Institute for Atom-efficient Chemical Transformations (IACT)

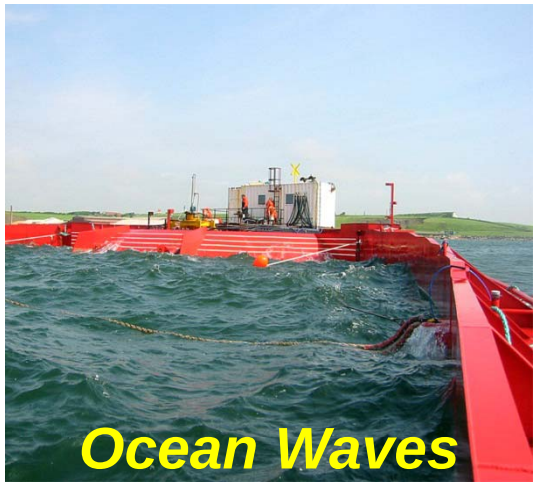
A joint DOE Energy Frontier Research Center (EFRC) with

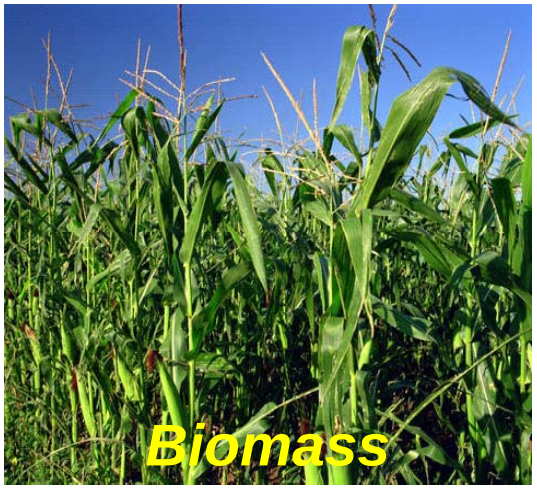
- ***Argonne National Laboratory***
- ***Northwestern University***
- ***Purdue University***
- ***University of Wisconsin***

APS Monthly Operations Meeting

February 23, 2011

Alternative Energy Sources: Renewable And Sustainable





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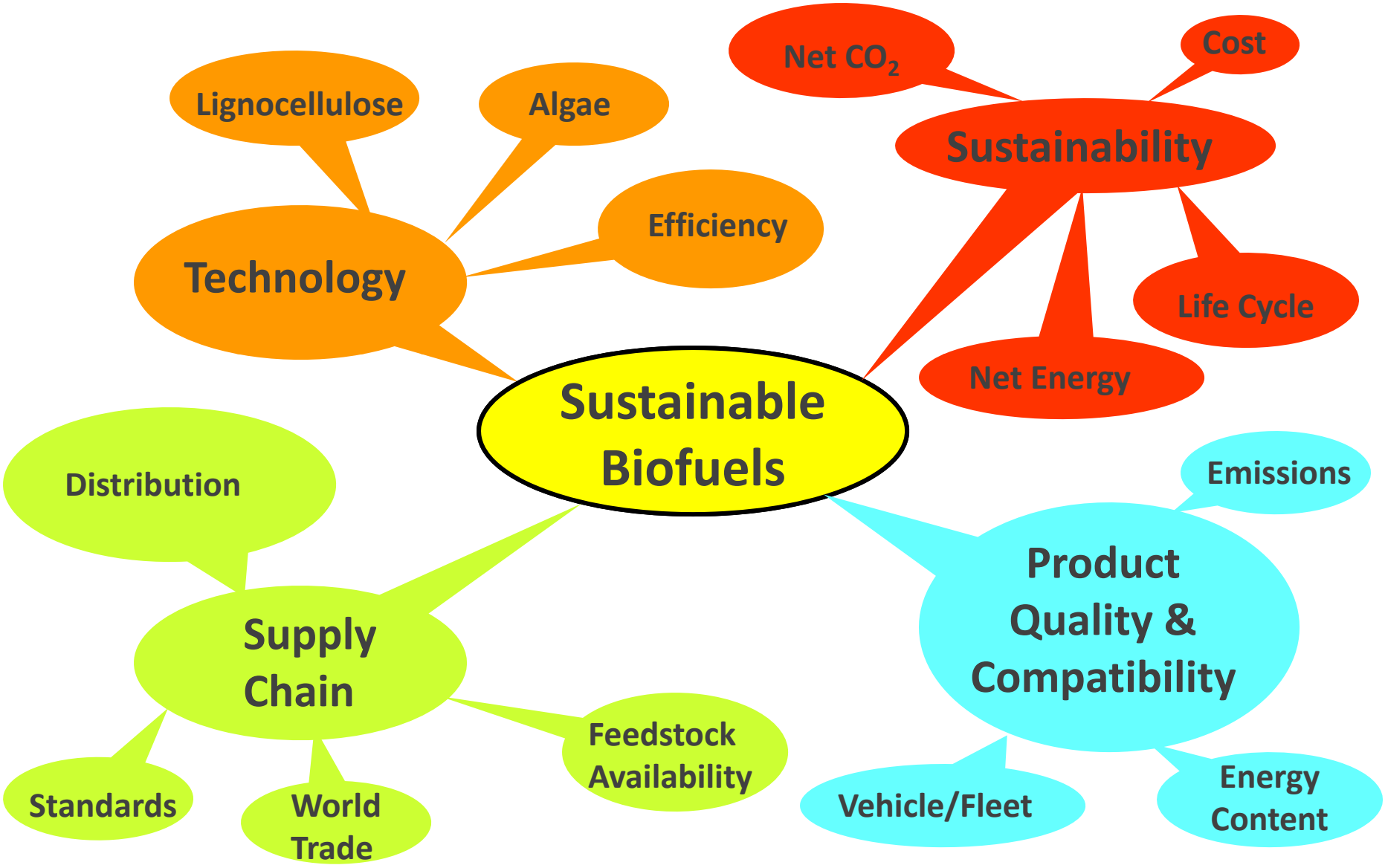
BioFuels: Great Potential - Much Work to Do



