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Tuesday, March 29th, 2022 at 4:00pm EST Virtual Meeting: Zoom

Dr. Manos Mavrikakis



Ernest Micek Distinguished Chair James A. Dumesic Professor Vilas Distinguished Achievement Professor Department of Chemical & Biological Engineering University of Wisconsin-Madison

An atomic-scale perspective on catalyst's stability and on the nature of the active site when the reaction is taking place

Addressing the question of the nature of the active site has been a central challenge in various types of catalysis (thermal heterogeneous, electrocatalysis, etc.) for a long time. With the advent of modern instrumentation providing atomic-scale information about catalytic surfaces, including under reaction conditions, and powerful spectroscopies combined with ever-increasing computational speed enabling extensive electronic structure calculations, addressing the question on the nature of the active site has become more viable. In this talk, we will discuss examples of

catalytic reactions, whereby a combination of reaction kinetics and characterization experiments with microkinetic modeling, informed by first-principles calculations, allows the derivation of insights on: (i) reaction mechanism at the elementary step level and (ii) the nature of the active site *when the reaction is taking place*. The role of spectator species versus active intermediates turning reactants over to products will be elucidated.

The second objective of this talk is to discuss catalyst's stability, a property equally important to its activity and selectivity, and which often determines whether a catalytic process becomes financially viable or not.

Speaker Bio

Manos Mavrikakis is the *Ernest Micek Distinguished Chair*, the *James A. Dumesic* Professor, and the *Vilas Distinguished Achievement* Professor of Chemical Engineering at the University of Wisconsin-Madison. He received a Diploma in Chemical Engineering from NTUA in Greece, and a PhD in Chemical Engineering & Scientific Computing from the University of Michigan, Ann Arbor. Following postdocs at the University of Delaware and the Technical University of Denmark, he joined the faculty of Chemical Engineering at UW-Madison. His main research interests include the elucidation of detailed reaction mechanisms for thermal heterogeneously catalyzed and electrocatalyzed reactions and the identification of improved catalytic materials from first-principles-based microkinetic modeling. Bridging the pressure gap between UHV experiments and atmospheric/higher pressure experiments in catalysis has been at the heart of his research.

Mavrikakis has been elected *Fellow* of *APS* (2013), *AAAS* (2014), and *AVS* (2016). He served as his Department Chair (2015-2018) and was a *Visiting Miller Research Professor* at UC Berkeley – Chemistry in 2019. He received the 2009 *Paul H. Emmett* award from the North American Catalysis Society, the 2014 *R. H. Wilhelm* award from AIChE, and the 2019 *Gabor A. Somorjai* award from ACS. Manos served as editor-in-chief of *Surface Science* between 2012 and 2020.

Presentation4:00 PMAnnual Membership Dues\$35 (Students = \$15)Deadline for reservations is 4:00PM Monday, March 28th, 2022
To make your reservation, fill out the online form.

Please refer to email announcement for login details.