"C^4E – Computational Chemistry of Compounds for Catalysis and Energy"

Wednesday
April 3, 2019
3:00 pm
Wu and Chen Auditorium
Levine Hall

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Abstract

At the forefront of contributing to solve the sustainable energy puzzle, one now finds first-principles based computational methods, providing a good balance between accuracy and computational cost. With these computational approaches, one can not only describe and understand chemistries of already known materials, but also allow for prediction of new materials through a careful analysis of the surface chemistry at the atomic level. I will demonstrate how we have been able to computationally predict several new catalyst materials. This presentation will first focus on electrochemical reactions, including both of the water splitting subreactions: the hydrogen evolution reaction (HER) on 2D materials, and oxygen evolution reaction (OER) on a highly active earth abundant catalyst and the most active catalyst to date that all have been experimentally synthesized, characterized and tested. I will also share our recent insights on the stability and activity of a nanostructured OER catalyst system showing a new surface activation phenomenon. Finally, I will discuss our ongoing efforts on more complex compound materials' chemistries and geometries used in energy applications beyond catalysis, such as fuel cells and batteries.

Bio

Dr. Aleksandra Vojvodic is the Skirkanich Assistant Professor of Innovation in the Department of Chemical and Biomolecular Engineering at the University of Pennsylvania, since September 2016. Her research focuses on theoretical and computational-driven materials design, in particular, on studies of surfaces and interfaces of complex materials for chemical transformations and energy conversion and storage.

She is the recipient of the 2017 European Federation of Catalysis Societies (EFCATS) Young Researcher Award, and the MIT Technology Review 35 Award (2016), which recognized her work and innovative approaches by identifying her as a "computation whiz that speeds up the search for catalysts that will make green chemistry possible." She has also recently been selected as a CIFAR Bio-inspired Solar Energy program fellow and Scialog fellow in Advanced Energy Storage. She has published more than 65 papers in journal publications, including Science, Energy & Environmental Science, Nature Materials, Nature Energy, Nature Communications and JACS.

Before joining the University of Pennsylvania, she was a staff scientist at the SUNCAT Center for Interface Science and Catalysis at SLAC National Accelerator Laboratory, where she lead a group conducting research on oxide surface reactivity. She was the Swedish Research Council postdoctoral scholar in the Department of Chemical Engineering at Stanford University, and at the Center for Atomic-scale Materials Design at Technical University of Denmark. She received her Ph.D. in Physics from the Department of Applied Physics at Chalmers University of Technology and her Master of Science in Physics from Lund University in Sweden.

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