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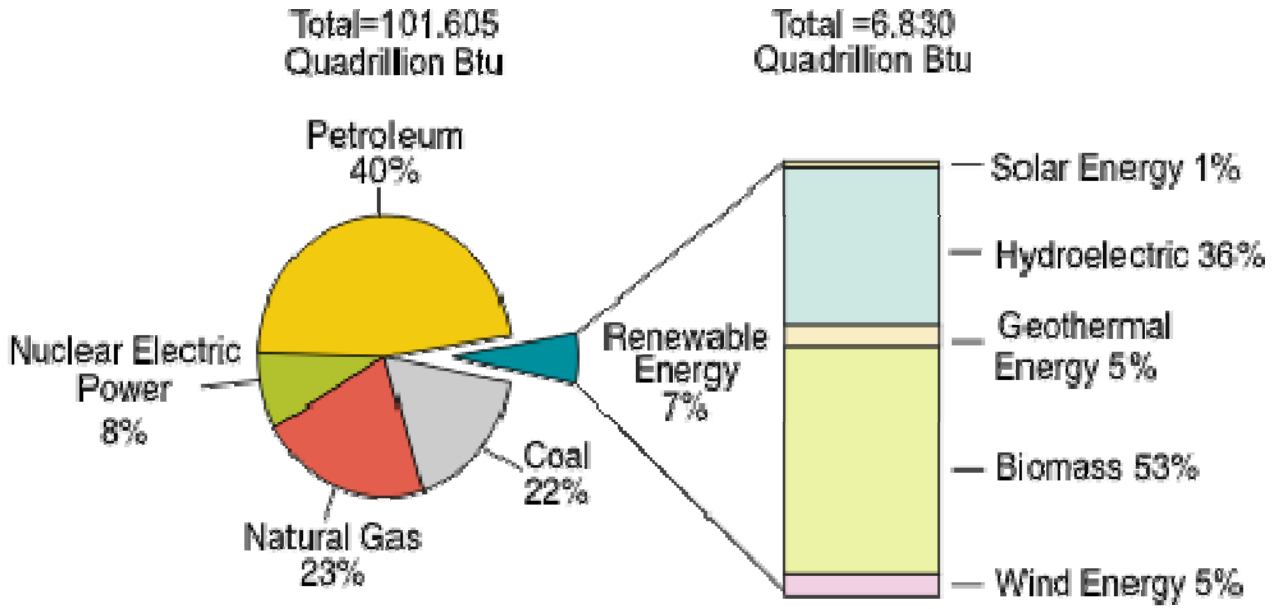
Current US Energy Demand



- 60% of petroleum is imported
  - A bio-fuels industry means **energy security**
- In the next 25 years, the US energy demand will grow by about 10% and world demand will double
  - A bio-fuels industry means stable, **growing economy**

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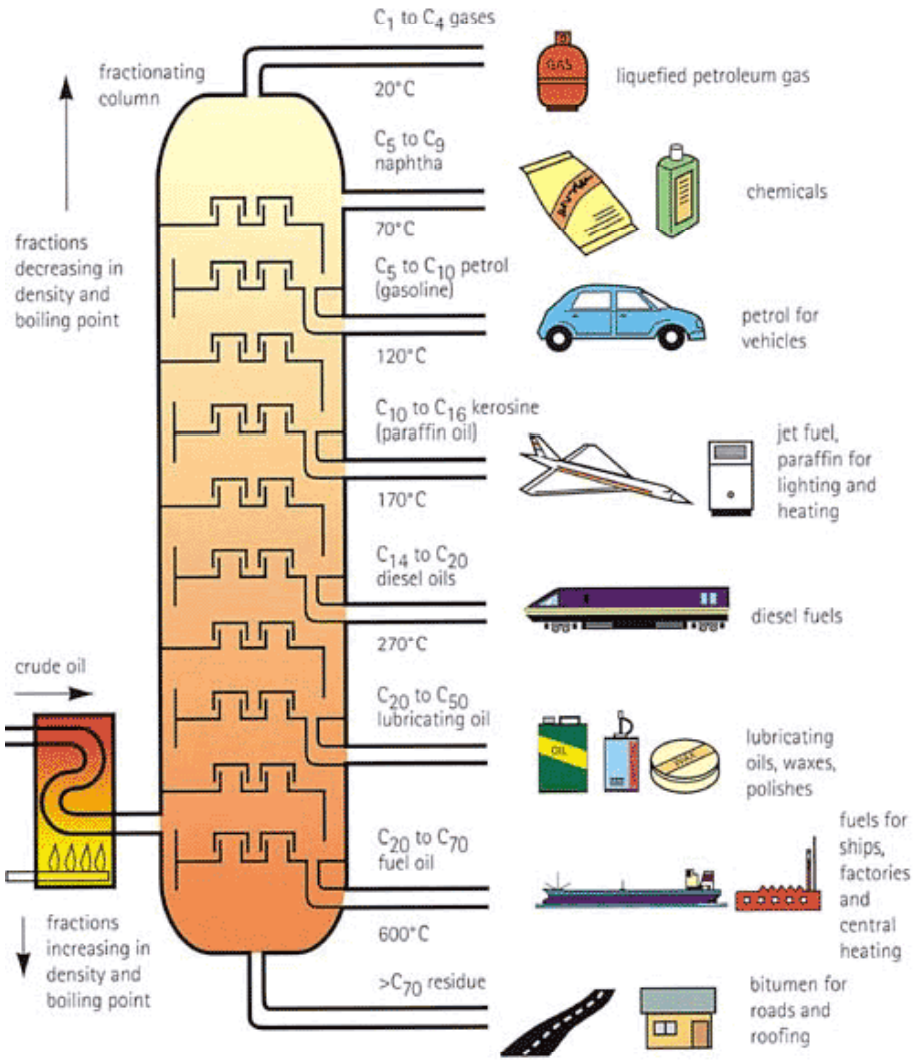
Oil and the Refining Industry

- Oil is the lifeblood of America's economy.
  - **HUGE INDUSTRY**
- Supplies more than 40% of our total energy demands.
- More than 99% of the fuel we use in our cars and trucks.
- Replacing the feedstock and infrastructure is a massive, multi-decade undertaking.
- Biofuels **MUST** be phased in to work with existing infrastructure.



