

Thursday Afternoon, November 10, 2022

Fundamental Discoveries in Heterogeneous Catalysis Focus Topic

Room 321 - Session HC+AS+NS+SS-ThA

Special Session and Reception for the HC Community and to Celebrate Robert Madix

Moderators: Liney Arnadottir, Oregon State University, Dan Killelea, Loyola University Chicago, Jason Weaver, University of Florida

2:20pm HC+AS+NS+SS-ThA-1 Gaede-Langmuir Award Talk: Not a Divide - A Continuum: Surface Science to Heterogeneous Catalysis, Robert J. Madix¹, Harvard University **INVITED**

The science of surface reactivity demands control of surface structure and surface composition. Surface science methods thus enable the investigation of reactions, including oxidations, hydrogenation, and coupling, on well-characterized single-crystal surfaces by providing molecular level insight into the bond breaking and formation on surfaces that are the basis for heterogeneous catalysis. The ultimate goal of such research is to provide benchmarks for theory, forming a firm basis for *a priori* catalyst design. In the nearer term it provides a kernel of information which can be combined with theory to accurately predict rates and selectivities for extended series of analogous reactions outside the data set. In this talk, these concepts will be discussed, linking fundamental surface science studies on Au single crystals with the performance of dilute Au-based dilute metal alloy catalysts operating at elevated temperature and 1 atm pressure. The use of key surface-science methods, including XPS, vibrational spectroscopy and temperature programmed reaction spectroscopy, will illustrate the methodology for understanding catalytic reactions. This work demonstrates the ability to successfully predict surface reactivity across vast regimes of pressure, temperature and materials complexity.

¹ Gaede Langmuir Award Winner

Author Index

Bold page numbers indicate presenter

— M —

Madix, R.: HC+AS+NS+SS-ThA-1, **1**