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Wednesday, Dec 1st, 2021 at 4:00pm EST
Virtual Meeting: Zoom

Prof. Ya-Huei (Cathy) Chin



Professor of Chemical Engineering & Applied Chemistry
University of Toronto

A Generalized Mechanistic Framework for C-H Bond Formation and C-O Bond Cleavage Catalysis on Transition Metal and Metal Sulfide Surfaces

Activation of hydrogen on transition metal, metal oxide, and metal sulfide catalysts that forms reactive hydrogen species and their sequential attack to organic moieties are ubiquitous catalytic events in hydrogenation, hydrodeoxygenation, and hydrodesulfurization reactions. Introduced in this lecture are the mechanistic similarities among the various classes of reactions, focusing on their common initiation step of hydrogen activation, which occurs via mechanistically distinct steps that lead to reactive H species of different electron densities, depending on the chemical identity and oxidation state of their binding ligands ($\text{Metal}^{\delta+}$, O^{2-} , S^{2-}) and solvation environment. In this lecture, I will share our journey to unravel the charge of the reactive hydrogen species and their catalytic roles in reducing polar C=O moieties at different interfaces, from vapor- to liquid-transition metal, as the chemical potential of the solvent increases, and in vapor-RuS_x interface, at which hydrogen activation forms proton-hydride pairs. Depending on these various factors that influence the thermodynamics and kinetics of hydrogen activation

steps, the reactive H may acquire the character of hydrogen adatom, proton, or hydride; these distinct H species participate in H attack events with different catalytic requirements, and together they complete a catalytic sojourn that reduces organic feedstocks. Through understanding the electronic charges, acidity, and catalytic roles, we could rationalize the catalytic fates of the organic reactant fragments, establish the structure and property relationships, as illustrated in this talk through the hydrogenation of carbonyls, hydrodeoxygenation of substituted phenols, and phenol deuteration reaction.

Speaker Bio

Ya-Huei (Cathy) Chin is Professor of Chemical Engineering and Applied Chemistry at the University of Toronto. She is a Canada Research Chair (Tier II) in Advanced Catalysis for Sustainable Chemistry. She joined the University in 2011, after receiving her Doctor of Philosophy (Ph.D.) degree in Chemical Engineering from the University of California, Berkeley. Before then, she was a research engineer (2000-2002) and then senior research scientist (2002-2005) at Pacific Northwest National Laboratory (PNNL), one of the ten National Research Laboratories for the U.S. Department of Energy. Her recent work focuses on elucidating the molecular events during alkane oxidation on Group VIII metal clusters and conversion of oxygenates to value-added chemicals and liquid fuels. Specifically, she applies isotopic, kinetic, and density functional theory methods to study the dynamics of catalyst surfaces and catalytic pathways.

Please refer to email announcement for login details.

Presentation	4:00 PM	Annual Membership Dues	\$35 (<i>Students</i> = \$15)
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Deadline for reservations is 4:00PM Monday, November 29th, 2021

To make your reservation, fill out the [online form](#).
