

# Unifying Principles in Hydrotreating Catalysis

## Research Themes

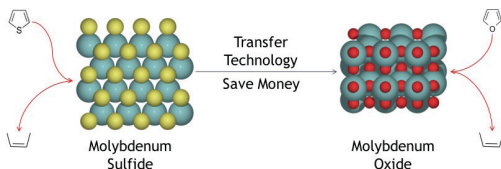
- Efficient heterogeneous catalysts for the upgrade of bio-oil to renewable fuels and chemicals
- Discovery of catalytic similarities and differences between hydrodeoxygenation and hydrodesulfurization from first principles
- Computational investigation of reaction mechanism and active sites on metal oxide catalysts
- Computational screening of transition metal promoter materials
- Predicting metastable active catalytic phases using structure prediction and ab-initio thermodynamic phase diagrams

## Recent Accomplishments

- Developed a rigorous ab-initio thermodynamic phase diagram and relevant computational kinetic studies to resolve remaining ambiguities in the literature regarding the nature of oxygen vacancy sites on Molybdenum oxide catalysts
- Funding for travel, GRC conference on Catalysis (Sawyer College, MD, June, 2016)
- AIChE CRE Travel award (Salt Lake City, UT, Nov. 2015)
- Best Poster Awards (OChEGS at UH - Sep. 2015, and CAMD at DTU Denmark – Aug. 2014)

## Issues

- Molybdenum oxide catalysts have complicated structures and many active site configurations are possible
- Stability of catalysts under prolonged exposure to very acidic pyrolysis oil
- Over utilization of H<sub>2</sub> and low activity of metal oxide catalysts
- Role of mixed oxycarbide phases formed reversibly under reaction conditions is still unknown



**Sashank Kasiraju**

Major/Field of Study: Chemical Engineering

College: Cullen College of Engineering

Professor: Dr. Lars C. Grabow

Email: [skasiraju@uh.edu](mailto:skasiraju@uh.edu)

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