



**Monday, April 10 2017, 12:00 pm**  
**Seaver Science Library, Room 150**  
*SSC Auditorium next to the library*

## **Professor Dominika Zgid**

*Department of Chemistry*  
*University of Michigan*

# **QM/QM Embedding Scheme for Strongly Correlated Problems**

### **Abstract:**

We present a detailed discussion of self-energy embedding theory (SEET), which is a QM/QM embedding scheme allowing us to describe a chosen subsystem very accurately while keeping the description of the environment at a lower cost. We apply SEET to molecular examples where commonly our chosen subsystem is made out of a set of strongly correlated orbitals while the weakly correlated orbitals constitute an environment. Such a separation is very general and can be applied to both molecules and solids.

On a set of carefully chosen molecular examples, we demonstrate that SEET, which is a controlled, systematically improvable Green's function method, can be as accurate as established wave function quantum chemistry methods. Finally, we discuss possible generalization of SEET to periodic problems.

Hosted by Professor Anna Krylov

*The scientific community is invited*