Quantum Science & Engineering Center

Quantum Computing Seminar Series

Snack &

GEORGE MASON UNIVERSITY

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Atomically Precise Nanochemistry and Quantum Computing: Where are we headed?

***Monday, February 20, 2023,*| 12:30–1:30pm | 3301 Exploratory Hall | Zoom**

Abstract

Atomically precise nanochemistry has become a widely studied subject by experimentalists and computational chemists alike. Often, researchers are interested in understanding structure-property relationships, which may include electronic structure, optical spectra, and electrochemical profiles. Computationally, researchers have relied on Density Functional Theory and Ab initio Molecular Dynamics (AIMD) to understand these critical relationships. While these methods do allow the community to gain some understanding, there are various shortfalls including chemical accuracy and the amount of time to obtain reliable results. Quantum Computing presents an opportunity to help reduce or eliminate the shortfalls of traditional computational chemistry approaches. In this talk, I will present some of our current work on atomically precise nanochemistry and give an outlook on how we envision quantum computing changing the landscape in the atomically precise nanochemistry.

Zoom link: https://go.gmu.edu/qcseminar

About the Seminar Series

The Quantum Computing Seminar Series are a series of working seminars organized and hosted by QSEC's quantum computing subgroup on Mondays. These events are free and open to the public. More information is available on QSEC's Computing Events and Mathematical Sciences Department's Quantum Computing Seminars. For any questions, contact qsec@gmu.edu.

Light snacks and coffee will be provided at the beginning of the seminar.