CME 522

Heterogeneous Catalysis & Surface Reaction

Credits and Contact hours: 3 credits; 2 hours 40 minutes weakly

Instructor: Tae Jin Kim (taejin.kim@stonybrook.edu, office # 218 at Old Eng. Bldg.)

Pre-requisites: CME504

Textbook: Julian R.H. Ross, Heterogeneous Catalysis: Fundamentals and Applications, 2011, Elsevier Publications, ISBN 978-0444533630

Suggested Materials

1. C.H. Bartholomew, R.J. Farrauto, Fundamentals of Industrial Catalytic Processes, 2005, Wiley Publications, ISBN 978-0471457138
2. Gadi Rothenberg, Catalysis: Concepts and Green Applications, 2008, Wiley-VCH Publications, ISBN 978-3527318247
3. J. W. Niemantsverdriet, Spectroscopy in Catalysis, 2007, Wiley-VCH Publications, ISBN 978-3527316519
4. H.S. Fogler, Elements of Chemical Reaction Engineering, 4th ed, 2006, Prentice Hall, ISBN 0-13-047394-4.

Week 1.	History and Background of catalysis
Week 2.	The basic of heterogeneous catalysis, homogeneous catalysis and biocatalysis
Week 3.	Synthesis of Catalysts: Bulk catalysts and Impregnated catalysts
Week 4.	Spectroscopy in Catalysis: Characterization Conditions (Ex-situ, In-situ, Operando) and Tools
Week 5.	Heterogeneous Catalysis: Fundamental
Week 6.	Guest speaker & **Midterm Exam**
Week 7.	Heterogeneous catalysis: catalysts and surface characterization
Week 8.	Heterogeneous catalysis in practice: oil refining and petrochemistry
Week 9.	Heterogeneous catalysis in practice: environmental catalysis
Week 10	Homogeneous and biocatalysis: industrial applications and catalyzed reactions
Week 11	Biomass conversion into biochemical and biofuel: heterogeneous and homogeneous catalysis

Week 12.	Kinetics and rate equations in catalysis: The reaction order: zero, first and second order kinetics
Week 13	Catalysis Reactors
Week 14	Electrocatalysis, Computational modeling
Week 15	Student final project presentations, final quiz, and reports
Week 16	Case study & **Final Exam**

Course Description:

Heterogeneous catalysis is central to the petroleum chemical industry and it is directly related to products efficiency. This course will emphasize the fundamental and application of heterogeneous catalysis and introduce the catalytic reaction mechanism. Students who complete the course will have attained the following outcomes: 1) Basic of heterogeneous catalyst and catalysis 2) Kinetics of heterogeneously catalyzed reaction 3) Surface characterization by spectroscopic techniques 4) Knowledge of supported metal oxide and zeolites 5) Application of theoretical calculations 6) Industrial applications of heterogeneous catalyst.

Students Learning Outcomes:

1. To know fundamental principles and experimental techniques used to study the five steps in a heterogeneously catalyzed reaction.
2. To be able to give a quantitative description of adsorption/desorption and the kinetics of catalytic reactions on a surface.
3. To be able to describe how quantum chemistry, statistical thermodynamics, and transition state theory are combined to calculate the rate of surface reactions.
4. To be able to account for how the catalytic activity and selectivity is influenced by the physical and electronic surface properties of the catalyst.
5. To be able to account for the physical and/or chemical phenomena behind important techniques for the characterization of catalysts and catalytic reactions and the information offered by these techniques.