# CORE-CM SEMINAR
# Michigan State University — Department of Chemistry


## Dr. Benjamin Schwartz
## UCLA


# To Be or Not to Be a Cavity: The Hydrated Electron Dilemma


The hydrated electron -- the species that results from the addition of a single excess electron to liquid water -- has been the focus of much interest both because of its role in radiation chemistry and other chemical reactions, and because it provides for a deceptively simple system that can serve as a means to confront the predictions of quantum molecular dynamics simulations with experiment. Despite all this interest, there is still considerable debate over the molecular structure of the hydrated electron: does it occupy a cavity, have a significant number of interior water molecules, or a structure somewhere in between? The reason for all this debate is that different computer simulations have produced each of these different structures, yet the predicted properties for these different structures are still in reasonable agreement with experiment. This talk will explore the reasons underlying why different structures are produced when different pseudopotentials are used in quantum simulations of the hydrated electron. It also will explore the agreement between different hydrated electron models and certain key experiments, such as resonance Raman spectroscopy and the temperature dependence and degree of homogeneous broadening of the optical absorption spectrum, in order to distinguish between the different simulated structures. Taken together, the results suggest that the hydrated electron likely has a significant number of interior water molecules.


**Thursday, January 23, 2014**
**12:00 PM**
**Room 1400 – BPS**
**Professor Warren Beck – Host**

*Accommodations for persons with disabilities may be requested by calling the Chemistry Department at (517) 355-9715, X191 two days prior to the event to ensure sufficient time to make arrangements. Requests received after this date will be met when possible.*