Surface Science
Room 120 - Session SS-ThA

Celebration of Robert J Madix and his Contributions to Surface Science & Reception

Moderators: Liney Árnadóttir, Oregon State University, **Dan Killelea**, Loyola University Chicago

2:15pm **SS-ThA-1 Alkane Activation and Oxidation on Solid Surfaces*, Jason Weaver,*** University of Florida **INVITED**

In this talk, I will discuss pioneering advances made in Bob Madix's group to understand the mechanisms for alkane activation on metal surfaces and how this knowledge has guided my group's studies of alkane chemistry on late transition-metal oxide surfaces. Madix's work was among the first to distinguish direct vs. trapping-mediated mechanisms for alkane activation on surfaces, and clarify dynamic factors that influence these reactions. My talk will provide an overview of Madix's key findings about alkane adsorption and activation determined from supersonic molecular beam studies and molecular dynamics simulations, including mechanisms for alkane adsorption and initial C-H cleavage, energy exchange processes in alkane trapping and dynamic effects in direct alkane dissociative chemisorption. I will lastly discuss how this fundamental knowledge has influenced my research on the surface chemistry of late transition-metal oxides, and enabled new discoveries.

2:45pm **SS-ThA-3 Thermodynamics and Kinetics of Elementary Reaction Steps on Late Transition Metal Catalysts: A Tribute to R. J. Madix*, Charles T. Campbell,*** University of Washington **INVITED**

I will review experimental and theoretical results from my own group concerning the thermodynamics and kinetics of elementary chemical reactions of importance in catalysis on late transition metal surfaces. I will focus on topics wherein my interest was inspired by work from Madix's group. These include: (1) the first proposed mechanism for methanol synthesis catalyzed by Cu, (2) measurements of pre-exponential factors and their interpretations through transition-state theory (TST), (3) measurements of the entropies of adsorbates and their trends, (4) using these together with elementary-step rate measurements and adsorbate energies to build microkinetic models for multi-step catalytic reactions, (5) a method for analyzing these that quantifies the extent to which the energy of each elementary-step transition state and intermediate controls the net rate, called the degree of rate control (DRC), and (6) interpreting kinetic isotope effects (KIEs) through DRC analysis.Work supported by NSF and DOE-OBES Chemical Sciences Division.

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