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Will present a seminar on

"SURFACE SCIENCE APPROACHES FOR BIOREFINING CATALYST DESIGN"

The development of “biorefining” processes for production of fuels and chemicals from biomass presents a number of interesting challenges for heterogeneous catalysis. Some of these challenges are similar to those encountered in traditional processing of hydrocarbon feedstocks. For example, there is a need to produce catalysts that can tolerate key contaminants such as sulfur. Other challenges are relatively unique to biorefineries. In particular, biomass-derived intermediates often contain multiple functional groups that can bind strongly to catalytic metal surfaces. Selective conversion of a single functional group in a multifunctional carbohydrate is often desired, but designing catalysts for such selective conversions is difficult. For example, the production of high-value chemical products from several of the carbohydrates identified as the top chemicals from biomass requires that a carbon-carbon double bond be selectively reduced while retaining the oxygenate functionality of the molecule (or *vice versa*). Such conversions are desired for reactions in the “derivative trees” of biomass-derived carbohydrates such as itaconic acid, levulinic acid, 2,5-furandicarboxylic acid, and fumaric acid. A major complication in catalyst development efforts is that metals which traditionally show excellent C=C hydrogenation activity (e.g., Pt) are also reactive toward oxygen-containing functional groups.

Our group aims to approach design of catalysts for these applications through surface-level studies of reaction mechanisms. To identify mechanisms, a combination of ultrahigh vacuum spectroscopies and molecular modeling simulations is used. Although the model systems leave out some of the complexity of the “real” catalytic systems, they offer the opportunity to unambiguously identify reaction intermediates on well-defined surfaces. After identifying the relevant mechanisms, technical catalysts can be designed from a more rational basis. This presentation will focus on our progress in designing improved catalysts for several reactions of highly functional oxygenates, and will cover multiple design approaches for tailoring surface reactivity; these approaches range from relatively conventional methods involving multimetallic surfaces to more novel designs that employ organic modifiers. The potential importance of catalyst designs for biorefining platform chemistries will be discussed.

THURSDAY, OCTOBER 8, 2009
COOKIES AND COFFEE -- 2:45 P.M.
SEMINAR -- 3:00 P.M.
SARKEYS ENERGY CENTER, ROOM M-204

THIS IS A REQUIRED SEMINAR FOR CHE 5971