



## ICDC Catalysis Crash Course

**May 30 - 31, 2015**  
**The Commons Hotel**  
**Minneapolis, Minnesota**

**INSTRUCTOR:** ICDC co-Principal Investigator Bruce Gates, University of California, Davis

**NOTE:** All sessions (except Session VI) are 90 minutes lecture, 30 minutes discussion

### **Saturday, May 30**

7:30 am - 8:30 am      **Registration**, Continental Breakfast Available  
Pinnacle Ballroom

8:30 am - 10:30 am      **Session I**  
Pinnacle Ballroom

- I. Definition of catalysis and basis for understanding
    - a. Cycles
    - b. Active centers
    - c. Fundamentals of reactors and kinetics
    - d. Rate equations and Arrhenius equation
      - i. Reaction networks
      - ii. Kinetics and thermodynamics
        - 1. Catalytic cycles
        - 2. Definitions (turnover frequency, etc)
        - 3. Conversion and selectivity
    - e. Reactors
      - i. Batch
      - ii. Flow
        - 1. Tube (no mixing)
        - 2. Tank (well mixed)
- Discussion -

10:30 am - 10:45 am      **Break**  
Pinnacle Ballroom

## **Saturday, May 30 (continued)**

10:45 am - 12:45 pm      **Session II**  
Pinnacle Ballroom

- II. Catalysis in solution
  - a. Acid-base catalysis
    - i. Brønsted relationship
    - ii. Hammett acidity function
  - b. Metal complex (organometallic) catalysis
  - c. Lewis acid catalysis
  - d. Transport (diffusion) influence on reaction rate
    - *Discussion* -

12:45 pm - 1:45 pm      **Lunch**  
Pathways Room

1:45 pm - 3:45 pm      **Session III**  
Pinnacle Ballroom

- III. Catalysis in gels and solution-like environments
  - a. Acid-base catalysis
  - b. Metal complex catalysis
  - c. Lewis acid catalysis
  - d. Transport (diffusion) influence on reaction rate
    - i. Extraparticle (fluid-phase) mass transport influence
    - ii. Intraparticle mass transport influence
  - e. Heat transfer influence
    - *Discussion* -

3:45 pm - 4:00 pm      **Break**  
Pinnacle Ballroom

4:00 pm - 6:00 pm      **Session IV**  
Pinnacle Ballroom

- IV. Catalysis in molecular-scale cages (e.g., zeolites)
  - a. Acid-base catalysis
  - b. Metal complex catalysis
  - c. Lewis acid catalysis
  - d. Transport effects: shape selectivity
    - *Discussion* -

7:00 pm      **Dinner**  
Pathways Room

**Sunday, May 31**

7:30 am - 8:30 am                    **Registration**, Continental Breakfast Available  
Pinnacle Ballroom

8:30 am - 10:30 am                **Session V**  
Pinnacle Ballroom

- V. Catalysis on surfaces
- a. Adsorption and surface area
  - b. Heterogeneity of surfaces
  - c. Methods for identifying and counting catalytic sites
  - d. Examples of reactions and processes
- Discussion -*

10:30 am - 11:00 am               **Break and Group Photo**  
Pinnacle Ballroom

11:00 am - 12:00 noon            **Session VI**  
Pinnacle Ballroom

- VI. Opportunities associated with catalysts that have well-defined surfaces
- a. Single crystals
  - b. Well-defined crystalline solids (e.g., zeolites)
  - c. Metal-organic frameworks
- Discussion -*

12:00 noon                            **Adjourn**