

# Thesis Defense in Chemistry

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Monday, July 8, 2019 at 2:00pm

Room 501 NW Corner

\*\*\*Please note location\*\*\*

Towards an accurate description of strongly correlated chemical systems with phaseless auxiliary-field quantum Monte Carlo - Methodological advances and applications

**Presented by James Shee**

*Friesner & Reichman Groups*

Abstract: Solving the electronic Schrodinger equation for chemical systems is a long-standing problem, due primarily to the fact that the complexity grows exponentially with the number of electrons. I will introduce a method called phaseless auxiliary-field quantum Monte Carlo, which after a number of recent developments, is capable of producing accurate predictions in a reasonable amount of wall-clock time, scaling as a low-polynomial of system size. Promising results are obtained even in the regime of strong electron correlation - as exemplified by transition metals, singlet biradicals, and bond-breaking events - which opens the door to a wide variety of applications relevant to drug design, catalysis, and optical devices.



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