MATERIALS SEMINAR

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"Selective Passivized Catalysis: Methane as an In-Situ Hydrogen Donor"

Hydrogen-intensive refining processes such as hydrogenation and hydrocracking depend on costly H_2 produced by steam methane reforming, while methane itself remains inexpensive and underutilized. We investigate whether CH_4 can serve directly as an *in-situ* hydrogen donor. We propose a catalyst design principle to achieve it: Selective Passivized Catalysis (SPC), a strategy developed in my group in which a fraction of the active sites is deliberately shielded, attenuated, or modified, either before the reaction (ex-situ) or during it (in-situ). We hypothesize that SPC breaks the activity-selectivity-stability trade-off, so selectivity and stability improve at once rather than being traded against each other. SPC will be illustrated using the methane-assisted semi-hydrogenation (MASH) of acetylene, $2CH_4 + 2C_2H_2 \rightarrow 3C_2H_4$, over Pt nanolayer catalysts supported on MXene and high-entropy MXene. This work combines synchrotron EXAFS/XANES, DRIFTS, XPS, and ToF-SIMS with kinetic and transport modeling, including a Multicomponent Diffusion with Decay Criterion (MDDC) developed to handle evolving pore structure. I will close with PAME-CARE (**P**rocess-Oriented **A**daptive **M**ulti-Scale **E**ngine for **CA**talysis and **R**eaction **E**ngineering), an open-source Python platform that carries this research data into the reaction engineering and process design curriculum and interfaces with commercial process simulators such as Aspen Plus.