PennState College of Engineering | CHEMICAL ENGINEERING

Chemical Engineering Seminar Series

Computational prediction of complex materials and their chemistries – Creating possibilities for materials design

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Abstract

Fueling the planet with energy, chemicals and food are central challenges of the 21st century. In our chemical industry most materials we see in our everyday life have seen at one point or another a catalyst material of a complex nature. I will demonstrate how we can computationally predict new catalyst materials through a careful analysis of their surface chemistry at the atomic-scale level enabled by access to advanced computational approaches and illustrate how this can be used to design new materials systems.

I will present our studies on electrochemical water splitting including both of its subreactions: the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Computationally we have identified a new highly active two-dimensional (2D) transition-metal carbide HER catalyst and transition-metal oxide OER catalysts that have been experimentally synthesized, characterized and tested. The OER catalysts belong to the perovskite group of oxide materials or are oxides based on earth abundant metal elements. I will also share our recent insights on the reactivity and activity of metal-supported thin layers, nanoparticles of oxides and heterostructured oxide systems. Finally, I will discuss our recent findings on oxygen incorporation chemistry of non-stoichiometric oxides.

Biosketch

Dr. Aleksandra Vojvodic is the Skirkanich Assistant Professor of Innovation at 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 the 2017 European Federation of Catalysis Societies (EFCATS) Young Researcher Award and of the MIT Technology Review 35 Award 2016 which recognized her work and innovative approaches by identified 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 60 papers in journals including Science, Nature Materials, Energy & Environmental Science, Nature Energy, Nature Communications and JACS.

Before joining U Penn 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 at 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.

Friday, April 6, 2018

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11:00-12:00 p.m.