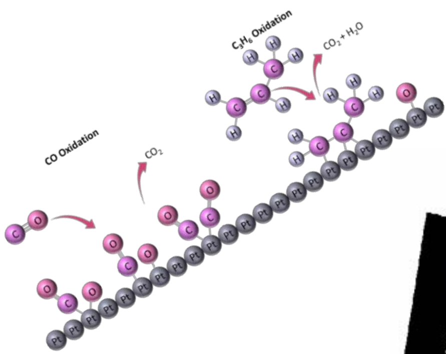

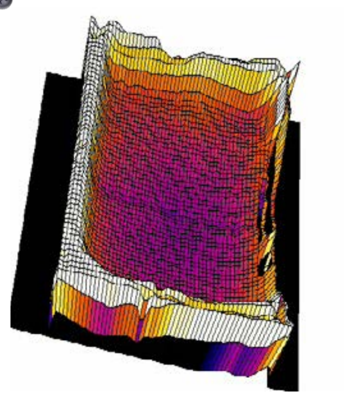

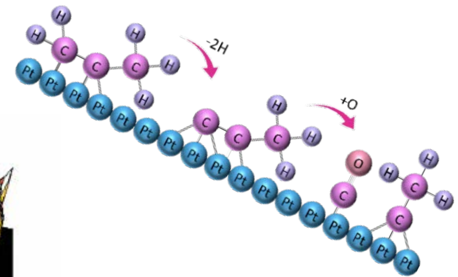

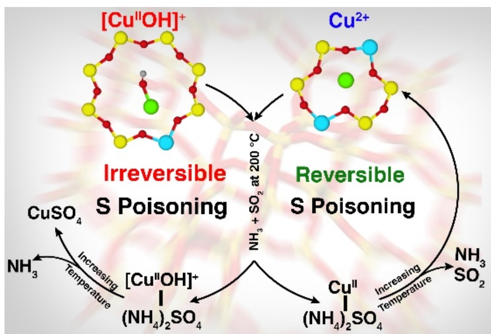

Catalysis is ubiquitous in manufacturing, with estimates that 90% of all products involving chemical processes include a catalytic step. Our research group focuses on understanding and engineering the reaction process on and along a catalyst surface, and how these change as a function of catalyst degradation modes. This encompasses the preparation of novel catalyst materials, the fundamental characterization of catalyst surfaces, and developing new analytic techniques, processes or devices, such that we can tailor design catalysts at the atomistic and reactor levels. All of which results in our ability to obtain and translate in-depth fundamental catalyst knowledge to practical, industrially relevant applications Of late, our focus is on eliminating pollutants from energy sources, diesel engines in particular, converting methane to higher value chemicals, and understanding and mitigating catalyst degradation in general.

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"Catalyst designs for the reaction and the reactor, from the atomistic to full scale."

University of Virginia
School of Engineering & Applied Science

Reducing NOx Emissions – Selective Catalytic Reduction (SCR)

With the world's increasing desire for mobility and thus transportation, more cars and trucks than ever are on the road. And with these come NOx emissions, which contribute to smog and ground level ozone formation and therefore the increasingly stringent regulations world-wide to combat NOx emissions and maintain air quality. Furthermore, with greater recognition of climate change, more efficient engines are being developed to reduce fuel use and thus CO_2 output. Our research seeks to predict NOx reduction catalyst performance changes as a function of new engine exhaust compositions, develop operating strategies to improve reduction performance and increase performance longevity. We use standard and novel catalyst and reaction characterization techniques to determine the reaction mechanisms, and to determine how catalyst performance decays. For example, a common degradation process is sulfur poisoning. We study the mechanisms behind this process and then design methodologies to reverse its impact. Our research is therefore focused on decreasing the stability of adsorbed sulfur species on the active catalyst surface so that its efficiency can be maintained. This work is motivated by the need to improve air quality, and to understand the fundamental reaction mechanisms behind sulfur poisoning and thus catalyst decay.

Tailor-designing Catalysts

Catalyst poisoning or other forms of catalyst degradation do not homogeneously affect industrial-scale systems. So, although most systems operate in a steady-state mode, the integral nature of catalyst systems needs to be modeled. We use and develop new tools, functionally-specific techniques and processes to monitor changes in catalyst reaction chemistry as a function of both catalyst life and position in the catalyst bed. These results are used as inputs for time-dependent control strategies and for designing and engineering better catalysts. Current applications include catalysts for after treatment systems and light alkane upgrading. An extension of this work includes pulsed/transient operation of catalyst systems. By controlling the introduction of reactants, periodic temperature and concentration gradients within a catalyst system can be established resulting in changed catalytic activity. This change can be associated with both selectivity and conversion to the desired products. Using experimental techniques designed to be functionally specific, we monitor the transient operation and optimize the strategy toward better performance. This also allows insight to reactor-level catalyst design, which includes gradients in active site densities. These themselves result in improved performance and significantly improved catalyst lifetimes.

RECENT RESEARCH DEVELOPMENTS

- Recent work demonstrates that two SCR sulfur poisoning degradation modes exist, yet the reversible and easier to regenerate mode can be designed to dominate.
- Tailor-designing hydrocarbon oxidation catalysts with multiple zones containing different distributions of active material decreased light off temperatures by >25°C.

RECENT GRANTS

- Cummins Inc – Chemical DeSOx of SCR Catalysts

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