Tamkang University Academic Year 104, 1st Semester Course Syllabus

Course Title	ATOMISTIC SIMULATION OF OPTOELECTRONIC MATERIALS	Instructor	HSUEH, HUNG-CHUNG
Course Class	TSPXM1A MASTER'S PROGRAM, DEPARTMENT OF PHYSICS, 1A	Details	◆ Selective ◆ One Semester ◆ 3 Credits

Departmental Aim of Education

Ⅰ. Conveying professional knowledge: Teach the students to learn the core knowledge of physics, to obtain the basic skills needed for physics research, and to apply the professional knowledge to physics related technologies.

Ⅱ. Analyzing and solving problems: Guide the students to analyze problems, and to acquire the mathematical ability to quantify conceptual models and also the capability needed to think and to innovate in solving various scientific and engineering problems.

Ⅲ. Training for experimental techniques: Teach the students on how to carry out and to verify various experiments, and at the same time to have the mentality of working cautiously and the awareness in operating safely.

Ⅳ. Expressing personal characteristics: Help the students to use their personal characteristics, like resolution, sincerity, and concentration, plus their professional skills to gain recognition among the executives and their peers.

Ⅴ. Cultivating team spirit: Train the students to have the organizational ability and the communicational skills to let them have the adaptability to integrate into a professional team, and to obtain the ability to bring out and to put to use the strength of.

Ⅵ. Building international views: Comply to the trends of globalization to build an international learning environment and opportunities in order to educate the students to continue in their self-advancements, to absorb new worldwide knowledge, and to become.

Departmental core competences

A. To acquire the core basic knowledge in the field of physics.

B. To understand the overall features of specific fields of physics.

C. To obtain the mathematical ability to quantify concepts, models, and practical problems.

D. To cultivate the basic ability to discover, to analyze, and to solve problems.

E. To practice the actual handling of physics problems, and to have the ability to analyze and to interpret experimental data.

F. To have the mentality to work cautiously and the awareness to operate safely.

G. To comprehend the trend of technological development and to acquire the knowledge and skills of other fields needed in their professional career.

H. To have the spirit and capability in team cooperation.

Course Introduction	Students could get insight into all the characteristics of opto-electronic materials (eg. structural, electronic-structure, magnetic, and optical properties) by means of both fundamental solid-state theory and ab-initio calculations.

The Relevance among Teaching Objectives, Objective Levels and Departmental core competences

I.Objective Levels (select applicable ones) :

(i) Cognitive Domain : C1-Remembering, C2-Understanding, C3-Applying, C4-Analyzing, C5-Evaluating, C6-Creating

(ii) Psychomotor Domain : P1-Imitation, P2-Mechanism, P3-Independent Operation, P4-Linked Operation, P5-Automation, P6-Origination

(iii) Affective Domain : A1-Receiving, A2-Responding, A3-Valuing, A4-Organizing, A5-Charaterizing, A6-Implementing

II.The Relevance among Teaching Objectives, Objective Levels and Departmental core competences :

(i) Determine the objective level(s) in any one of the three learning domains (cognitive, psychomotor, and affective) corresponding to the teaching objective. Each objective should correspond to the objective level(s) of ONLY ONE of the three domains.

(ii) If more than one objective levels are applicable for each learning domain, select the highest one only. (For example, if the objective levels for Cognitive Domain include C3,C5,and C6, select C6 only and fill it in the boxes below. The same rule applies to Psychomotor Domain and Affective Domain.)

(iii) Determine the Departmental core competences that correspond to each teaching objective. Each objective may correspond to one or more Departmental core competences at a time. (For example, if one objective corresponds to three Departmental core competences: A,AD, and BEF, list all of the three in the box.)