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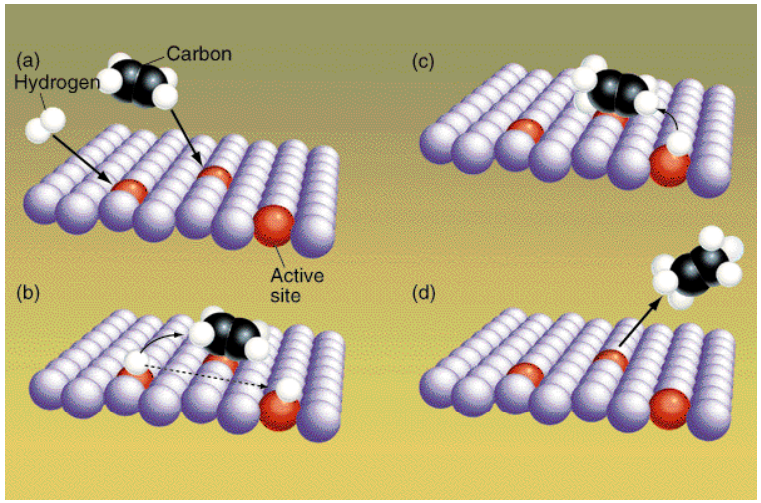
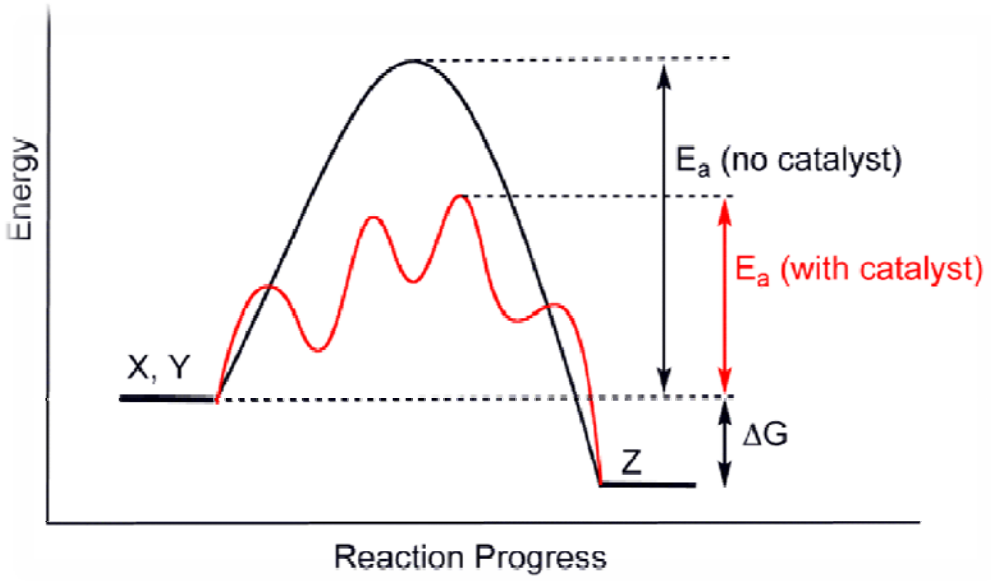
What Do Catalysts Do?





- Catalysts bind the reactants thereby facilitating their reaction to form products, **i.e., the catalyst is a molecular match maker**
- Catalysts lower the activation barriers to be surmounted between reactants and products
- Catalysts promote preferred pathway, minimizing the formation of byproducts

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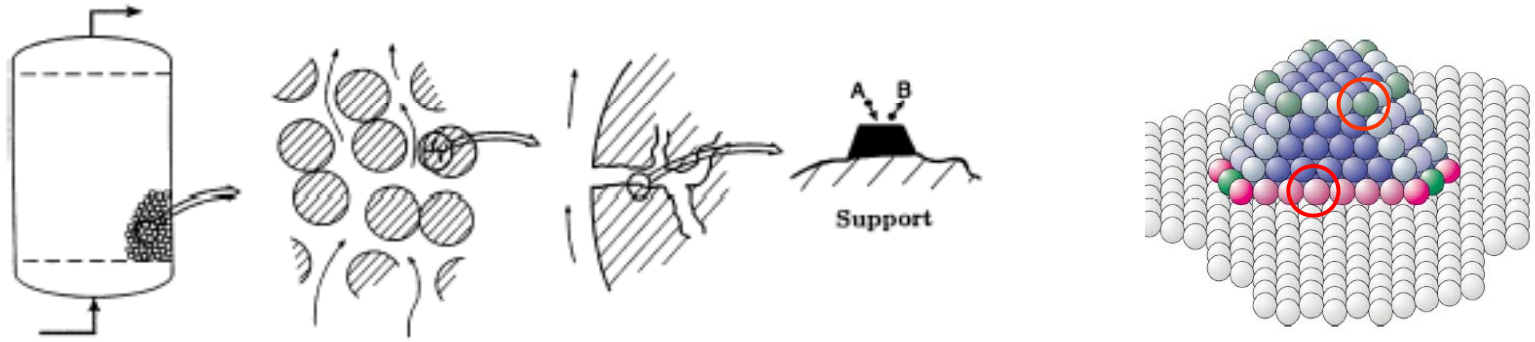
Catalysts – Nanoscale Materials that Enable Chemical Transformations

• Virtually all chemical transformation carried out in the energy and chemical industries depend on catalysis (>90%)

- Generate U.S. sales in excess of **$400 billion per year**.
- Net positive balance of trade of **$16 billion annually**.

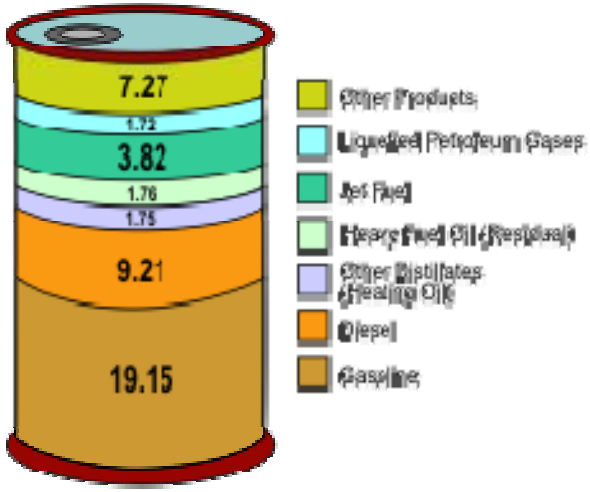
• Catalyst activity and selectivity affect capital and operating costs of industrial processes

• The performance of catalysts is strongly linked to the physical and chemical properties of the active phase(s) of a catalyst



Reactor (meters) | **Pellets (2-20 mm)** | **Pores (2-50 nm)** | **Catalyst particles (1-20 nm)** | **Supported nanoparticle**

Impact on Catalysts on Fuel Production from Crude Oil



(42 gal/bbl)

- Catalysts
  - Increase yield
  - Meet performance demands
  - Reduce environmental impact

Biomass MUST be brought into this infrastructure in order to make a major impact.

