

# Materials Seminar

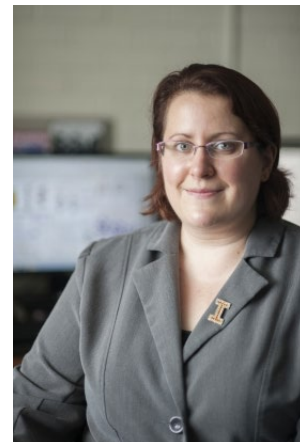
## Professor Sara Mason

University of Iowa  
Department of Chemistry

*“Modeling Cation Release of Compositionally-Tuned Complex Metal Oxides from First-Principles and Thermodynamics”*

Nanoscale complex metal oxides have transformed how technology is used worldwide. The most widespread examples are the electroactive components of Li-ion batteries found in portable electronic devices. As the number of portable devices is projected to increase, so too will the inadvertent release of complex metal oxide nanomaterials into the environment. This is a pressing problem because the environmental and biological impact of complex metal oxide nanomaterials are most times unknown, since they are subject to transform rapidly with changes in pH and concentration. This brings us to a looming problem that needs to be solved on a global scale. There is a fundamental knowledge gap in developing sustainable nanotechnology because there is not yet a systematic method to predict how the properties of a complex metal oxide will change with changes in chemical environment. We have developed a modeling approach, based on Hess's Law, which combines DFT-computed total energies and experimentally adjustable reaction conditions to compute the surface dissolution of complex metal oxides. We focus on the materials found in a Li-ion battery cathode, namely  $\text{LiCoO}_2$  and compositionally tuned variants with general chemical formula  $\text{Li}(\text{NixMnyCoz})\text{O}_2$ . We find that adjusting surface terminations, compositions and pH will change the dissolution properties of this family of materials, and yields insights into the nanoscale transformations that may take place under a given set of conditions. Not only can these results be used to improve environmental fate and toxicity models, but we are able to use the results of our analysis to create a set of rational design rules to govern the creation of the next-generation of Li-ion battery cathodes that will be benign by design.

Host: Prof. Bob Hamers



Thursday  
October 18<sup>th</sup>

12:15 p.m.  
1315 Chemistry

Coffee & cookies  
at 12 p.m.



DEPARTMENT OF  
Chemistry  
UNIVERSITY OF WISCONSIN-MADISON