CHE, MT, EN, CH, NANO 555
Catalysis and Characterization of Nanoparticles
Fall 2011

Instructor: Prof. Simon Podkolzin
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Textbook:

"Concepts of Modern Catalysis and Kinetics" by I. Chorkendorff , J. W. Niemantsverdriet, Wiley-VCH; 2nd, Revised and Enlarged Edition (2007), ISBN-10: 3527316728, ISBN-13: 978-3527316724.

Additional recommended reading (optional):

"Heterogeneous Catalysis for the Synthetic Chemist" Robert L. Augustine, CRC Press; 1st edition (1995), ISBN-10: 0824790219, ISBN-13: 978-0824790219.

Class schedule:

Thursday at 6:15 - 8:45 pm in Burchard-430

Prerequisites:

CH-115 General Chemistry I or equivalent.
CH-116 General Chemistry II or equivalent.
CHE-234 Chemical Engineering Thermodynamics or equivalent.

Registration: If you have taken the prerequisite courses at a different university, please send this information to the instructor (Simon.Podkolzin@Stevens.edu) to receive a waiver. Use the E-mail confirmation with the waiver from the instructor to have the prerequisite restrictions removed by your Department office (CHE and MT student should contact Ms. Nancy Webb at the CEMS office).

Grading:

Homework	25
Class participation	25
Project and presentation	25
Midterm exam	25

Homework is due in class on Thursday. No late homework will be accepted for any reason. Each student may miss 1 homework assignment and still receive full credit for it. For students who complete all assignments, the homework with the lowest grade will be adjusted to 100%.

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Course Outline

1) Introduction to catalysis. Use of metal and metal oxide nanoparticles in catalysis. Homogeneous, heterogeneous and bio catalysis. Catalysis in energy research and green chemistry for sustainability.

(2) Kinetics of catalytic reactions. Integrated rate equations. Mean field approximation. Langmuir-Hinshelwood and Eley-Rideal reaction models. Steady-state approximation.

(3) Kinetics of catalytic reactions at nanoscale. Reaction rates based on the transition state theory.

(4) Elementary reaction steps. Adsorption on crystal planes and nanoparticles. Reactions between adsorbed species. Catalyst deactivation and regeneration.

(5) Characterization of nanoparticles for adsorption and catalysis applications: XRD, XPS, EXAFS. Description of the techniques, the nature of information obtained with these techniques, interpretation of results for establishing structure-catalytic activity relations. Usefulness and limitations.

(6) Characterization of nanoparticles for adsorption and catalysis applications: electron microscopies and Mossbauer spectroscopy. Usefulness and limitations.

(7) Characterization of nanoparticles for adsorption and catalysis applications with vibrational spectroscopies (HREELS, Raman and IR) and DFT calculations. Usefulness and limitations.

(8) Characterization of nanoparticles for adsorption and catalysis applications: SIMS, LEIS, and RBS ion spectroscopies; temperature programmed reactions. Usefulness and limitations.

(9) Catalysis with metal and metal oxide nanoparticles. Preparation and testing methods. Common catalyst supports. Zeolites as catalysts and catalyst supports. Inhibitors, promoters and poisons.

(10) Physisorption, chemisorption, dissociation. Reactions on surfaces at nanoscale. Bridging the scale gap between molecular reaction mechanisms and observable reaction rates.

(11) Kinetic modeling based on elementary reaction steps at the molecular level. Activation energy and reaction orders. Deriving kinetic expressions from elementary reaction mechanisms.

(12) Examples of commercial applications with catalytic nanoparticles. Catalytic reactions with hydrogen: steam reforming, methanol synthesis, synthetic fuels with Fischer-Tropsch chemistry, fuel cells.

(13) Examples of commercial applications with catalytic nanoparticles. Oil refining: hydrotreating, fluid catalytic cracking, reforming. Challenges for new technologies for green chemistry and sustainability: oxygen and hydrogen peroxide as benign oxidants with water as the only byproduct.