City University of Hong Kong
Course Syllabus

offered by Department of Materials Science and Engineering
with effect from Semester A 2023/24

Part I   Course Overview

Course Title:	**Functional Properties of Materials**
Course Code:	**MSE8019**
Course Duration:	**One semester**
Credit Units:	**3**
Level:	**R8**
Medium of Instruction:	**English**
Medium of Assessment:	**English**
Prerequisites: *(Course Code and Title)*	**Nil**
Precursors: *(Course Code and Title)*	**Nil**
Equivalent Courses: *(Course Code and Title)*	**Nil**
Exclusive Courses: *(Course Code and Title)*	**Nil**

Part II   Course Details

1.   Abstract

This course applies basic quantum mechanics principles (Schrödinger wave equation and perturbation theory, classical and quantum free-electron theories, band theory for solids) to understand the functional properties of materials (including electrical, optical, optoelectronic, magnetic and topological properties etc.). Topics in this course include single-particle Schrodinger equation and its applications in several typical quantum mechanical systems and realistic quantum materials and advanced characterization techniques; non-degenerate and degenerate (time-independent) perturbation theories, and their applications in the ground state of helium atom, Stark effect, and Zeeman splitting; classical free-electron gas model, quantum free-electron theory, quantum density of states, Fermi-Dirac distribution, Maxwell Boltzmann distribution, Fermi energy, and Fermi surface; Bloch's theorem, approaching band model through Schrödinger equation, nearly free-electron model, tight binding model, Kronig-Penney model for deriving the formation of discrete energy levels and band structures of crystalline solids; apply band structures to classify materials and understand electrical, optical, and topological properties of recently emerging materials systems (two-dimensional materials and topological insulators etc.).

2.   Course Intended Learning Outcomes (CILOs)
(CILOs state what the student is expected to be able to do at the end of the course according to a given standard of performance.)

No.	CILOs	Weighting* (if applicable)	Discovery-enriched curriculum related learning outcomes (please tick where appropriate)		
			A1	*A2*	*A3*
1.	Describe the fundamental concepts of quantum mechanics and single-particle Schrodinger equation and its applications in several typical quantum mechanical systems and realistic quantum materials and advanced characterization techniques	30%	✓	✓	✓
2.	Introduce Dirac notation, non-degenerate and degenerate (time-independent) perturbation theories and their applications in the ground state of helium atom, Stark effect, and Zeeman splitting	10%	✓	✓	✓
3.	Describe the classical free-electron gas model and the quantum free-electron theory; Introduce the quantum density of states, the Fermi-Dirac distribution function, and determine Fermi energy and Fermi surface	30%	✓	✓	✓
4.	Describe the formation of discrete energy levels and the band structure of crystalline solids based on Bloch's theorem, nearly free-electron model, tight-binding model, and Kronig-Penney model	20%	✓	✓	
5.	Apply band structure to classify materials and understand their electrical, optical (absorption, emission, and amplification of optically active materials), optoelectronic (devices), and topological properties	10%	✓	✓	✓
If weighting is assigned to CILOs, they should add up to 100%.		100%			

A1:   Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2:   *Ability*
        Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to self-life problems.

A3:   *Accomplishments*
        Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

3. Teaching and Learning Activities (TLAs)

(TLAs designed to facilitate students' achievement of the CILOs.)

TLA	Brief Description	Hours/week (if applicable)					
		1	2	3	4	5	
Lecture	Explain key quantum mechanics principles, single-particle Schrodinger wave equation, classical and quantum free-electron theories, statistical mechanics, solid-state band theories, and their applications in understanding the multi-physical properties of crystalline solids	✓	✓	✓	✓	✓	2 hrs/wk
Tutorial	Discuss tutorial questions and assignments, and provide consultation	✓	✓	✓	✓	✓	0.5 hrs/wk

4. Assessment Tasks/Activities (ATs)

(ATs are designed to assess how well the students achieve the CILOs.)

Assessment Tasks/Activities	CILO No.					Weighting*	Remarks
	1	2	3	4	5		
Continuous Assessment: 50%							
Assignments	✓	✓	✓	✓	✓	30%	
Midterm test	✓	✓				20%	
Examination: (duration: 2 hours)	✓	✓	✓	✓	✓	50%	

* The weightings should add up to 100%. | 100% |

5. Assessment Rubrics

(Grading of student achievements is based on student performance in assessment tasks/activities with the following rubrics.)

