ChemE MIT Chemical Engineering

Seminar Series
Spring 2026

The Secret Lives of Oxidation Catalysts

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Friday, April 3, 2026
3pm, Reception 2:45pm
66-110

We describe the mechanistic role of lattice oxygen and solid state and gas phase promoters in oxidation catalysis in context of two case studies. First, we demonstrate the proficiency of Bi_2O_3 to selectively (>99%) combust acetylene in mixtures with ethylene. Measured rate constants for acetylene combustion are ~3000× those for ethylene in line with DFT studies suggesting heterolytic C–H activation transition states favor the activation of more acidic C–H bonds in C_2H_2. These heterolytic reactivity channels are also available for larger aliphatic and aromatic terminal alkynes demonstrating the utility of chemical looping combustion for purifying olefin gas streams containing trace alkyne impurities. Second, we rationalize the role of promoters in silver-catalyzed propylene epoxidation, wherein high selectivity (~60%) for epoxidation is only observed in the presence of four promoters viz., potassium (~0.02 g K $(g_{cat})^{-1}$) as well as gaseous co-feeds—2–10 vol% carbon dioxide, 5–20 ppmv allyl chloride, and 100–1000 ppmv nitric oxide. Allyl chloride (~2 Pa or ~20 ppm C_3H_5Cl) is shown to deposit ~0.15 mol Cl (mol Ag_{surf})$^{-1}$ Cl adatoms, monitored in-situ via Cl mole balances, and result in an increase in the epoxidation-to-combustion ratio ~20× without significantly altering rate-determining O_2 activation. Co-promoting nitric oxide, carbon dioxide, and potassium are required in addition to Cl promotion for selective epoxidation. We illustrate that threshold concentrations of these co-promoters result in crowded catalytic surfaces that are selective for both propylene (~60% selectivity) and ethylene epoxidation (~90% selectivity) which share common oxidants and common active sites.

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