理　學　院
109 學年度第一學期模組化課程

應用第一原理於凝態材料理論與實作(一)
Applications of First-Principles methods to Condensed Materials：Theory and Practice(I)

授課教師	任職單位	畢業學校
鄭靜	**國立成功大學理學院兼任教授**	**英國劍橋大學**

課程類別	學分數	選必修	開課人數	其他注意事項
Lecture + Recitation	**2**	**選修**	**35**	**學生需自備筆電。實作軟體以 Material Studio 為主，軟硬體需求請見本課程綱要最後一頁。**

先修課程或先備能力：

無

建議修課年級：

大三、大四、碩士班

建議修課學生背景：

理學院、工學院、電資學院

欲修習「應用第一原理方法於凝態材料性質研究的理論與實作(二)」學生者，需先選修本課程。

教學方法：

講授 50%、實作 30%、討論 20%

評量方式：

問題考試 30%、報告 30%、實驗操作 40%

補充說明：

The Q/A will be taken at the end of each 3.5-hour lectures (30%).
The final report is about the implementation of the first-principles methods to a project identified by the course takers (30%).
The experimental practice is about evaluation of the performance in the hands-on sessions (40%).

學習規範：

無

課程概述(中文)：

本課程的目的在提供修課者，應用第一原理方法於凝態系統研究相關物理性質的理論背景知識和實際執行操作。

課程概述(英文)：

The aim of the course is to provide the course takers both theory and practice of the applications of first-principles methods to condensed materials.

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課程進度：

堂次	時數	進 度 說 明
8/3	9:00-12:40 14:00-17:40	**A. Many-electron systems: Introduction (Lectures)** **1. From classical continuum to quantum world** **2. Complexity of many-electron systems : from on-electron, two-electron to many-electron systems** **3. Density Function Theory : exchange-correlation energy functionals**
8/4	9:00-12:40 14:00-17:40	**B. Electronic Structures (Lectures)** **1. What is the classical picture?** **2. "one-electron systems" to "few-electron systems" to "condensed systems"** **3. Periodic systems : real-space atomic structures → reciprocal space** **4. Electronic structures → band structures** **實作 B1：Stability of bulk materials; geometry optimization; numerical accuracy**
8/5	9:00-12:40 14:00-17:40	**B. Electronic Structures (Lectures)** **5. Electronic spectra → electronic density of states (DOS)** **6. Excitations : HOMO and LUMO** **實作 B2：Electronic structures of bulk materials; pseudopotentials**
8/6	9:00-12:40 14:00-17:40	**C. Thermal vibration (Lectures)** **1. 2-atom systems** **2. Clusters** **3. Periodic systems : lattice vibration → phonon dispersion** **實作 C1：molecular vibrations**
8/7	9:00-12:40 14:00-17:40	**4. Phonon energy spectra → phonon density of states (DOS)** **5. IR spectra and Raman spectra** **實作 C2：elastic properties, IR and Raman spectra of bulk materials, phonon dispersion**

課程學習目標：

1.Equipped with the basic knowledge of the quantum theory for many-electron systems
2.Capable of implementing the first-principles methods to condensed material science
3.Carrying out the application to the course takers' interested material systems and properties

課程的重要性、跨域性與時代性：

Researchers, notably material experimentalists, usually search for an alternative or/as well as side-by-side theoretical rationalization to their experimental outcome.

At the same time, the progress of the first-principles methods, along with the computational hardware and the development of the friendly interfaces, has reached a point such that some physical

properties of condensed materials can be obtained by reasonable standard procedures.

However, the theories behind these first-principles methods and the complex implementation involved still prove hindering its application by the experimental researchers.

The aim of the course is to bridge the gap in between the experimental researchers and the applications of the first-principles methods.

The focus will be providing the most essential theoretical background of the first-principles methods and, through the hands-on sessions, demonstrating as well as supervising the course takers to carry out implementations on the material systems of their interested research fields.

The corresponding topics of applications include the physical properties which are usually encountered by the researchers in the departments of material science, chemical engineering, resource engineering, earth science, to name a few.

The course is expected to facilitate, for the experimental researchers, understanding and interpreting the studied condensed-material systems using the first-principles methods.

其他備註:

參考書目：

Structure and dynamics by M. T. Dove (Oxford University Press);
Band theory and electronic properties of solids by J. Singleton (Oxford University)

學生自備之筆電軟硬體需求：

Materials Visualizer Requirements

This section describes the requirements of the Materials Visualizer *only*. The Materials Visualizer is the core client module in Materials Studio; providing modeling, analysis, and visualization tools. It cannot set up or launch jobs *unless* installed in conjunction with Materials Studio Server.

Supported Operating Systems

Operating System	Supported Versions	Notes
Microsoft Windows Professional & Enterprise	10	64-bit only

Hardware Requirements

Component	Minimum Hardware	Recommended
Processor	Intel® Core™ i5 or equivalent	Intel Core i7 or equivalent
RAM	4 GB	16 GB
Available hard disk space for installation	1 GB	4 GB
	The hard disk space required for installation can vary between 1 GB for Materials Visualizer only and 4 GB if you install the complete Materials Studio server and client. The Materials Visualizer can only be installed on Windows. Additional space will be required if system updates are necessary, for example for .NET, runtimes, and libraries.	
Display	1366 × 768 display resolution 24-bit	1920 × 1080 display resolution 32-bit