



MIT ChemE

Spring 2025 Seminars

Unravelling Structure-function Relationships Through Kinetic and Spectroscopic Assessments for Sustainable, Atom-efficient Chemical Processes



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This talk will explore how isolated metal sites within well-defined coordination environments can be systematically controlled, how dynamic these sites are under process conditions, and how governing material properties can be engineered to improve activity. To this end, we utilize rigorous spectroscopic and kinetic assessments to elucidate how material properties dictate molecular-scale behavior and to define reaction, adsorption, and deactivation mechanisms that inform a broader material and application portfolio.

Using crystalline MOFs (porous) and perovskites (non-porous) as model materials with isolated metal sites in well-defined atomistic arrangements, we can exploit their tunable physicochemical properties to build structure-function relationships in catalytic and adsorptive applications. For example, we utilize probe reactions (e.g., hydrocarbon oxidations) to unravel how metal identity and coordination environments affect reaction rates and product selectivity, with metal valency, electron affinities, oxygen mobility, and ligand effects playing key roles. Further, we examine site evolution and prominent deactivation mechanisms (like metal leaching in liquid systems) and by identifying underlying causes, propose mitigating strategies to improve material stability and efficiency. For adsorptive systems, we utilize CO₂ capture to exemplify how metal sites within differing coordination environments exhibit disparate CO₂ uptake capacities and propensities to stabilize additional uptake centers (e.g., amine species) for improved oxidative degradation resistance and site efficiency.

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