CHEMISTRY & BIOCHEMISTRY

SEMINAR PROGRAM

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We Are Pleased to Announce a Seminar
Presented By

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Chemical, Biological & Materials Engineering

Friday, March 3, 2023
4:15 pm
NWC 1313

Deconvoluting the many roles of water and confinement in zeolite catalysis

Zeolites are among the most important catalysts in use today, with applications ranging from petroleum processing to biomass conversion and waste polymer upcycling. Here we discuss the many ways that water, which is inherently present in many of these streams, can influence reactions over these catalysts. First, we provide an overview of the consequences of confinement on activity for zeolite catalyzed coupling and C-C bond cleavage reactions over Bronsted acid sites. We discuss the modification of adsorbate and transition state enthalpies due to the local confining environment as well as corruption of rates due to diffusion limitations and incorrect interpretations of intrinsic rates that often result if not properly accounted for. We then show how, after these aspects have been accounted for, the incorporation of water in these confined environments can influence the chemistry in many interesting ways. We discuss the delocalization of protons around framework acid sites and consequences on catalytic activity, as well as the ways in which these delocalized protons may influence competition for active sites and stabilize reactive intermediates. These effects are decoupled from modifications in catalyst deactivation rates that are often confused with rate modifications. We further show how, for some reactions where water does not directly modify kinetically relevant transition states, it can induce structural modifications that lead to unique active sites with greatly enhanced activities for some demanding reactions.

Refreshments will be served

(Biography on back)