Advanced Computational Chemistry

Course Outline

This coursework will cover the following topics: (1) Mapping the Reaction Paths with the Artificial Force Induced Reaction (AFIR) Method, (2) Calculation of Excited State Species and Design of Heterogeneous Catalysts, (3) Chemoinformatics: In silico design of new molecules, materials and reactions, (4) Theoretical Calculation of Polymer Materials and Macromolecules, (5) "Data-driven prediction" and "optimal design of experiments" in chemistry with machine learning.

Instructor (Institution)

Kimichi SUZUKI (Associate Professor, Institute for Chemical reaction Design and Discovery, Hokkaido University)

Andrey LYALIN (Associate Professor, Institute for Chemical reaction Design and Discovery, Hokkaido University)

Alexandre VARNEK (Professor, Laboratory of Chemoinformatics, University of Strasbourg)

Michael RUBINSTEIN (Professor, Department of Chemistry and Departments of Mechanical Engineering and Materials Science, Biomedical Engineering, and Physics, Duke University)

Ichigaku TAKIGAWA (Researcher, Center for Advanced Intelligence Project, RIKEN)

Type of Class

Lecture (✓) Seminar ( ) Experiment [Lab work] ( ) Practical Training ( )

Credit

1

Duration

24 / AUG - 26 / AUG , 2020

Organizing Institution

Institute for Chemical Reaction Design and Discovery

Level

Graduate Level

Place

✓	Sapporo Campus		Hakodate Campus		Other;

Tuition (No additional fee for HU students)

¥14,800

Language

English

Capacity

50

Target Group (Prerequisites)

This course is intended for master course and PhD students with a background in theoretical chemistry, quantum chemistry, computational chemistry, chemoinformatics, and machine learning.

Non-Students Application		Not Applicable

Key Words

Theoretical Chemistry, Quantum Chemistry, Computational Chemistry, Artificial Force Induced Reaction Method, Reaction Dynamics, Reaction design, Chemoinformatics, Materials informatics, Bioinformatics, Quantitative Structure-Activity Relationships, Condensed Graph of Reaction, Chemical Space analysis, Machine learning, Data mining, Big Data, Artificial Intelligence

Course Objectives

The development of new chemical reactions is intrinsically entangled with the prosperity of humanity and the preservation of the environment. However, the currently used methods for the design and development of bespoke chemical reactions is highly inefficient. Usually, these methods are based on trial and error, which is not only very laborious and time-consuming, but the discovery of truly innovative reactions is relatively rare. As the development and implementation of new chemical reactions often takes decades in reality, fundamentally new scientific approaches are required.

In this lecture, the development of new chemical reaction by using computational chemistry and information science will be discussed. In particular, "Artificial Force Induced Reaction" (AFIR) method to calculate chemical reaction-path networks, Calculation of Excited State Species, Theoretical Calculation of Polymer Materials and Macromolecules and information science such as chemoinformatics and machine learning, for chemical reaction prediction will be discussed.

Course Goals

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

1. understand Mapping the Reaction Paths with the Artificial Force Induced Reaction (AFIR) Method
2. understand Calculation of Excited State Species and Design of Heterogeneous Catalysts
3. understand Chemoinformatics: In silico design of new molecules, materials and reactions
4. understand Theoretical Calculation of Polymer Materials and Macromolecules
5. understand "Data-driven prediction" and "optimal design of experiments" in chemistry with machine learning.

Course Schedule

This Course is focused the development of new chemical reaction by using computational chemistry and information science.
In particular, this course is organized as follows:

1. Mapping the Reaction Paths with the Artificial Force Induced Reaction (AFIR) Method (2 lectures).
2. Calculation of Excited State Species and Design of Heterogeneous Catalysts (2 lectures).
3. Chemoinformatics: In silico design of new molecules, materials and reactions (1 lecture).
4. Theoretical Calculation of Polymer Materials and Macromolecules (1 lecture).
5. "Data-driven prediction" and "optimal design of experiments" in chemistry with machine learning (2 lectures).

Preparation and Homework

Students need the preparations for discussion about Computational chemistry, theoretical calculation, Chemoinformatics and machine learning.
You will be asked to write a page (A4) of report at the end of each lecture.

Grading System

Grading will be based on the reports submitted regarding Computational chemistry, Theoretical calculation, Chemoinformatics and machine learning (60%).
In addition, we also consider it as the important factor for assessment how actively students participate in each class (40%).

Related Course (HSI)

Mandatory Course (Course required to be taken together with this course):

Recommended Course (Course highly recommended to be taken together with this course):

Textbooks

No textbook required. Handout will be distributed.

Reading List

Required Equipment for a class (Laptop, etc.)

Website of Laboratory

https://www.icredd.hokudai.ac.jp/

Additional Information

Contact Information for Inquiries

Update

5/Dec/2019