Theme 1. Amorphous catalytic solids: beyond ordered materials

Amorphous catalysts are widely used in industry and are often superior to crystalline catalysts.

- The research objectives are to increase understanding of catalysis by metal ions and metal clusters dispersed on amorphous solids.

- Amorphous oxide catalysts and supports
- Metas isolated and dispersed on amorphous supports
- Metal oxides on amorphous supports

Amorphous Oxides as Catalyst Supports: Development of Improved Models

Atomically Dispersed Catalysts on Amorphous Supports

\[ \text{WO}_x \text{S}_y \text{O}_z \] supported on \( \text{SiO}_2 \), for the formation of propene from ethene and butene

The nature of the active site(s) of \( \text{WO}_x \text{S}_y \text{O}_z \) is still a matter of debate.

WO crystallite can be ruled out as the catalytically active species.

Methods A. First-principles modeling and molecular simulation techniques

A detailed understanding of catalysts and materials requires an accurate description of their electronic and geometrical properties under realistic conditions.

- Density functional theory
- Ab initio molecular dynamics
- Minima and saddle search algorithms

Cluster models

Slab models

Ab initio thermodynamics and rate theories

Methods B. Data science and machine learning for materials

Data analytics tools applied to materials data offers opportunities to accelerate materials discovery.

The primary goal of this research is to develop and apply machine learning tools to find materials science insights.

- Subgroup discovery
- Apply subgroup discovery to examine 24,480 metal-gas-phase grid-cluster configurations (of data S-26 atoms).

- Find relations between geometrical and electronic properties.

Theme 2. Single atom and nanocluster catalysis

Catalysis is prerequisite for more than 20% of all production in the industrial world.

- The objectives of this research are to understand single atoms, nanoclusters, and nanoparticles dispersed on metal oxides.

- We recently reported the use of isolated Pt atoms as active sites on silica and metal oxides and their circumventions to Pt clusters, which is well documented.

Single Atom and Nanocluster Catalysis

Single Pt atoms on \( \text{Fe}_2\text{O}_3 \).

Rh nanocluster supported by a zeolite.

Gold nanoparticle supported by \( \text{CO}_3 \).

We recently reported the use of isolated Pt atoms as active sites on silica and metal oxides and their circumventions to Pt clusters, which is well documented.

Methods C. Principles Modeling of Catalysts and Materials

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

Theme 3. Electrocatalysis for waste remediation and energy

Electrocatalysis can use renewable energy to drive sustainable chemical transformations.

Understanding metal and bimetallic surfaces for enhanced-efficiency electrocatalysts to drive hydrogen production.

- Electrochemical Reduction of NO to \( \text{N}_2 \) for Wastewater Remediation: Closing the Nitrogen Cycle

Goldsmith Lab (Fall 2019)

- 5 PhD students and 1 MS student
- 5 Undergraduate students

Goldsmith Lab (Spring 2022)

- 100 Undergraduate students

First-Principles Modeling of Catalysts and Materials

The Goldsmith Lab

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