Mesoscale Priority Research Direction

Design of Mesoscale Catalytic Processes

Opportunity

Scientific challenge: Understand the design principles for creating efficient catalytic processes to convert feedstock materials to fuels and chemicals. Molecular science has made great strides in understanding how individual active sites promote bond breaking/making processes. Control of catalytic conversions, which involve multiple reaction steps, will require understanding how to transport intermediates between active sites with differing functions as well as designing active sites for specific transformations. Biology has mastered such complex conversions by using a variety of mesoscale processes to control coupled reaction and transport processes at the level of enzymes and cells. We have the opportunity to learn from nature to design new inorganic catalytic materials and processes.

Current state of understanding: Although progress towards the understanding of catalytic processes at individual active sites has been significant, we currently we do not know how to control interactions between active sites that is needed to direct the cascade of reactions in complex, multi-step catalytic conversions.

Meso Challenge

What makes it meso? The goal is to learn how to control coupled reaction and transport over 10s to 100s of nanometers, rather than macroscopic levels encountered in scale-up of catalytic processes. We expect new emergent behavior from reaction/transport coupling at this scale.

Approach

What can be done to address the challenge? An integrated approach is needed to address this challenge, which includes novel synthesis approaches to create nanostructured catalytic materials with controlled distributions of active sites, multimodal characterization techniques that allow the observation of coupled reaction/transport under real operating conditions, and new theory and computational approaches that span molecular to meso scales. Only through this integrated approach can we develop an understanding of the 'design principles' for controlling emergent behavior arising from complex networks of reactions and transport. Parallel efforts are also needed to gain better understanding of coupled enzymatic reactions in cells and how biological systems control transport processes and their coupling to chemical transformations.

Impact

How will pursuit of the research direction, including the meso opportunity, impact the scientific challenge? Detailed understanding leading to control of coupled reaction/transport processes will enable the design of entirely new catalytic processes for efficient conversion of complex feedstock materials to fuels and chemicals.

References: DOE/BES Workshop Report on "Basic Research Needs: Catalysis for Energy" (2007)

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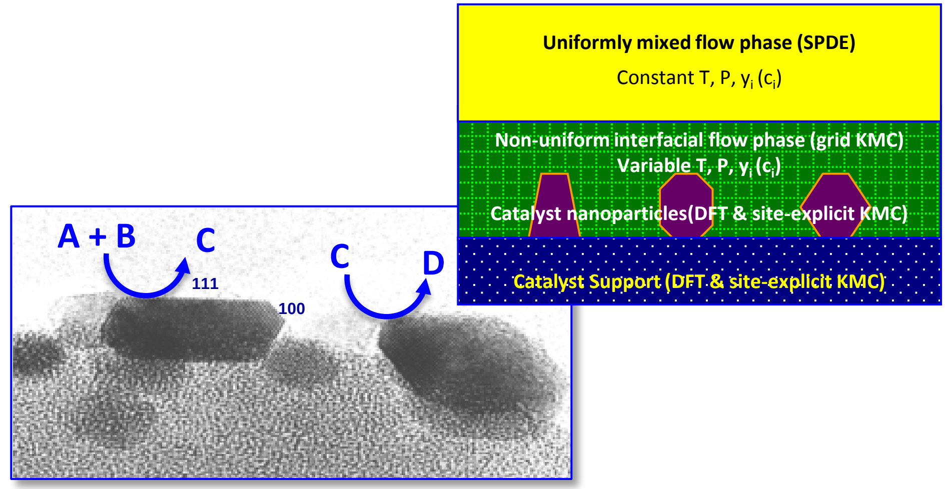
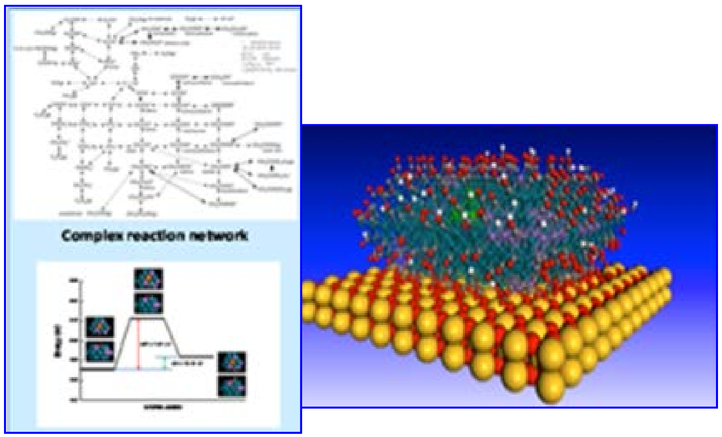
The mesoscale of catalysis with multiple functions



Target applications:

Transformation of alternate feedstocks (e.g., biomass, syn gas, pyrolysis oils and CO_2) to fuels



Molecular scale:

Thermodynamic and kinetic parameters from electronic structure calculations for first principles-based KMC simulations

Mesoscale:

- *Extended KMC Modeling* of complex catalysis with multiple functions to capture: i) intrinsic heterogeneities of particles and support; ii) transport in multiple phases; iii) inhomogeneities in surface chemistry and flow chemistry; iv) dynamic morphology of particles and system.
- Reactivity, transport, and system dynamics span varied length and time scales
- *High resolution imaging with time / ensemble sampling* is critical to model validation
- *Controlled synthesis / assembly / deposition* of catalytic scaffold is critical to model validation

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