

**SEMINARS IN  
CHEMICAL AND BIOMOLECULAR ENGINEERING****Friday, February 05, 2016 10:00AM****PENTHOUSE****BH8500**

Presented by

**L**uke Roling

Ph.D. Candidate, Chemical Engineering

**U**niversity of Wisconsin-Madison***“First-Principles Design of Fuel Cells Catalysts with Reduced Platinum Dependence”***

*Fuel cells have great potential to revolutionize the energy sector and replace fossil fuels, particularly in portable applications such as vehicles. However, their commercialization is limited by the high cost of the platinum catalysts required at the electrodes as well as infrastructural challenges related to fuel transportation and storage. In this seminar, I describe first-principles density functional theory (DFT) calculations to address these challenges facing the design of more practical fuel cell catalysts. I focus particularly on the structure sensitivity of fuel cell reactions to leverage recent advances in shape-selective catalyst synthesis toward the design of lower-cost catalysts with improved activity and durability. First, I present dimethyl ether as a candidate fuel cell feed and examine the structure sensitivity and potential dependence of its detailed decomposition mechanism on representative crystal facets of platinum nanoparticles. Next, I describe the computational design of improved palladium-platinum core-shell catalysts for the cathodic oxygen reduction reaction, which reduce the materials cost of fuel cells. Innovative theoretical models are combined with novel synthesis techniques to yield new classes of highly active and stable electrocatalysts with greatly reduced platinum dependence. In addition to predicting reactivity, computations identify fundamental processes occurring during nanocrystal formation that enable the formation of the novel catalyst structures. Together, these studies provide critical atomic-scale insight towards identifying economical, optimized fuel cell catalysts.*

**Luke Roling** is a PhD Candidate under Professor Manos Mavrikakis at the University of Wisconsin-Madison. He received a B.S. degree in chemical engineering and a B.S. degree in mathematics from Iowa State University in 2011. His research interests include heterogeneous catalysis and alternative energy.