

Molecular-Level Foundations of Sustainable Catalytic Transformations: A Tale of Reactive Oxygen versus Reactive Hydrogen in Catalytic Cycles

Ya-Huei (Cathy) Chin

Department of Chemical Engineering and Applied Chemistry

University of Toronto, Toronto, Canada

Abstract:

Catalytic technology development spans multiple disciplines, from elucidating atomistic and electronic phenomena to reactor engineering and process optimization. In this talk, I will present an overview of current research challenges in uncovering the structure and dynamics of catalytic surfaces and the resulting molecular dance steps of chemical building blocks that govern the sustainable synthesis of value-added chemicals and next-generation fuels. The focus is on engineering reactive surfaces with atomic precision and on reshaping the reaction free-energy landscape, enabling the discovery of new chemistry and catalytic pathways. Illustration includes two contrasting examples—the roles of reactive oxygen in oxidation of alkanes and alkanols and those of reactive hydrogen in hydrogenation and hydrodeoxygenation, both on transition metals and oxides. This molecular level knowledge guides us to discover and design of active sites and reaction environment for effective catalytic transformation.

Biosketch: Ya-Huei (Cathy) Chin is Professor and Canada Research Chair (Tier II) in Advanced Catalysis for Sustainable Chemistry at the University of Toronto. She is currently a visiting Global Fellow at TU Wien. Her research focuses on establishing mechanistic linkages and developing kinetic–thermochemical frameworks to understand catalytic events and surface dynamics during the transformation of molecular building blocks into value-added chemicals and liquid fuels. She integrates isotopic labeling, kinetic analysis, and density functional theory to interrogate catalyst surface dynamics and reaction pathways at vapor–solid and liquid–solid interfaces.



Professor Chin serves as an Associate Editor for the *Journal of Catalysis* and as an advisory board member for several leading journals in the field, including *Applied Catalysis B: Environmental, Reaction Chemistry and Engineering*, *Chem Catalysis*, and the *Canadian Journal of Chemical Engineering*.