Intensive Course Schedule for Spring and Summer terms
in International Physics Course (IPC) and Special Integrated Science Course (SISC)
at the Graduate School of Science at Osaka University

Updated: 2018.7. 27

Courses (Code)	Instructors (Affiliation)	Date	Period	Classroom
Current Topics Ⅰ Carbohydrates:biofunction and chemical synthesis (24S014)	**Prof. Koichi FUKASE** (Osaka University)	April 19 (Thu) April 20 (Fri)	2 ～5 2 ～4 (-15:25), 16:00～1730: open lecture Details are shown on the attached file	D401
Current Topics Ⅲ How plants recognize circumstances (24S016)	**Associate prof. Izumi MORI** (Okayama University)	July 2 (Mon) July 3 (Tue)	3 ～5 1 ～5 (-17:05)	E204
Current Topics Ⅳ Introduction to Computational Chemistry (24S017)	**Associate Prof. Hajime HIRAO** (City University of Hong Kong)	August 21 (Tue) August 22 (Wed) August 23 (Thu)	3 ～4 3 ～4 3 ～5 (16:20- Research seminar) ※ Details are shown on the next pages	【Toyonaka】Lec Room 3, 7F, Interdisciplinary Research Building 【Suita:**Video Lecture Only**】 Room F390, First Research Building of I.S.I.R
Current Topics Ⅴ Recent Topics of Molecule-based Magnets (24S018)	**Prof. Joel S. Miller** (University of Utah)	July 11 (Wed) July 18 (Wed) July 25 (Wed)	1 ～2 1 ～4 (-15:25) 1 ～2	E204

IMSC
INTERACTIVE MATERIALS SCIENCE CADET

インタラクティブ物質科学・カデットプログラム
平成30年度物質科学特別講義（化学系）
Topical Seminar for Materials Science, 2018

Dr. Hajime Hirao
Department of Chemistry,
City University of Hong Kong

Introduction to Computational Chemistry

Course Objective:

Computational chemistry is nowadays an indispensable tool for investigating a variety of chemical phenomena at the atomic level. The availability of many elaborate software packages allows us to apply computational chemistry techniques to specific problems immediately without paying much attention to underlying theories. Although this black-box-like nature is in a sense a good aspect of computational chemistry, in this course, emphasis will be placed rather on discussing derivation processes and other details of a few fundamental concepts.

Schedule

Day 1: Aug. 21, 13:00-14:30, 14:40-16:10
Day 2: Aug. 22, 13:00-14:30, 14:40-16:10
Day 3: Aug. 23, 13:00-14:30, 14:40-16:10

Research seminar:

"Applications of Computational Chemistry to Chemical Reactions"
Aug.23,16:20-

Place

<TOYONAKA> Lec Room 3, 7F, Interdisciplinary Research Building
（豊中・文理融合棟7階・講義室３）
<SUITA>Room F390, First Research Building of I.S.I.R ※
(吹田・産研・第一研究棟３階・F390)　※Video Lecture Only

More info. about Dr. Hirao:
https://www.cityu.edu.hk/chem/profile/drhirao.html

Hong Kong City UniversityのDr. Hajime Hiraoをお招きし、物質科学特別講義を開催します。
希望者には物質科学特別講義（1単位）の付与が可能、
カデット生以外の受講も受け付けますので、
お気軽にお問い合わせください。沢山のみなさまのご参加をお待ちしております。

問合せ先：未来戦略第三部門インタラクティブ物質科学カデットプログラム事務局
mirai-jimu-dai3@office.osaka-u.ac.jp　内線・6403（豊中）

Introduction to Computational Chemistry

Hajime Hirao
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Course Objective

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Expected Learning Outcomes

1. To understand key mathematical tools and fundamental quantum mechanical concepts, which are closely related to quantum chemistry.
2. To understand key concepts and formalisms in quantum chemistry and computational chemistry (Hartree approximation, Hartree–Fock equations, density functional theory (DFT), hybrid quantum mechanics and molecular mechanics (QM/MM) methods, etc.).
3. To be able to solve relevant quiz questions and explain.
4. To get prepared for further learning of computational chemistry in the future.

Schedule

Day 1: introduction; key mathematical tools and techniques; (quantum chemistry 1)
Day 2: quantum chemistry 1; research seminar (recent applications of computational chemistry to be showcased)
Day 3: quantum chemistry 2; other computational chemistry techniques

Recommended Reading

1. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (A. Szabo and N. S. Ostlund)
2. A Chemist's Guide to Density Functional Theory (W. Koch and M. C. Holthausen)
3. Essentials of Computational Chemistry: Theories and Models (C. J. Cramer)

Grading Policy

50% class participation (presentation, quiz, etc); 50% final report (assignment).