

# Catalysis Principle and Catalyst Design

## Course Outline

This course provides lectures on catalysis principles and methods for catalyst design. The lectures are appropriate for master and Ph.D. students and covers electronic structure theory of catalysis, catalytic mechanism, surface structure analysis, and high-throughput screening method for catalyst development.

## Instructor

Jochen LAUTERBACH (University of South Carolina, College of Engineering and Computing)  
Sergey LEVCHENKO (Fritz-Haber-Institute, Theory Department)  
Kiyotaka ASAKURA (Hokkaido University, Institute for Catalysis)  
Jun-ya HASEGAWA (Hokkaido University, Institute for Catalysis)

## Type of Class and Class Hours [One class hour = Two hours (90 minutes of actual instruction)]

Lecture ( 8 ) Seminar ( ) Experiment ( ) Practical Training ( )

## Credit

1

## Duration

18/Jul/2017 - 27/Jul/2017

## Organizing Institution

Institute for Catalysis

## Level

Graduate Level

## Place

Sapporo

## Tuition (No additional fee for HU students)

¥14,800

## Language

English

## Capacity

20

## Target Group (Prerequisites)

This course is useful for master and PhD students with a strong interest in catalysis.  
A basic understanding of physical and inorganic chemistry is a prerequisite for successful course completion.

## Key Words

Electronic structure theory, Catalytic mechanism, Surface structure analysis, High-throughput screening

## Course Objectives

Materials that promote chemical reactions are called Catalyst. Because many useful chemical compounds are produced, catalysts have been highly interesting in scientific and industrial points of view. Catalysts provide environmentally-friendly ways of chemical synthesis, because catalysts do not change their catalytic properties and drive the chemical reaction with less energy. Therefore, catalysis is the indispensable for realizing sustainable human society. However, due to the complexity in catalyst structure and in catalysis reaction, the research on the catalytic mechanism is still in progress.

Another important aspect is catalyst design. More efficient catalysts are desired for keeping the existing human society that is based on the energy consumptions. Therefore, both rational and efficient methods for the catalyst development are highly desirable.

For this event, Institute for Catalysis (ICAT) invites the top level scientists for the catalysis theory and catalysis design. This lecture provides electronic structure theory of catalysis, catalytic mechanism, surface structure analysis, and high-throughput screening method for catalyst development. We also show a current status of catalyst development. This lecture provides a unique opportunity to explain the forefront by the frontrunners in the field of catalysis science.

## Course Goals

By the end of this course you will be able to explain

1. the electronic structure method that are widely used in computer programs.
2. the catalytic mechanism underlying the catalytic reactions.
3. the methods for surface structure analysis and X-ray absorption spectroscopy.
4. the high-throughput screening methods for efficient catalyst design.

#### Course Schedule

1. Density-Functional Theory for Materials
  2. Ab initio atomistic thermodynamics
  3. Potential energy surface of chemical reactions
  4. Electronic structure of catalytic surfaces
  5. Introduction to surface structure analysis :
  6. Principle and applications of X-ray absorption spectroscopy
  7. In situ spectroscopic techniques for surface processes
  8. The high-throughput screening methods for efficient catalyst design
- Since the course schedule may be changed, please confirm final schedule.

#### Preparation and Assignments

Students will be asked to write a report at the end of each lecture.

#### Grading System

Grades are judged based on attendance records and reports in which the students will be requested to explain

1. the electronic structure method that are widely used in computer programs (25 %)
2. the catalytic mechanism underlying the catalytic reactions (25 %)
3. the methods for surface structure analysis and X-ray absorption spectroscopy (25 %)
4. the high-throughput screening methods for efficient catalyst design (25 %).

#### Related Course(HSI)

None

#### Textbooks

None

#### Reading List

None

#### Equipment

None

#### Additional Information

None

#### Update

1/Dec/2016