

Tamkang University Academic Year 108, 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	<ul style="list-style-type: none"> ◆ General Course ◆ Selective ◆ One Semester

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 the team to solve professional problems.
- 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 a professional with international views in their future perspective careers.

Subject Departmental core competences

- A. To acquire the core basic knowledge in the field of physics.(ratio:20.00)
- C. To obtain the mathematical ability to quantify concepts, models, and practical problems.
(ratio:30.00)
- D. To cultivate the basic ability to discover, to analyze, and to solve problems.(ratio:30.00)
- E. To practice the actual handling of physics problems, and to have the ability to analyze and to interpret experimental data.(ratio:20.00)

Subject Schoolwide essential virtues

2. Information literacy. (ratio:40.00)
3. A vision for the future. (ratio:30.00)
5. Independent thinking. (ratio:30.00)

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.
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The correspondences between the course's instructional objectives and the cognitive, affective, and psychomotor objectives.

Differentiate the various objective methods among the cognitive, affective and psychomotor domains of the course's instructional objectives.

- I. Cognitive : Emphasis upon the study of various kinds of knowledge in the cognition of the course's veracity, conception, procedures, outcomes, etc.
- II. Affective : Emphasis upon the study of various kinds of knowledge in the course's appeal, morals, attitude, conviction, values, etc.
- III. Psychomotor: Emphasis upon the study of the course's physical activity and technical manipulation.

No.	Teaching Objectives	objective methods
1	Students could get the ability of both fundamental theory and computational skill of electronic properties calculation of materials.	Cognitive

The correspondences of teaching objectives : core competences, essential virtues, teaching methods, and assessment

No.	Core Competences	Essential Virtues	Teaching Methods	Assessment
1	AD	2	Lecture, Practicum	Testing, Practicum

Course Schedule

Week	Date	Course Contents	Note
1	108/09/09 ~ 108/09/15	Introduction	
2	108/09/16 ~ 108/09/22	An overview of computational material science	
3	108/09/23 ~ 108/09/29	Density Functional Theory	
4	108/09/30 ~ 108/10/06	Density Functional Theory	

5	108/10/07 ~ 108/10/13	Atoms in crystals (supercell, k-points, ...)	
6	108/10/14 ~ 108/10/20	Pseudopotential vs. atomic orbital	
7	108/10/21 ~ 108/10/27	Computational procedure (Methodolgy)	
8	108/10/28 ~ 108/11/03	Electronic band structure calculation I	
9	108/11/04 ~ 108/11/10	Electronic band structure calculation II	
10	108/11/11 ~ 108/11/17	Electronic band structure calculation III	
11	108/11/18 ~ 108/11/24	Structural properties calculation I	
12	108/11/25 ~ 108/12/01	Structural properties calculation II	
13	108/12/02 ~ 108/12/08	Magnetic properties calculation I	
14	108/12/09 ~ 108/12/15	Magnetic properties calculation II	
15	108/12/16 ~ 108/12/22	Optical properties calculation I	
16	108/12/23 ~ 108/12/29	Optical properties calculation II	
17	108/12/30 ~ 109/01/05	Beyond Density Functional Theory I	
18	109/01/06 ~ 109/01/12	Beyond Density Functional Theory II	
Requirement	Since topics included in this lecture are rather broaden, please try your best to attend each lecture.		
Teaching Facility	Computer, Projector, Other (PC cluster)		
Textbooks and Teaching Materials	Teaching note as enclosed in the iClass platform		
References			
Number of Assignment(s)	(Filled in by assignment instructor only)		
Grading Policy	◆ Attendance : 10.0 % ◆ Mark of Usual : % ◆ Midterm Exam : 30.0 % ◆ Final Exam : 30.0 % ◆ Other 〈Hand-ons〉 : 30.0 %		

Note	<p>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 .</p> <p>※ Unauthorized photocopying is illegal. Using original textbooks is advised. It is a crime to improperly photocopy others' publications.</p>
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