

Modern Paradigms for Computational Catalyst Design in Energy Transition

Speaker: Prof. Lars Grabow

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Abstract: Efficient heterogeneous catalysts are crucial for renewable energy and sustainable feedstock. Traditional computational catalyst design optimizes binding energies of surface intermediates to achieve optimal catalytic activity, guided by the Sabatier principle. The Open Catalyst Project (OCP) has revolutionized this field by providing a powerful screening framework. Using OCP and machine learning, we predicted electrocatalysts for the oxygen evolution reaction (OER) in water electrolysis, evaluating 4,728 oxide materials and over 4 million surface intermediate predictions. Our criteria included synthesizability, stability, cost, and overpotential, leading to new candidate materials verified by density functional theory (DFT). Additionally, we collaborate with the Center for Programmable Energy Catalysis (CPEC) to enhance catalyst activity beyond the Sabatier limit by modulating surface binding properties using a catalytic condenser. This approach, tested in steam methane reforming (SMR), shows promise for capturing methane emissions and improving catalytic activity through dynamic modulation. Our combined strategies aim to accelerate the transition to a sustainable future.



Biography:

Prof. Lars Grabow is the Dan Luss Professor in the William A. Brookshire Department of Chemical and Biomolecular Engineering at the University of Houston. 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 and electro-catalysis, surface science, and energy transition. His papers have been cited more than 9,100 times (Google Scholar) 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), the NSF CAREER Award (2015), and most recently, the Andrea Prosperetti Research Computing Faculty Award from the Cullen College of Engineering at the University of Houston (2021). He currently serves as Editor-in-Chief of ChemistryEurope, and was previously Editor of Surface Science.