TcSUH Bi-Weekly Seminar

Computational Design of Functional Materials in Catalysis and Electrochemical Energy Storage

Prof. Lars Grabow

Dan Luss Associate Professor of Chemical and Biomolecular Engineering; Associate Professor of Chemistry (by courtesy); TcSUH PI

Friday, February 7, 2020

Room 102, Houston Science Center

12:00 p.m. – 1:00 p.m.

RSVP for sandwich by 12 p.m. Thurs. Feb. 6th:

cblake3@central.uh.edu

Abstract: Advanced functional materials are at the heart of nearly any solution to challenges in clean energy, health, national security or human welfare in general. Unfortunately, their discovery often happens "by accident" in repeated trial-and-error experimentation. Through the Materials Genome Initiative (MGI) launched in the U.S. in 2011 large scale efforts were made to discover, manufacture and deploy advanced materials twice as fast, at a fraction of the cost (www.mgi.gov). Most of the funded research under the MGI, as well as many other parallel efforts, exploited computational and data-science approaches to increase the rate of materials discovery with variable success.

In our group we use a combination of predictive ab initio simulations coupled to statistical analysis tools to guide the discovery and development of new functional solid-state materials. For the design of heterogeneous catalysts used in the treatment of diesel exhaust emissions, we have used density functional theory (DFT) simulations to calculate reaction pathways and identify reactivity descriptors that allow rapid screening of the binary metal alloy space. Through our computational study we discovered a new metal alloy that shows great promise to meet the U.S. Department of Energy 150°C challenge for diesel oxidation catalysis, and the results were confirmed in bench scale reaction experiments. In contrast, we bypass any physical knowledge of the system in our attempts to discover solid state electrolytes to be used as ion conductors in all solid-state Li-ion batteries. Instead, we rely on statistical models and jump directly from the electronic structure of the material to the macroscopically observable conductivity. Finally, we combine a physical model for the stability of dilute surface alloys with an error correction term, that is trained using black box machine learning methods. The results are encouraging in that the model can extrapolate to new materials with reasonable accuracy and predictive power. Overall, these examples demonstrate that computational materials design has many merits, but there are many limitations and challenges that still need to be addressed for a successful implementation of artificial intelligence in the design of advanced materials.

BIO: Prof. Lars Grabow is the Dan Luss Associate Professor in the Department of Chemical and Biomolecular Engineering at the University of Houston and holds a courtesy appointment in the Department of Chemistry. He received his PhD in Chemical Engineering from the University of Wisconsin in 2008, followed by postdoctoral appointments at the Technical University of Denmark and Stanford University. His expertise is the application of electronic structure calculations, kinetic modeling, data science and transient kinetic characterization to problems in heterogeneous catalysis, surface science and electrochemical energy storage. His papers have been cited more than 4,000 times and he was elected into the 2018 Class of Influential Researchers by Industrial and Engineering Chemistry (IE&C) Research. Prof. Grabow won the prestigious U.S. Department of Energy (DOE) Early Career Award (2014) and the NSF CAREER Award (2015), the Excellence in Research Award at the assistant professor level from the University of Houston (2017). Currently, he serves as Chair of the Southwest Catalysis Society (SWCS) and is the Past Chair of the AIChE Catalysis and Reaction Engineering (CRE) Division. He is a member of the International Advisory Board of ChemCatChem, the Editorial Advisory Board of Surface Science, and a past member of the Early Career Advisory Board of ACS Catalysis.

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