



THE UNIVERSITY OF  
**CHICAGO**

THE COMMITTEE ON  
COMPUTATIONAL AND  
APPLIED MATHEMATICS

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The Reichman Group  
Columbia University

## **Auxiliary-Field Quantum Monte Carlo for Electronic Ground State and Thermal Electronic States**

FRIDAY, March 17, 2022 at 4:00pm  
Jones 303, 5747 S. Ellis Ave. Chicago, IL 60637  
OR  
via Zoom

Quantum chemistry has become an indispensable tool in revealing the microscopic details of molecules and materials such as barrier heights, interaction energies, and correlation functions. Obtaining an accurate approximate solution to the electronic Schrödinger equation has been an active research area in quantum chemistry. In this talk, I will discuss an accurate, scalable approximation to the electron correlation problem known as auxiliary-field Quantum Monte Carlo (AFQMC). I will discuss its power for electronic ground states and thermal electronic states as well as related algorithmic developments.

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Organizer:

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