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Problems with blending biomass with gasoline and diesel

- Oxygen content
  - Sugar and gasoline don't mix
- Volatility
  - C_6 sugars are solids & C_6 hydrocarbons are vapors
- Solubility
  - Ethanol adsorbs water into gasoline
- Low H/C ratio
  - Lower energy content
  - MPG of E85 is 70% of gasoline
- Location
  - H_2O content of biomass requires local processing

Selective oxygen removal

MW modification

Higher hydrocarbons or alcohols

Added hydrogen

Low severity processing

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Catalyst Technology for Future Biofuels

- There are many possible routes for production of the next generation of bio-fuels
  - Multi-step and complex (high capital)
  - Many separations (low energy efficiency)

- Transformative technology will:
  - Reduce complexity by combining reaction steps or finding new, more efficient reaction pathways
  - Require new catalytic materials
  - Accelerate technology discovery with advanced simulation methods

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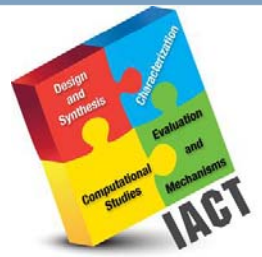
Institute for Atom-efficient Chemical Transformations (IACT)



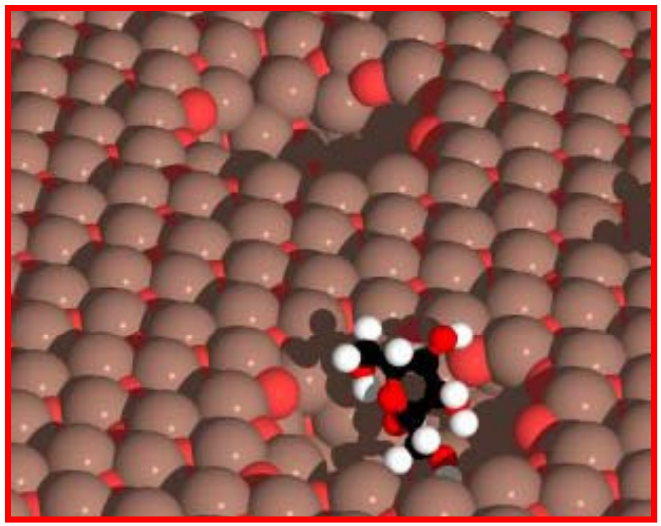
RESEARCH TEAM

Argonne National Laboratory

Northwestern University

Purdue University

University of Wisconsin



Vision:

- Chemical selectivity comparable to that demonstrated by nature.

Mission:

- Advance the science of catalysis for efficient conversion of bio-resources
- Improve the efficiency for conversion of biomass to fuels
- Promote the selective removal of oxygen.

Argonne NATIONAL LABORATORY

NORTHWESTERN UNIVERSITY

PURDUE UNIVERSITY

THE UNIVERSITY of WISCONSIN MADISON

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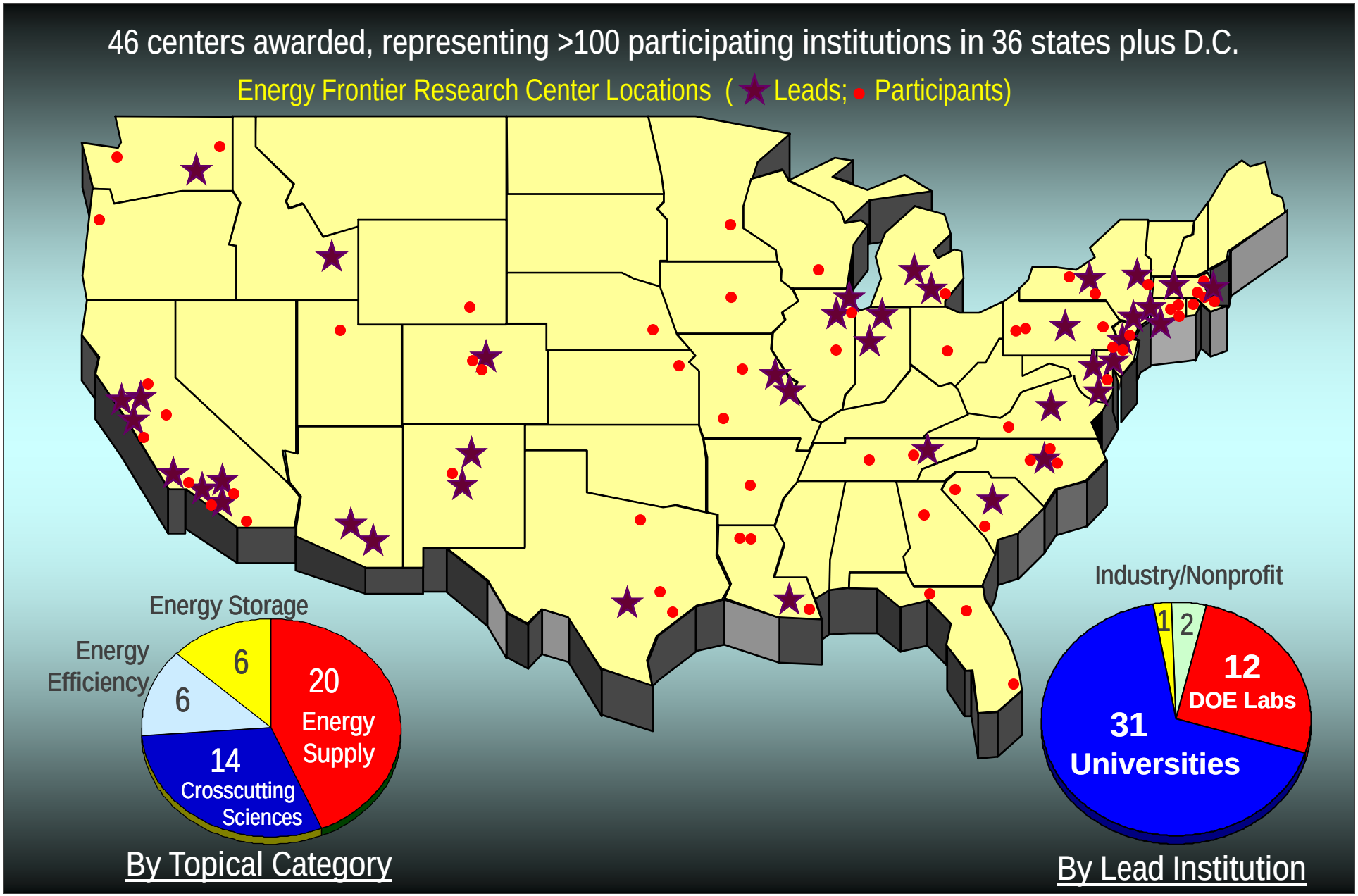
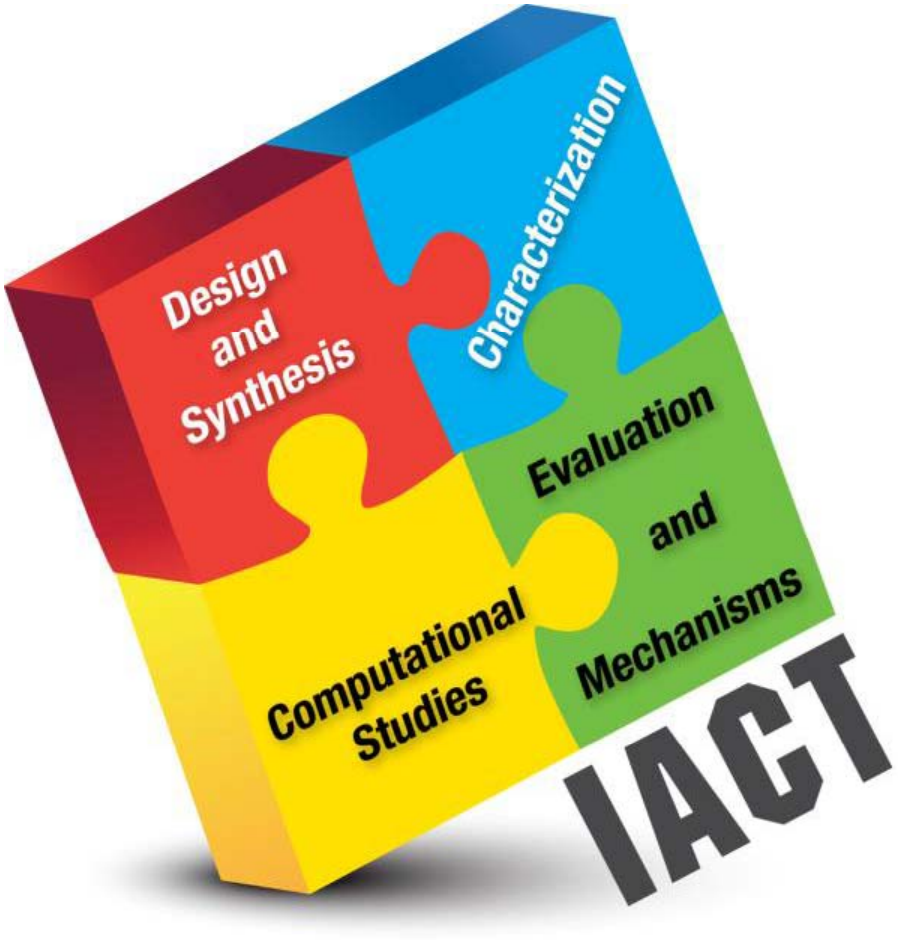
Energy Frontier Research Centers



