## The Goldsmith Lab

**First-Principles Modeling of Catalysts and Materials**

University of Michigan – Ann Arbor, Department of Chemical Engineering

### Theme 1: Catalysis for Air and Water Pollution Reduction

**Single Atom and Nanocluster Catalysis for CO₂ reduction**

- CO₂ can be reduced via H₂ to produce either methane (CH₄) or carbon monoxide (CO). Depending on the presence of nanoclusters or single atoms.
- What impact on catalytic activity and selectivity can be seen from varying the metal nanocluster size and support surface?

**Pl₃Ru₃ alloys for electrocatalytic nitrate reduction**

- Aqueous nitrate (NO₃⁻), a major water pollutant, can be remediated with electrocatalytic nitrate reduction.
- Metal alloys can perform this reaction with higher activity (higher turnover frequency, TOF) than their pure-metal counterparts.
- What alloy compositions make the most active and selective catalyst?

### Theme 2: Machine Learning to Accelerate Catalyst Design

**Interpretable, Theory-Guided Machine Learning for Chemisorption on Alloys**

- The objective of this research is to develop physically transparent and accurate structure-property models for understanding chemical interactions on alloy surfaces.

**Machine Learning Enabled High-Throughput Evaluation of Catalysts**

- Machine learning applied to alloys yields insights into the effect of the number of d-electrons in the ligand metal for various adsorbates.

### Theme 3: Catalysis for Renewable Energy Generation, Use, and Storage

**Redox Flow Batteries for Large-Scale Energy Storage**

- Redox flow batteries are used to match power grid supply to demand, which is increasingly relevant as we transition to intermittent renewable energy sources.

**Metal and Bimetallic Catalysts for Bio-Oil Hydrogenation**

- Biomass-derived molecules can be upgraded to fuels and industrially relevant chemicals using aqueous-phase electrocatalytic hydrogenation driven with renewable electricity.

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### Methods A: First-principles modeling and molecular simulation techniques

- Cutting-edge computational techniques yield an accurate description of catalyst and material electronic and geometric properties under realistic conditions.
- Minima and saddle search algorithms

### Methods B: Data science and machine learning for materials

- Data analytics applied to catalyst data offers opportunities to advance discovery.
- We develop and apply machine learning approaches to uncover catalytic insights.

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**The Goldsmith Lab**

- 5 PhD students
- 4 Undergraduate students

**Goldsmith Lab (Fall 2020)**

Combining first-principles (electronic-structure theory) modeling and data science to understand catalysts and materials.