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RESEARCH & COLLABORATION PROFILE

KEY WORDS: CO_2 Hydrogenation, Liquid Organic Hydrogen Carrier, Heterogeneous Catalysis, Sustainable Aviation Fuel, Metal Oxide, Zeolite



Research Snapshot. Dr. Kim designs multifunctional heterogeneous catalysts and reaction systems to address global carbon neutrality and clean energy storage challenges. His research focuses on active phase manipulation and interfacial engineering for direct CO_2 hydrogenation to value-added hydrocarbons and sustainable aviation fuels (SAF), hydrogen storage/generation from liquid organic hydrogen carriers (LOHCs), and value-addition of chemical feedstocks via heterogeneous catalysis.

RESEARCH EXPERTISE

- **CO_2 hydrogenation to value-added chemicals:** development of multifunctional oxide and composite catalysts for direct conversion of CO_2 into liquid hydrocarbons (C_{5+}) and SAF.
- **LOHC systems:** catalytic hydrogenation and dehydrogenation of homocyclic and heterocyclic LOHCs (e.g., methylbenzyl naphthalene, piperidine derivatives) with high efficiency and suppressed side reactions.
- **Dynamic catalytic phase engineering:** in-situ understanding and kinetic control of active phase evolution, metal-support interactions, and hydrogen spillover in multi-component heterogeneous catalysts.
- **Industrial feedstock and byproduct upcycling:** gas-phase aldol condensation for acrylic acid production and catalytic dehydration of ether byproducts for olefin recovery.
- **Porous nanomaterial design:** synthesis and morphological control of mesoporous zeolite, hollow silica spheres, and bimetallic spinel oxides for energy and catalytic applications.

RECENT RESEARCH HIGHLIGHTS

- **Dynamic phase evolution in CO_2 catalysis (Adv. Funct. Mater. 2026):** elucidated the dynamic active phase transformation of Fe-based catalysts during CO_2 hydrogenation, establishing foundational data-driven catalyst design principles (Selected as Cover).
- **Hydrogen spillover-mediated selectivity control (Chem. Eng. J.):** demonstrated precise steering of hydrocarbon product distribution from olefins to paraffins via controlled hydrogen spillover on multifunctional FeK/$CuAl_2O_4$ catalysts during CO_2 hydrogenation.
- **Byproduct-minimized LOHC dehydrogenation (Appl. Surf. Sci. 2025):** demonstrated that sulfur-doped Pt/TiO_2 catalysts dramatically suppress undesirable high-temperature side reactions during H_2 release from methylbenzyl naphthalene.

POTENTIAL COLLABORATION RESEARCH

Best-fit collaborator areas: synchrotron operando/in-situ characterization | computational calculation (DFT) | reaction engineering & scaling | data-driven catalyst discovery

- **1. Operando and in-situ synchrotron analysis:** tracking dynamic phase transitions, active carbide restructuring, and local electronic states under high-pressure CO_2 hydrogenation via synchrotron XAS, XRD, and XPS.
- **2. DFT calculation & microkinetic modeling:** theoretical elucidation elementary reaction pathways, adsorption geometries, and hydrogen spillover energy barrier on bimetallic interfaces and defective metal oxides
- **3. Data-driven catalyst discovery:** collaborative construction of catalyst property descriptors and machine learning workflows to accelerate the discovery of high-performance catalysts for SAF.
- **4. Reaction system & LOHC module engineering:** multi-scale reaction engineering, continuous-flow process optimization, and system-level thermal coupling for mobile/stationary clean hydrogen delivery module.

SELECTED RECENT PUBLICATIONS

- **Adv. Funct. Mater. 2026, Accepted —** Dynamic Phase Evolution of Fe-Based Catalysts during CO_2 Hydrogenation: Implications for Data-Driven Design
- **Chem. Eng. J. 2024, 498, 152614 —** Consequence of controlled hydrogen spillover on FeK/$CuAl_2O_4$ in CO_2 hydrogenation
- **J. Mater. Chem. A 2022, 10, 21862 —** Multifunctional long-lived catalysts for direct hydrogenative conversion of CO_2 to liquid hydrocar-bons with upscaling C_{5+} productivity

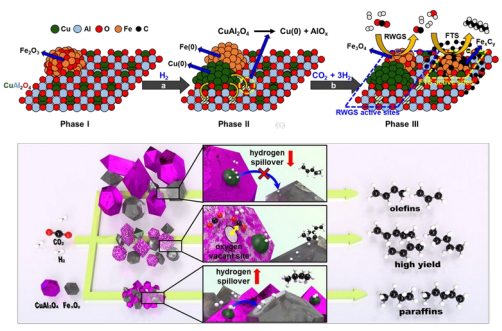
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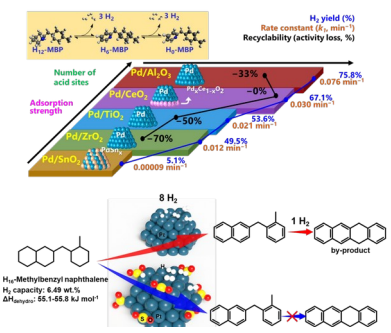
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REPRESENTATIVE RESEARCH FIGURES / SCHEMES

CO_2 hydrogenation to value-added chemicals



LOHC systems



Industrial feedstock and byproduct upcycling

