



DR. EDWARD VALEEV

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“PREDICTIVE AB INITIO QUANTUM CHEMISTRY FOR LARGE MOLECULES AND MATERIALS”

November 22nd, 2019 ~ 11:30AM
Life Science Center II, Room 130

Abstract: Despite its massive success in enabling accurate in-silico chemistry and materials science, the Density Functional Theory (DFT) has many known shortcomings. While the search for the exact density functional is continuing unabated, dramatic advances have recently occurred in the development of wave function electronic structure methods. While traditionally much more expensive than the DFT methods and limited to systems with 20-30 atoms, the recent improvements in the wave function-based methods have enabled accurate description of systems with thousands of atoms. These developments position the new generation of the wave function methods as a viable alternative to the approximate DFT. In this talk I will review the recent advances that made the predictive ab initio quantum chemistry methods possible and preview applications of these methods to problems in chemistry and materials science.

FALL 2019 CHEMISTRY SEMINAR SERIES

**HOST:
DR. MICHELE
PAVANELLO**

**COFFEE SOCIAL
11:00 AM
OLSON HALL, 338**

**ALL THOSE
INTERESTED ARE
WELCOME TO
ATTEND**

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