課程綱要與教學日誌

101 學年度第 1 學期

課程名稱：（中文）**電腦輔助材料設計** （英文）Computer-aided Design of Materials		開課單位	光電工程學系
		永久課號	

授課教師：黃中垚

學分數	3	必/選修	選	開課年級	大四、研究所

先修科目或先備能力：
近代物理 (或量子力學)、固態物理 (或材料力學、統計物理、熱力學等)

課程概述與目標：
This course provides the background and an extensive set of examples of how computational methods are applied to modern design of materials with desired functionality. The methods span multi-length and time scales, including molecular dynamics simulations, first-principles approaches, stochastic methods for optimization and sampling, and continuum elasticity theory. The examples will include problems in electronic and photonic devices, materials for energy conversion, storage, and environmental protection, and those related to mechanical strength of materials.

After taking this course, hopefully students are able to:
• Apply computational methods, such as molecular dynamics simulations, first-principles approaches, stochastic methods, and continuum elasticity theory, to modern design of materials;
• Effectively design materials of desired functionality;
• Design experimental studies of materials with better physical insights;
• Interpret experimental data based on related theoretical modeling and simulations.

教科書	Following books are helpful for references: 1. Density-Functional Theory of Atoms and Molecules, Robert G. Parr, Weitao Yang (Oxford University Press, 1989). 2. Atomic and Electronic Structure of Solids, Efthimios Kaxiras (Cambridge University Press, 2003). 3. Introduction to Surface Chemistry and Catalysis, Gabor A. Somorjai (Wiley, 1994). 4. Introduction to Nanoscience, Steve Lindsay (Oxford University Press, 2010). 5. Nano Mechanics and Materials: *Theory, Multiscale Methods, and Materials*, Wing Kam Liu, Eduard G. Karpov, Harold S. Park (Wiley, 2006).

課程大綱		分配時數				備註
單元主題	內容綱要	講授	示範	習作	其他[1]	

1. Principles of computational materials design	1.1 Kohn-Sham density functional theory 1.2 Molecular Dynamics Simulation 1.3 Transition-state search with Nudged elastic band method 1.4 Kinetic Monte Carlo simulations 1.5 Multi-scale materials modeling: sequential approaches 1.6 Multi-scale materials modeling: concurrent approaches	15				
2.Computational design of materials for desired mechanical properties	2.1 *Ab initio* elasticity of single-crystal solids 2.2 Superhard materials 2.3 Modeling Brittle and Ductile Behavior of Solids	6				
3. Computational design of semiconductor systems	3.1 Stable versus unstable growth in strained systems 3.2 Fabrication of ordered semiconductor quantum dots 3.3 Interface control of semiconductor multilayers 3.4 Morphological evolution on stepped surfaces 3.5 Bandgap engineering of low-dimensional semiconductors 3.6 Doping control of oxide semiconductors for energy applications 3.7 Diluted magnetic semiconductors (DMS)	9				
4. Computational design of metal systems	4.1 Pre DFT Model for Metal: 4.1.1 Jellium model (focus on electrons) 4.1.2 Effective Medium Model (EMM, focus on ions) 4.1.3 Embedded Atom Model (EAM, focus on ions) 4.2 Magic Clusters 4.3 Metal Wires 4.4 Quantum Size Effects (Stability, Work Function) of Metallic Films and Alloys 4.5 Plasmonic materials and Metamaterials	6				
5. Computational design of catalytic materials	5.1 Fundamentals of catalysis 5.2 *d*-band theory of surface catalysis 5.3 Photocatalysis 5.4 Novel quantum materials for environmental cleanup	6				

6. Computational Design of Clean Energy-related Materials	6.1 Atomistic Simulation Methods for Energy Materials 6.2 *ab initio* design of photovoltaic materials 6.3 Solid Ion Conductors for Fuel Cells: 6.3a Proton transport through perovskite oxides (ABO_3) 6.3b Oxide-ion transport through apatite silicates 6.3c Cathode Materials for Lithium Batteries 6.4 Water splitting with Photocatalysis and Hydrogen Storage Materials 6.5 Thermoelectric Materials and Applications	6				
7. Project Presentation Session of Students					6	

1. 教學要點概述 (請填寫教材編選、教學方法、評量方法、教學資源、教學相關配合事項等)：

Students must actively participate the lectures and discussions. The overall performance of a student will be evaluated by two homeworks (40%) and the final project (60%) she or he completes as a team effort. Projects combining experimental data and simulations are particularly encouraged.

教學日誌(進度)

週次	上課日期	課程進度、內容、主題
1-2		**1. Principles of computational materials design)** 1.1 Kohn-Sham density functional theory 1.2 Classical and ab initio molecular dynamics 1.3 Nudged elastic band method for atomistic rate processes
3		1.4 Kinetic Monte Carlo simulations 1.5 Multi-scale materials modeling: sequential approaches 1.6 Multi-scale materials modeling: concurrent approaches
4-5		**2. Computational design of materials for desired mechanical properties** 2.1 Ab initio elasticity of single-crystal solids 2.2 Superhard materials 2.3 Modeling Brittle and Ductile Behavior of Solids
6		**3. Computational design of semiconductor systems** 3.1 Fabrication of ordered semiconductor quantum dots 3.2 Interface control of semiconductor multilayers 3.3 Bandgap engineering of low-dimensional semiconductors
7		3.4 Doping control of oxide semiconductors for energy applications 3.5 Diluted magnetic semiconductors (DMS)
8-9		**2. Computational design of metal systems** 2.1.1 Jellium model 2.1.2 Effective Medium Theory 2.1.3 Embedded Atom Model

		2.2 Magic Clusters 2.3 Metal wires 2.4 Quantum size effects of metallic films and alloys 2.5 Plasmonic materials and Metamaterials
10-11		**4. Computational design of catalytic materials** 4.1 Fundamentals of catalysis
12		4.2 *d*-band theory of surface catalysis 4.3 Photocatalysis 4.4 Novel quantum materials for environmental cleanup
13		**6. Computational design of Clean Energy-related Materials** 6.1 *Ab initio* design of photovoltaic materials 6.2 Solid Ion Conductors for Fuel Cells: 6.2a Proton transport through perovskite oxides (ABO3)
14-15		6.2b Oxide-ion transport through apatite silicates 6.2c Cathode Materials for Lithium Batteries 6.3 Photocatalysis, Water splitting, and Hydrogen Storage Materials 6.4 Thermoelectric Materials and Applications
16		**Project Presentation Session of Students: I**
17		**Project Presentation Session of Students: II**
18		**Project Presentation Session of Students: III**

備註：

1. 其他欄包含參訪、專題演講等活動。
2. 所有課程包括學系所開設必（選）修、選修課程，以及校際所開設課程，如共同必修科目、通識課程等，皆須填寫此表格。
3. 如需本課程綱要表格之電子檔，請至課務組網頁－＞各類申請表下載。
4. 請用電腦打字成檔案，於每學期末、初選前（1 月初及 6 月初），利用選課系統（http://cos.adm.nctu.edu.tw/）之「課程綱要上傳」將課程綱要 update 上網。