

### Center for Environmentally Beneficial Catalysis: Overview September 30, 2004











Designing environmentally responsible molecules, products, and processes – from the molecular scale to the plant scale.

Lead Institution: University of Kansas (KU)

**Core Partners:** University of Iowa (UI); Washington University in St. Louis (WUStL); Prairie View A&M University (PVAMU)

Director: Bala Subramaniam (KU); Deputy Director: Daryle Busch (KU)

Associate Directors: John Rosazza (UI); Milorad Dudukovic (WUStL); Irvin Osborne-Lee (PVAMU)

http://crelonweb.wustl.edu

## Developing Environmentally Beneficial Catalytic Processes: A Multiobjective Task



## Multiscale Approach & Multidisciplinary Research Thrust Groups



**Disciplines Represented in TGs** 

- Engineering: Chemical, Civil, Environmental
- Sciences: Chemistry, Biology

## Multi-University Partnership: A Unique Resource for Catalysis Research

#### University of Kansas

High-pressure reaction engineering
Benign reaction media and catalyst supports
Molecular modeling and reaction mechanisms
Transition-metal catalyst design & synthesis

#### University of Iowa

- Biocatalyst design & synthesis
- Biocatalytic processing

### Engineered

Catalytic System

### Multiphase reactor engineering

Washington

University in St. Louis

**Reactor scaleup** 

#### Prairie View A&M

- Environmental Engineering
- Bioengineering

# Near-Term (5 Yr) Goals

- Develop transformational catalytic technologies using CEBC's strategic research concept for the following classes of reaction systems (termed as *testbeds*)
  - Selective oxidations
  - Oxidative biocatalysis
  - Hydroformylations of olefins
  - Solid acid catalyzed alkylations & acylations

## R&D Challenges & Expected Outcomes

- Catalyst design for selective, stable and atom-economical reactions
  - Novel biocatalysts, solid acid catalysts, homogenous and heterogeneous catalysts with nanoscale properties
- Design of "green" solvent media and catalyst supports
   Water, CO<sub>2</sub>-based solvents, nanoporous polymeric hosts
- Fundamentals of reaction mechanisms and reactor hydrodynamics
  - Advanced experimental methods for probing reaction mechanisms, transport properties and reactor hydrodynamics
  - Molecular-scale and CFD models
- Reactor selection, design and scaleup
  - Advanced multifunctional reactors and novel bioreactors based on the use of benign media and catalysts

## **Strategic Research Plan**

