The role of chemical and steric environment of active sites for catalytic vectors | Similarities with active sites in enzymes

Abstract

Elementary organic transformations are catalyzed by enzymes at large unmatched rate and selectivity. The local constraints at active sites of enzymes and the local chemical environment are two key properties to achieve such extraordinary catalytic vectors. We use the sites in crystalline nanoporous materials to mimic such well-defined reaction space. Molecules experience constraints that can be subtly adjusted via direct synthesis, as well as via the addition of cations, oxidic clusters or organic fragments. The role of water and other solvents in such environments changes drastically the reaction pathways compared with the catalytic pathways in a homogeneous environment of chemistry in solution. The lecture will compare reactions such as elimination reactions of alcohols, alkylation of aromatic molecules and the role of acid sites for hydrogenation and hydrogenolysis. Experimental methods to define the state of the reacting molecules combined with detailed kinetic analysis and theory will be used to explain the principal contributions of the interactions and the confinement to determine reaction rates. It will be discussed how reaction rates and pathways can be tailored using the space available for a transition state and the chemical constituents around the active site.

Thursday, November 9th, 2017
2 Eaton Hall (Spahr Auditorium)
11:00 – 11:50AM