Multi-disciplinary Approach to Catalysis Research
Four Linked but Separate Subtasks



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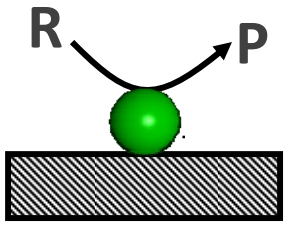
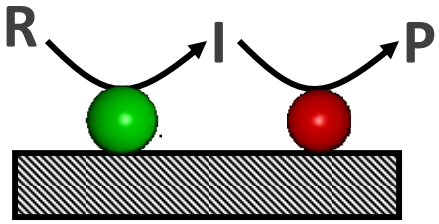
Subtask 1 (Synthesis)



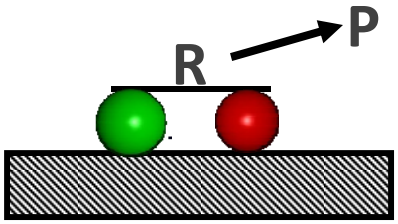
Isolated Mono-Functional Sites

- Conventional picture of heterogeneous catalysts, such as oxide-supported metal particles or an acid/redox site on a bulk oxide.



Proximate Multi-Functional Sites

- Multiple functions (e.g., metal and acid) are positioned in three dimensions with separations on the nanoscale or less.



Synergistic Multi-Functional Sites

- Two or more surface functionalities are in such close proximity that they act simultaneously on a single functional group in the reactant molecule.

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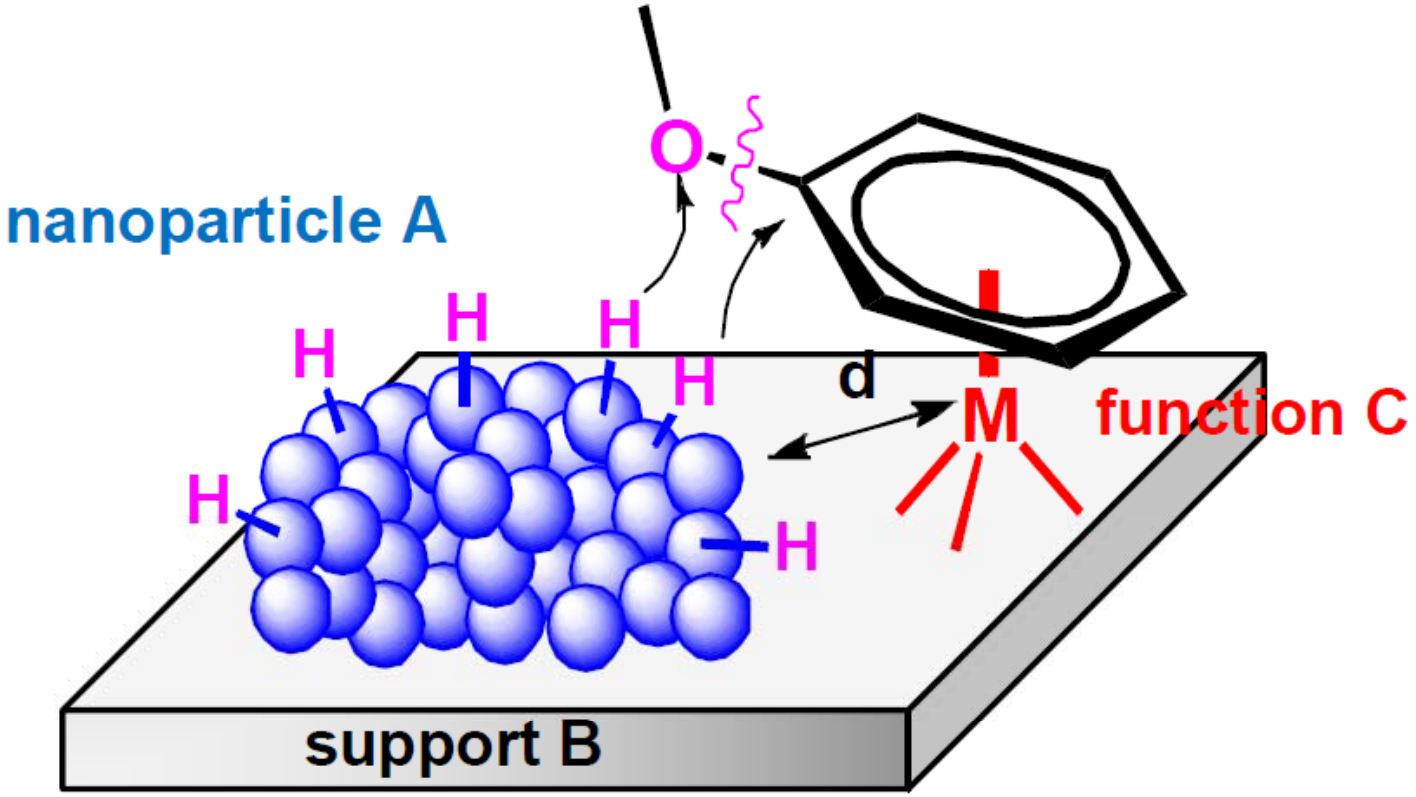
Subtask 1 (Synthesis)
Multifunctional Bimetallic Catalysts