Applicable to students admitted in Semester A 2022/23 and thereafter

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B)	Marginal (B-, C+, C)	Failure (F)
1. Assignments	Understand basic theories and principles, be able to apply them to solve relevant questions and explain relevant physical phenomena	High	Moderate	Basic	Not even reaching marginal levels
2. Midterm test	Demonstrate understanding of key quantum mechanics principles, single-particle Schrodinger wave equation, non-degenerate and degenerate (time-independent) perturbation theories, and be capable of solving relevant problems	High	Moderate	Basic	Not even reaching marginal levels
3. Examination	Describe basic quantum mechanical theories and principles, explain experimentally observed quantum mechanical and solid-state physical phenomena, draw schematic diagrams and perform calculations, and understand the working principles of typical quantum materials, devices and instrument	High	Moderate	Basic	Not even reaching marginal levels

Applicable to students admitted before Semester A 2022/23

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B, B-)	Fair (C+, C, C-)	Marginal (D)	Failure (F)
1. Assignments	Understand basic theories and principles, be able to apply them to solve relevant questions and explain relevant physical phenomena	High	Significant	Moderate	Basic	Not even reaching marginal levels
2. Midterm test	Demonstrate understanding of key quantum mechanics principles, single-particle Schrodinger wave equation, non-degenerate and degenerate (time-independent) perturbation theories, and be capable of solving relevant problems	High	Significant	Moderate	Basic	Not even reaching marginal levels
3. Examination	Describe basic quantum mechanical theories and principles, explain experimentally observed quantum mechanical and solid-state physical phenomena, draw schematic diagrams and perform calculations, and understand the working principles of typical quantum materials, devices and instrument	High	Significant	Moderate	Basic	Not even reaching marginal levels

Part III   Other Information (more details can be provided separately in the teaching plan)

1. **Keyword Syllabus**
    (An indication of the key topics of the course.)

*   Quantum behaviours, wave-particle duality relationship;
*   Heisenberg's uncertainty principle, quantum operators;
*   Single-particle Schrodinger wave equations for typical quantum systems and realistic quantum materials;
*   Dirac notation, non-degenerate and degenerate perturbation theories;
*   Ground state of helium atom, Stark effect in hydrogen atom, and Zeeman splitting
*   Classical free-electron gas model, quantum free-electron theory;
*   Quantum density of states, Fermi-Dirac distribution, Maxwell Boltzmann distribution;
*   Fermi energy, Fermi surface;
*   Three approximations for approaching band model through Schrodinger equation;
*   Bloch's theorem;
*   Nearly free-electron model;
*   Tight-binding model;
*   Kronig-Penny model;
*   Formation of discrete energy levels;
*   Band structures of typical crystalline solids (metals, insulators and semiconductors);
*   Band model interpretation of electrical conduction in solids, and crystal momentum and effective mass;
*   Band structures for understanding optical absorption, emission, and amplification of optical materials;
*   Emerging two-dimensional materials (graphene and TMDCs) and topological insulators;

2. **Reading List**
2.1 **Compulsory Readings**
    (Compulsory readings can include books, book chapters, or journal/magazine articles. There are also collections of e-books, e-journals available from the CityU Library.)

1.	Nil

2.2 **Additional Readings**
    (Additional references for students to learn to expand their knowledge about the subject.)

1.	Richard P. Feynman, "The Feynman Lecture Notes on Physics, Vol. III: Quantum Mechanics", Ingram Publisher Service, New York, US, 1971
2.	Hasse Fredriksson, Ulla Åkerlind, "Physics of Functional Materials", John Wiley & Sons Inc., 2008 (QC21.3.F74, 2008)
3.	Neil W. Ashcroft, N. David Mermin, "Solid State Physics", Saunders College Publishing, 1976 (QC176.A83, 1976)
4.	Charles Kittel, "Introduction to Solid State Physics", 8th Edition, John Wiley & Sons Inc. 1996/2005 (QC176.K57, 1996/2005).
5.	(E-Book) Rolf E. Hummel, "Electronic Properties of Materials", 4th Edition, Springer, New York, 2011 (QC176.H86, 2011)
6.	Robert Eisberg and Robert Resnick, "Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles", 2nd Edition, Wiley, 1985 (QC174.12.E34, 1985)
7.	Safa O. Kasap, "Principles of Electronic Materials and Devices", 3rd Edition, McGraw-Hill, 2006 (TK453.K26, 2006)

8.	Sara M. McMurry, "Quantum Mechanics", Addison-Wesley, Wokingham, c1994 (QC174.12.M38, 1996)