ETH zürich

Understanding and Designing Metal Oxide Behavior from the Ground up: Density functional theory as a critical tool for improving performance

Tuesday, 21st May 2019, 4 pm to 5 pm
ML J 25, ETH Zurich, Sonneggstrasse 3, 8092 Zurich

Host: Prof. A. Steinfeld, Professorship of Renewable Energy Carriers

Metal oxides are a wide class of materials characterized by oxidized metal centers and reduced oxygen centers. Within this group are a wide range of behaviors and applications to processes critical to sustainability on this planet, particularly renewable energy generation and storage and remediation of the environment around us. Due to their complexity and numerous compositional design space computational tools are critical in understanding the fundamental physics of their behavior and in the design and rapid screening of novel materials. Particularly the density functional theory (DFT) implementation of quantum simulations enables a priori examination of properties without the need for human input into the models which can predetermine the outcome. In this seminar, we will explore the use of DFT in understanding and design metal oxide materials for two classes of reactions: oxygen exchange materials for fuel production and selective adsorbents for aqueous toxic oxo-anions. In these cases, we will examine problems where DFT is highly successful as well as cases were additional techniques are required, and how we can use machine learning techniques to overcome these challenges. Through the understandings develop we are able to propose new materials designs that provide better performance which is validated experimentally.

Dr. Christopher Muhich is an Assistant Professor of Chemical Engineering within the School for the Engineering of Matter, Transport and Energy at Arizona State Univer- sity. He earned a B.S.E in Chemical Engineering from the University of Michigan (2009) and a Ph.D. in Chemical Engineering at the University of Colorado at Boulder (2014) under the su- pervision of Profs. Al Weimer and Charles Musgrave. He did postdoctoral work at ETH Zurich (Swiss Federal Institute of Technology) with Aldo Steinfeld before joining ASU in 2018.

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