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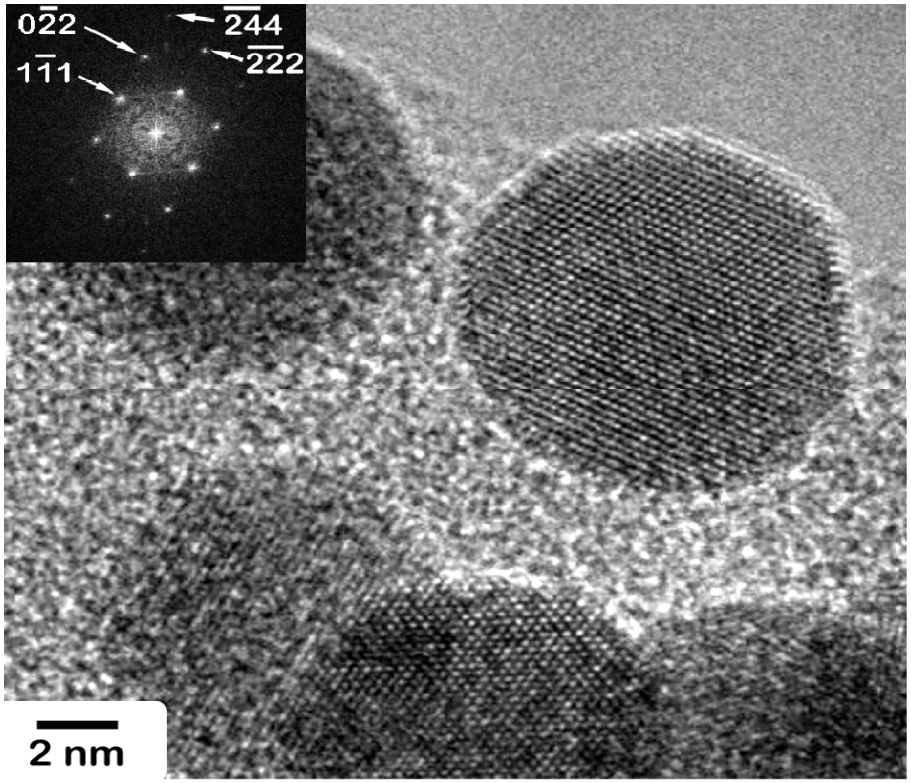
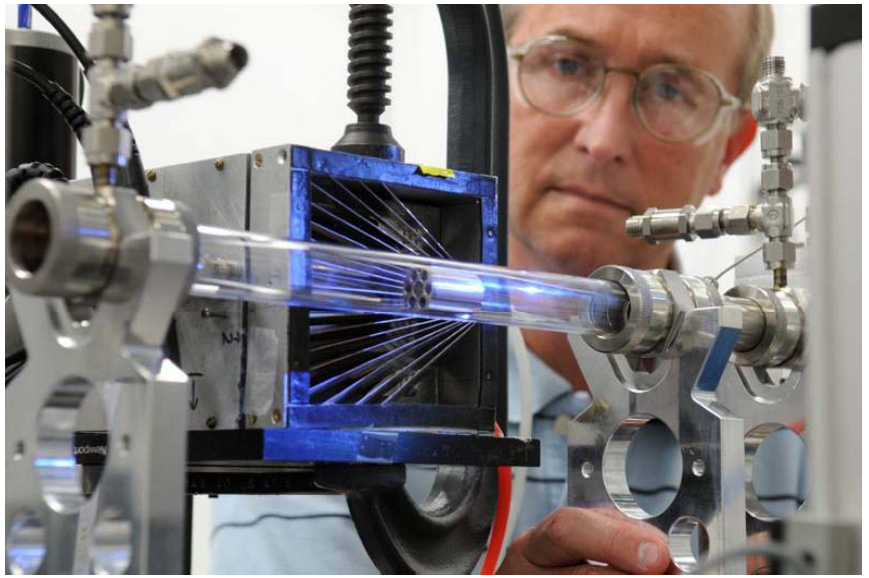
State of the Art Analytical Methods (under reaction conditions)





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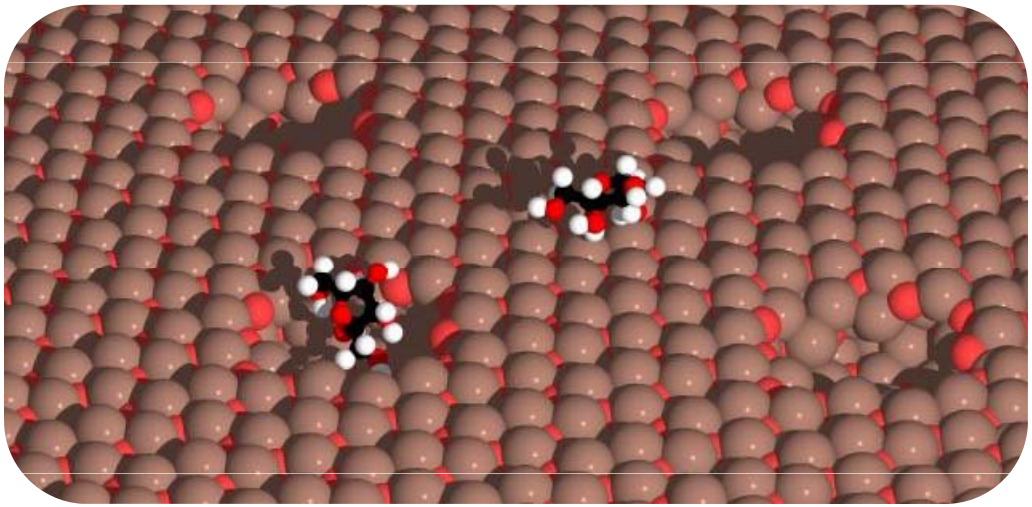
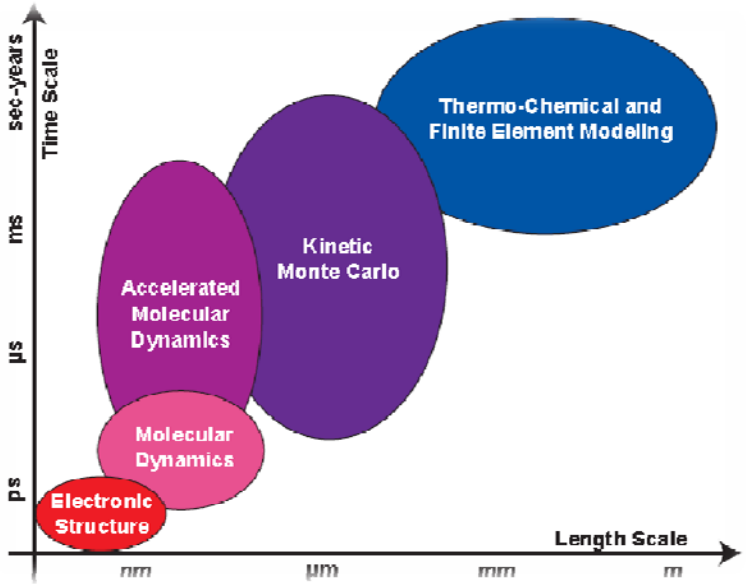
Theory, Modeling, and Simulation