No.	Teaching Objectives	Relevance	
		Objective Levels	Departmental core competences
1	Students could get the ability of both fundamental theory and computational skill of electronic properties calculation of materials.	C3	AEG

Teaching Objectives, Teaching Methods and Assessment

No.	Teaching Objectives	Teaching Methods	Assessment

1	Students could get the ability of both fundamental theory and computational skill of electronic properties calculation of materials.	Lecture, Discussion, Simulation	Practicum, Participation

This course has been designed to cultivate the following essential qualities in TKU students

Essential Qualities of TKU Students	Description
◇ A global perspective	Helping students develop a broader perspective from which to understand international affairs and global development.
◆ Information literacy	Becoming adept at using information technology and learning the proper way to process information.
◆ A vision for the future	Understanding self-growth, social change, and technological development so as to gain the skills necessary to bring about one's future vision.
◇ Moral integrity	Learning how to interact with others, practicing empathy and caring for others, and constructing moral principles with which to solve ethical problems.
◇ Independent thinking	Encouraging students to keenly observe and seek out the source of their problems, and to think logically and critically.
◇ A cheerful attitude and healthy lifestyle	Raising an awareness of the fine balance between one's body and soul and the environment; helping students live a meaningful life.
◆ A spirit of teamwork and dedication	Improving one's ability to communicate and cooperate so as to integrate resources, collaborate with others, and solve problems.
◇ A sense of aesthetic appreciation	Equipping students with the ability to sense and appreciate aesthetic beauty, to express themselves clearly, and to enjoy the creative process.

Course Schedule

Week	Date	Subject/Topics	Note
1	104/09/14 ~ 104/09/20	Introduction	
2	104/09/21 ~ 104/09/27	An overview of computational material science	
3	104/09/28 ~ 104/10/04	Density Functional Theory	
4	104/10/05 ~ 104/10/11	Density Functional Theory	
5	104/10/12 ~ 104/10/18	Atoms in crystals (supercell, k-points, ...)	
6	104/10/19 ~ 104/10/25	Pseudopotential vs. atomic orbital	
7	104/10/26 ~ 104/11/01	Computational procedure (Methodolgy)	
8	104/11/02 ~ 104/11/08	Electronic band structure calculation I	
9	104/11/09 ~ 104/11/15	Electronic band structure calculation II	

10	104/11/16～104/11/22	Electronic band structure calculation Ⅲ	
11	104/11/23～104/11/29	Structural properties calculation Ⅰ	
12	104/11/30～104/12/06	Structural properties calculation Ⅱ	
13	104/12/07～104/12/13	Magnetic properties calculation Ⅰ	
14	104/12/14～104/12/20	Magnetic properties calculation Ⅱ	
15	104/12/21～104/12/27	Optical properties calculation Ⅰ	
16	104/12/28～105/01/03	Optical properties calculation Ⅱ	
17	105/01/04～105/01/10	Quasiparticle GW calculations	
18	105/01/11～105/01/17	Beyond Density Functional Theory	

Requirement	Since topics included in this lecture are rather broaden, please try your best to attend each lecture.
Teaching Facility	Computer, Other (PC cluster)
Textbook(s)	Teaching note as enclosed in the teaching-add platform
Reference(s)	User manual of VASP (can be downloaded from http://www.vasp.at/index.php/documentation) Atomic and Electronic Structure of Solids /Efthimios Kaxiras, Cambridge University Press (2003)
Number of Assignment(s)	(Filled in by assignment instructor only)
Grading Policy	◆ Attendance： 20.0 % ◆ Mark of Usual： % ◆ Midterm Exam： % ◆ Final Exam： 30.0 % ◆ Other〈Hand-ons〉：50.0 %
Note	This syllabus may be uploaded at the website of Course Syllabus Management System at http://info.ais.tku.edu.tw/csp or through the link of Course Syllabus Upload posted on the home page of TKU Office of Academic Affairs at http://www.acad.tku.edu.tw/CS/main.php . **※ Unauthorized photocopying is illegal. Using original textbooks is advised. It is a crime to improperly photocopy others' publications.**