

# Chemistry Seminar

Electronic Structure as a Predictor of  
Hydrated Oxide Surface Reactivity

Dr. Sara Mason  
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Friday, Nov. 12

12:00 p.m.

WSB-119

(Note new date and room)

Abstract: It is now well-established that oxide surface structure is dependent on the conditions to which the surface is exposed, and that clean surface structures found in ultra-high vacuum conditions can evolve significantly as a function of water and oxygen exposure. However, the structure-property relationships of hydrated oxides remain poorly understood, limiting both the ability to interpret empirical trends in environmental interface reactivity and the rational design of hydrated surfaces with tailored reactivity. The oxide-water interface introduces complexity not found in analogous ultra-high vacuum surface science, complicating the goal to identify the key factors driving reactivity. When coupled with an ab initio thermodynamic framework, density functional theory can be used to study and predict structure and important classes of reactivity at hydrated oxide surfaces. Examples are presented in which electronic structure analysis is used to provide new molecular-level understanding of adsorption processes at oxide-water interfaces. The focus is on the uptake of heavy metal cations to form inner-sphere surface complexes, with implications for broader classes of reactivity.

Dr. Mason will meet with students at 1:00 p.m. in WSB-344.