- Geometric and Electronic Structure
- Reactant bonding and transition state
- Reaction intermediates
- Reaction rates
- Reaction mechanisms
- Prediction of new materials and reactivity





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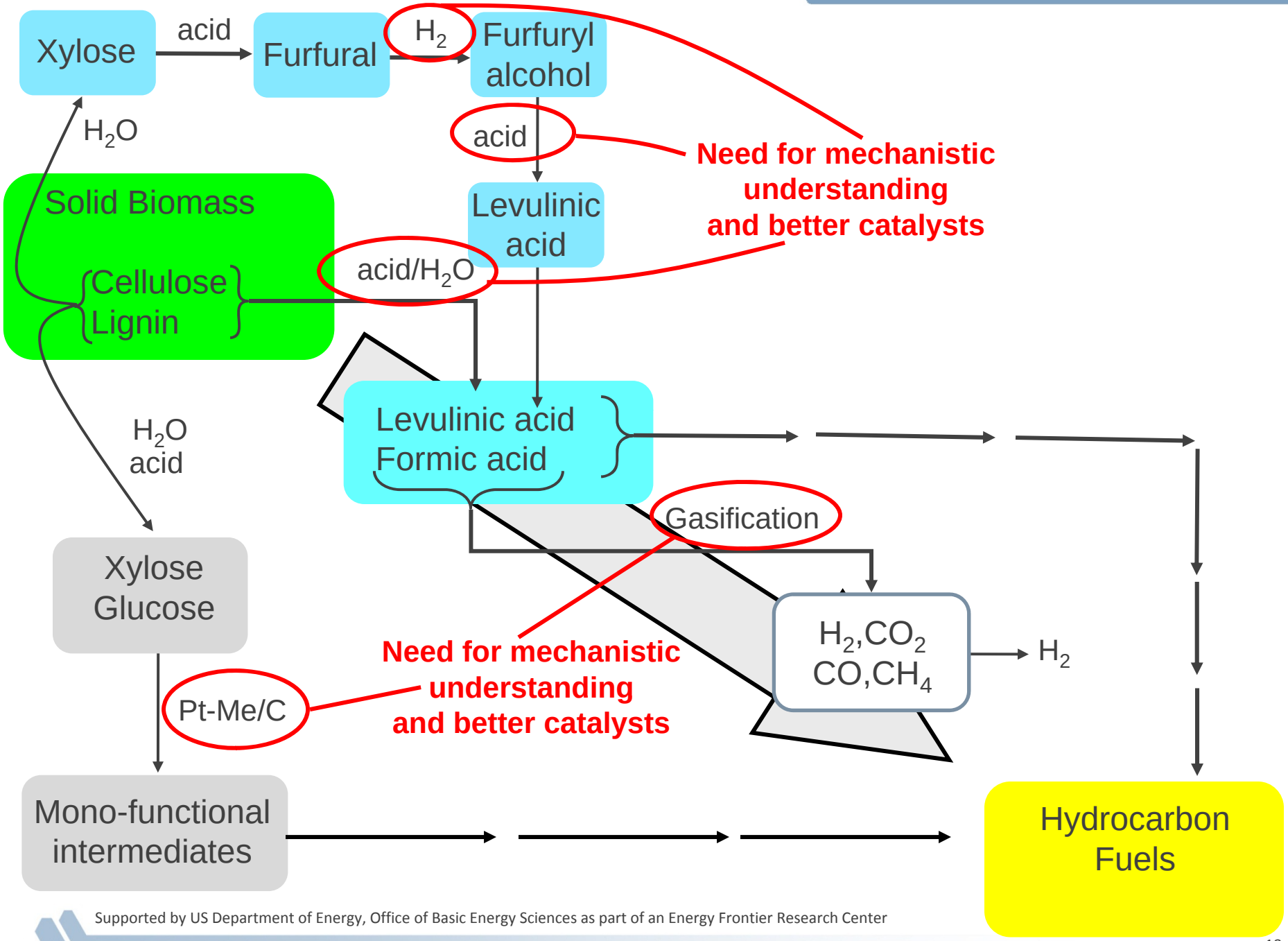

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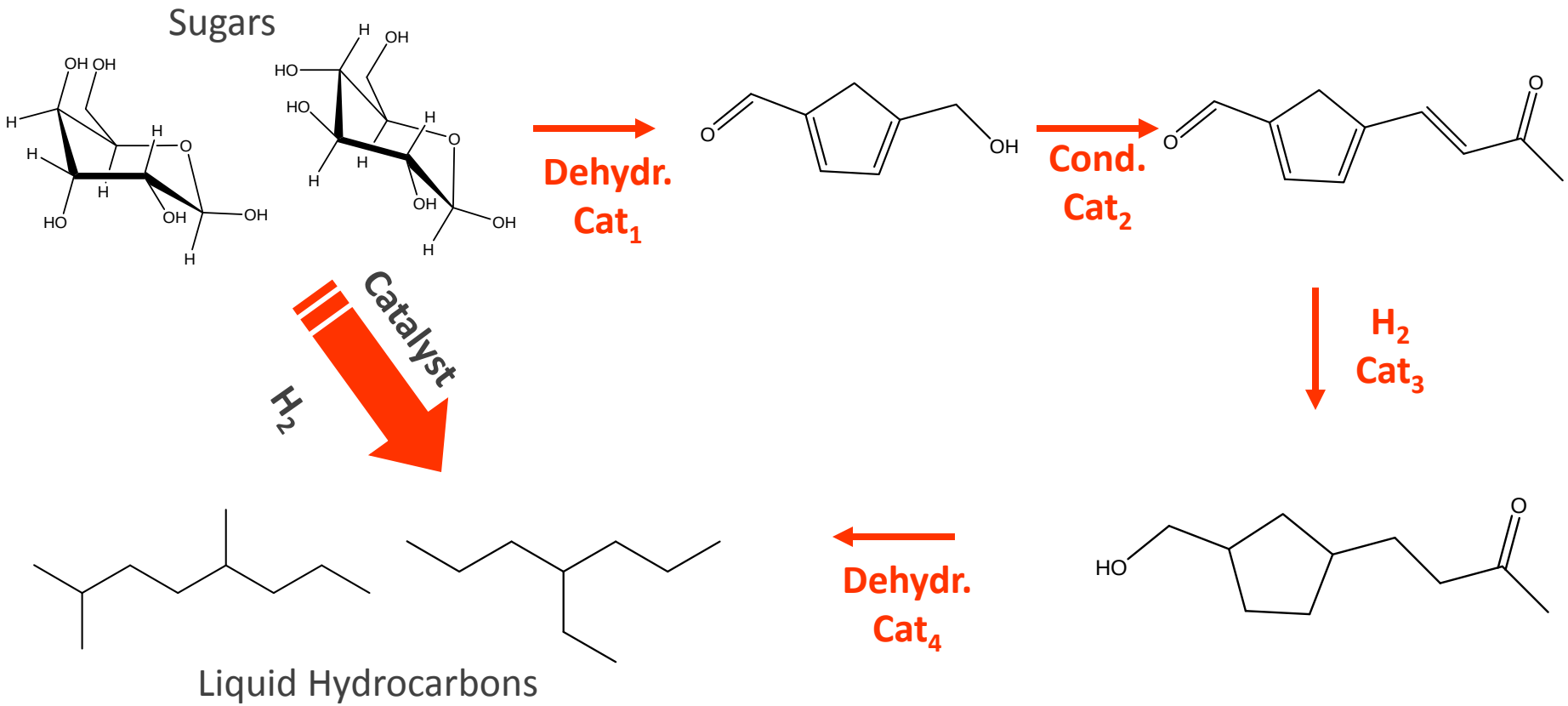
Institute for Atom-Efficient Chemical Transformations (IACT) Scheme for Bio-Fuel Production



