltonians may serve as stepping stones toward the use of trapped-ion simulators beyond the reach of classical-digital methods. Finally, we identify dynamical regimes where classical-digital simulations seem to have the weakest performance compared to analog-quantum simulations. These regimes may provide the lowest hanging fruit to exploit potential quantum advantages.

BIOGRAPHY

Mingyu Kang is a Physics PhD student at Duke University working with Prof Kenneth Brown. He does theoretical research on quantum control, quantum error correction, and quantum simulation. He is particularly interested in how theoretical ideas are experimentally implemented in quantum platforms, such as trapped ions.

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