

# Computational Materials Science for Photonics

Special Subjects  
Elective 2 credit

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## 1. Course Description

Students will learn the followings in this course,

- (1) Basics of the quantum theory of many electrons in matter
- (2) Matter-light interaction
- (3) Density functional theory (DFT)
- (4) Usage of DFT computation softwares.

This course is in accordance with diploma policy #2.

## 2. Course Objectives

Material properties that benefit us in everyday lives mostly originate from the microscopic behavior of the internal electrons.

Their simulation on computers thus will lead us to the better understanding of how these properties emerge and also the possible prediction of yet undiscovered superior materials.

In this course we shall learn the theory of electronic states of matter and know how to use DFT computation softwares for your own needs. We will also learn to simulate the behavior of matter under optical excitation.

## 3. Grading Policy

You will be graded by your exercise performances (50%) and lab reports (50%).

Comments are appropriately provided for feedback.

## 4. Textbook and Reference

Textbook

Kaoru Ohno et al. Computational Nanoscience (Japanese) Kindai Kagakusha

Reference

June Gunn Lee Computational Materials Science: An Introduction CRC Press

## 5. Requirements(Assignments)

Read the corresponding part of the lecture materials and the reference books carefully (~3 hours in total).

## 6. Note

None.

## 7. Schedule

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|------|--|
| [1]  | Basic quantum mechanics  |
| [2]  | Many electron systems, Hartree-Fock approximation  |
| [3]  | Density functional theory (DFT)  |
| [4]  | Representation of electron wavefunctions 1: atoms and molecules                                |
| [5]  | Representation of electron wavefunctions 2: solids   |
| [6]  | Self-consistent calculation  |
| [7]  | Calculation of forces, first principles molecular dynamics                                     |
| [8]  | Exercise #1: Usage of the computing environment  |
| [9]  | Exercise #2: Computation of electronic states via DFT software                                 |
| [10] | Second quantization  |
| [11] | Theory of quasi-particles  |
| [12] | Time-dependent density functional theory (TD-DFT)  |
| [13] | Exercise #3-1: Calculation of material optical properties via TD-DFT: weak excitation regime   |
| [14] | Exercise #3-2: Calculation of material optical properties via TD-DFT: strong excitation regime |
| [15] | Summary  |