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Resources and Infrastructure

- **Argonne**
  - Advanced Photon Source (APS)
  - Center for Nanomaterials (CNM)
  - CSE NMR facility
  - Atomic Layer Deposition (ALD)
  - Computing Facilities (ALCF)
- **Northwestern**
  - Crystal Growth Facility
  - Synthesis Labs
- **Purdue**
  - Environmental TEM
  - Combinatorial Reactors
- **Wisconsin**
  - Computing Facilities
  - Liquid Phase Reactor systems

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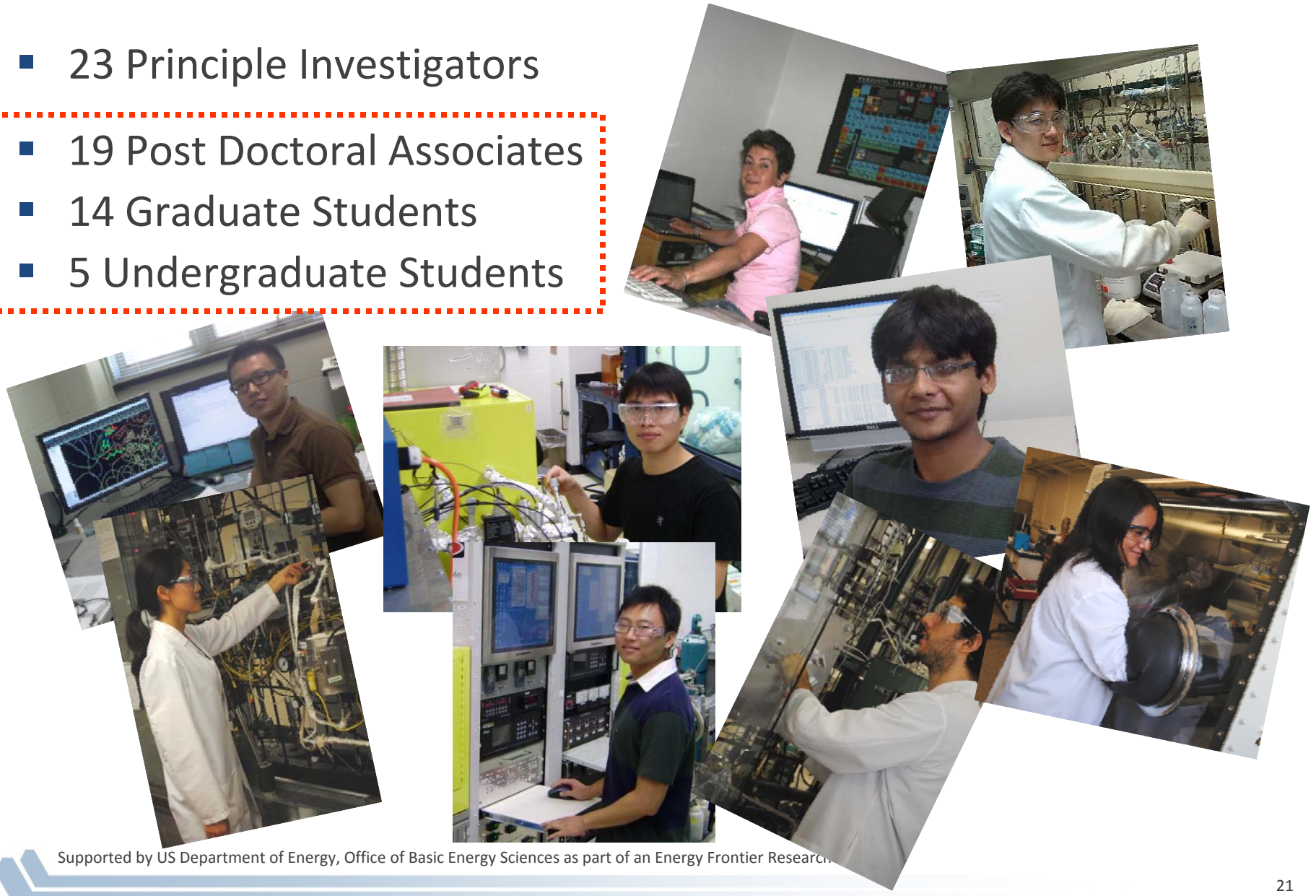
IACT Educational Component

- 23 Principle Investigators

- 19 Post Doctoral Associates
- 14 Graduate Students
- 5 Undergraduate Students



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Summary - IACT

- Advance the science of catalysis for the efficient conversion of energy resources
- Improve the efficiency for conversion of biomass to fuels

- Link and coordinate four distinct, but intimately interlinked subtasks:
  - Catalyst Synthesis
  - In situ Characterization
  - Computational Modeling
  - Catalytic and Chemical Reaction Science.

- Expertise of Four World Class Institutions
  - Argonne National Laboratory
  - Northwestern University
  - Purdue University
  - University of Wisconsin
- Highly Qualified Research Staff
  - 23 PIs
  - 19 Post Docs
  - 14 Graduate Students
- **http://www.iact.anl.gov**

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Questions?
Comments?