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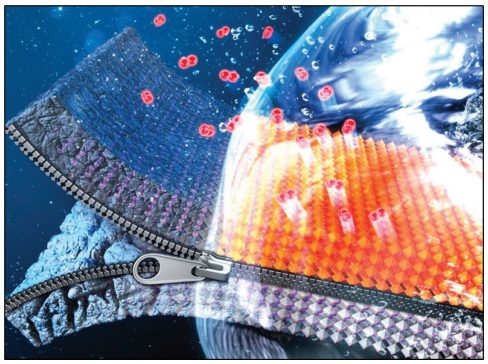
C^4E – COMPUTATIONAL CHEMISTRY OF COMPOUNDS FOR CATALYSIS AND ENERGY

The race to solve the sustainable energy puzzle is on. First-principles based computational methods, which balance accuracy and computational cost, are at the forefront for solving this puzzle. These computational approaches allow one to describe and understand chemistries of already known materials, and, importantly, they can be used to predict new materials. In this talk, I will first demonstrate how we have been able to computationally predict several new complex catalyst materials including metal oxides, which have been experimentally synthesized, characterized and tested. I then share recent insights on the stability and activity of computationally predicted catalyst systems and conclude with our new efforts to understand the dynamic behavior of these complex materials. Together, this research agenda aims to replace trial-and-error, time-consuming approaches as the main source of development for new materials and chemical routes with a systematic computational materials modeling strategy.



ABOUT THE SPEAKER

Dr. Aleksandra Vojvodic is the Rosenbluth Associate Professor at the Department of Chemical and Biomolecular Engineering and the Director of Penn Institute of Computational Science at the University of Pennsylvania. 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. Recently, she was recognized as the Trottier Fellow in Bio-inspired-solar-energy (2021) and one of the "Women Scientists at the Forefront of Energy Research" (2020). 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 led 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.