

PHYSICAL CHEMISTRY SEMINAR



Professor Jeff Greeley
Purdue University

Host Prof. J.R. Schmidt

“First principles studies of heterogeneous (electro)catalysis: incorporating structural complexity into catalyst reactivity and screening studies”

***Tuesday
November 6th
11:00 am***

***Room 1315
Chemistry
Building***

In his talk, Prof. Greeley will begin by discussing how his lab has applied strategies from computational heterogeneous catalysis to screening of electrochemical catalysts for the classic oxygen reduction reaction, and he will then explore challenges in extending such screening studies to more structurally and mechanistically complex catalytic processes. He will illustrate some of these challenges through a detailed analysis of electrocatalytic reactivity at bifunctional metal/(oxy)hydroxide interfaces in alkaline solutions, first describing the development of structural models of these interfaces, which involves a combination of ab-initio thermodynamic and molecular dynamic analyses, and then discussing how the mechanisms and rates of classical electrocatalytic processes, such as hydrogen evolution, may be significantly accelerated by these structures. He will close by illustrating how some of the insights gained from these studies might be extended to facilitate future catalyst screening studies on these fascinating molecular architectures.



Department of Chemistry
UNIVERSITY OF WISCONSIN-MADISON

Graduate students can meet with the speaker in Room 8305F at 1:00 pm