

# Joint Quantum Sciences Seminar

**Wednesday, November 6, 4:30 pm**  
**Jefferson 250**

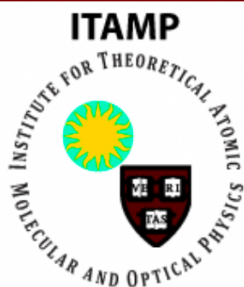
## Prof. Sabre Kais

Department of Chemistry, Department of Physics and Astronomy, and Brick  
Nanotechnology Center, Purdue University

### *“Quantum Information and Computation for Complex Chemical Systems”*

I will give a brief overview of the recent advances in quantum information and computation for chemistry. Then present the challenging problems in quantum computing for complex chemical systems focusing on electronic structure calculations and open quantum dynamics. I will present three related approaches to electronic structure calculations: The quantum circuit model with qudits, the adiabatic quantum computing model by transferring the electronic structure Hamiltonian to an Ising type Hamiltonian and the quantum machine learning approach. Quantum machine learning – a hybridization of classical machine learning techniques with quantum computation – is emerging as a powerful approach that may have impactful applications in chemistry particularly on electronic structure and quantum state classifications. Then I will present our recent developed quantum algorithm for evolving open quantum dynamics on quantum computing devices. Finally, I will discuss the opportunities, open questions and challenges in the field of quantum computing for complex chemical systems.

**There will be no student speaker**  
**Guest Presentation will begin at 4:30 PM**  
**Refreshments will be provided**



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