## Predictive Modeling of Adsorption and Reaction Equilibria in Nanoporous Materials

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Force-field-based and first principles Monte Carlo simulations are used to explore (a) the adsorption of complex mixtures in microporous and hierarchical zeolites (including multicomponent sour gas mixtures and aqueous solutions of alcohols and biorefinery compounds), (b) the adsorption of gas molecules in metal-organic frameworks with undercoordinated metal sites, and (c) the influence of nanoscale confinement and preferential adsorption sites on reaction equilibria. The talk will highlight simulation methodologies and microscopic-level origins of the observed thermodynamic behavior.