Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)

EFRC Director: Cynthia M. Friend
Lead Institution: Harvard University
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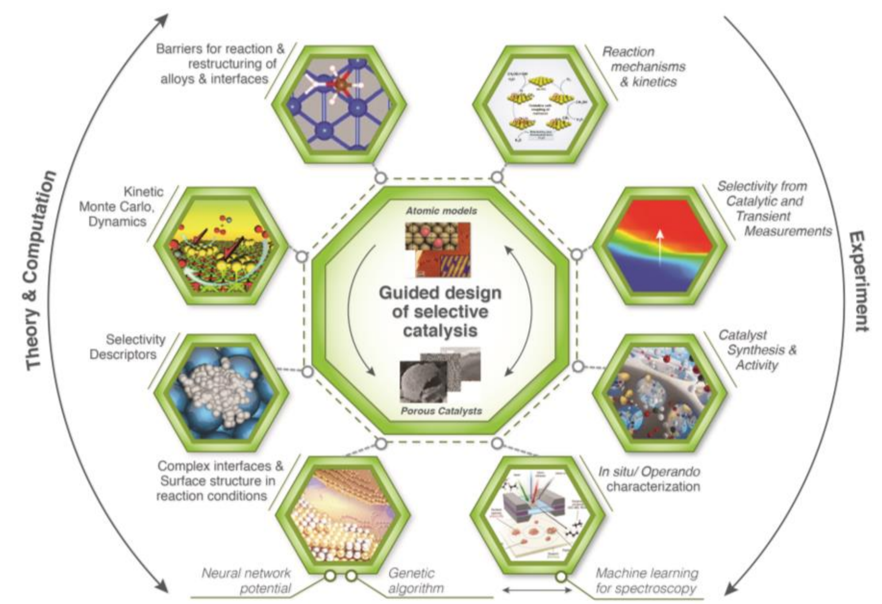
Mission Statement: *To establish design principles for highly selective catalytic transformations driven by nanoporous dilute alloys.*



Scheme 1: Schematic of approach to design of selective catalysts in IMASC. A powerful combination of experiment and theory will be brought to bear on understanding key catalytic synthesis reactions on model systems and on functioning porous catalysts as a means of improving selectivity.

The Center for Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC), an Energy Frontier Research Center, unites best-in-class researchers from universities and national laboratories to perform collaborative, innovative fundamental research at the intersection of surface chemistry and physics to transform how catalysts are designed. The integrated, Center-wide effort, built on a foundation of a well-managed matrix of projects and expertise, will enable us to reach ambitious strategic goals through innovative approaches and aggressive effort from a clear set of unified principles, fully committed collaborations and synergistic partnerships. The Center-wide goal is to develop the ability to improve catalytic selectivity by quantitatively scaling from model studies to catalytic conditions using advanced experiment and theory (Scheme 1). Improving reaction selectivity is extremely important because of the potential for increasing the efficiency of chemical production, which accounts for nearly 25% of energy use worldwide and which relies heavily on heterogeneous catalysis.

Heterogeneous catalytic processes are extremely complex, requiring optimization of factors across multiple scales of length, time, pressure and temperature. Hence, catalyst development requires the confluence of materials synthesis, mechanistic surface chemistry, and reaction kinetics. Complex metal/oxide interfaces are often present and may play an important synergistic role in the catalysis. Further, since the materials are often affected by the reaction environment, pre- and on-stream activation and optimization of performance is required. IMASC will capitalize on recent advances in theory and experiment to address these issues and thereby improve the efficiency of key catalytic processes.

The IMASC mission will be achieved by addressing several key scientific questions aimed at establishing principles for designing highly selective catalytic processes.

Key Scientific Questions:

1. How are the elementary steps in the reactive process affected by materials composition and structure?
2. What compositions, configurations, and structures of the alloy materials are optimal for high reactivity and high selectivity for specific reactions?
3. What is the effect of complex metal/metal oxide interfaces and how can they be controlled?
4. What is the state of the catalyst surface under reaction conditions and how does this affect selectivity and reactivity?

These questions will be addressed through the Center-wide projects that draw upon a range of experimental and theoretical expertise all managed in a matrix structure. Four cross-cutting methodological Expertise Areas will enable the research: EA1: Selectivity and Mechanism (Leads: Madix); EA2: Materials Synthesis (Lead: Biener); EA3: Theoretical Tools (Lead: Sautet); and, EA4: In Situ/Operando experiment (Lead: Stach).

Three **Center-wide projects** (thrusts) will focus IMASC efforts on critical catalytic transformations selected for their importance in chemical production.

A. Advancing the paradigm for mechanistic control of complex selective oxidation. (Lead: Madix)
B. Exploiting complex metal/oxide interfaces for challenging catalytic transformations. (Lead: Friend)
C. Directing selective hydrogenation: unsaturated oxygenates to nonthermodynamic products (Lead: Sautet)

The research in IMASC will culminate in a set of principles for designing dilute alloy catalysts capable of driving highly selective reactions. More broadly, an efficient methodology for understanding and improving catalytic processes will be established.

Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)	
Harvard University	Cynthia Friend (Director), Joanna Aizenberg, Boris Kozinsky, Robert Madix (Executive Committee Member)
UCLA	Philippe Sautet (Deputy Director)
Lawrence Livermore National Laboratory	Juergen Biener (Executive Committee Member)
University of Pennsylvania	Eric Stach (Executive Committee Member)
Tufts University	Maria Flytzani-Stephaopoulos, Charles Sykes
Brookhaven National Laboratory	Anibal Boscoboinik, Dario Stacchiola
Stony Brook University	Anatoly Frenkel
University of Florida	Jason Weaver
University College London	Michail Stamatakis

Contact: Leah DeFrancesco, Program Assistant, defrancesco@chemistry.harvard.edu
617-495-4198, https://efrc.harvard.edu/