课程大纲
COURSE SYLLABUS

1.	**课程代码/名称** **Course Code/Title**	PHY5009/密度泛函方法和固态电子结构 Fundamentals of electronic structures and density functional theory
2.	**课程性质** **Compulsory/Elective**	专业选修课 Elective Course
3.	**课程学分/学时** **Course Credit/Hours**	3/48
4.	**授课语言** **Teaching Language**	中文 Chinese
5.	**授课教师** **Instructor(s)**	张文清 Wenqing Zhang
6.	**是否面向本科生开放** **Open to undergraduates or not**	是 YES
7.	**先修要求** **Pre-requisites**	（如面向本科生开放，请注明区分内容。 If the course is open to undergraduates, please indicate the difference.） 量子力学 I PHY206-15 Quantum Mechanics

8. **教学目标**
Course Objectives

（如面向本科生开放，请注明区分内容。 If the course is open to undergraduates, please indicate the difference.）

本课程是专为物理学，材料科学，化学和电气工程专业的高年级本科生及一年级研究生开设的。该课程主要涵盖以下内容：材料（主要是无机晶体）的晶体结构和化学键基础，化学键与能带结构之间的关系，密度泛函理论（DFT）的基础，以及如何应用有效的密度泛函方法在物理和材料科学的研究中对材料结构与特性之间的联系进行理解。这些教学内容将帮助学生和初涉该领域的研究人员将这种基于 DFT 的重要计算技术应用于广泛的物理和材料科学研究中。此外，我们还将在课程中对密度泛函理论的基础以及实际应用中的相关计算软件包进行介绍和解释。

This course is designed for senior undergraduates and first-year graduate students majoring in physics, materials science, chemistry, and electrical engineering. The course mainly covers the following topics: crystalline structure and chemical bond fundamental of materials especially inorganic crystals, relationship between chemical bonds and band structures, fundamental of Density functional theory(DFT), and applications of the powerful density-functional approach in understanding the structure-property relationship of materials for physics and materials science research. The topics makes it possible for students and junior researchers to apply this important DFT-based computational technique to a broad range of physics and materials science problems. We will also spend some time in explaining the fundamental of density functional theory and the related software packages for real applications.

9. **教学方法**
Teaching Methods

（如面向本科生开放，请注明区分内容。 If the course is open to undergraduates, please indicate the difference.）

课堂介绍 +小组讨论 +上机课

Class teaching +Group project+ Computer practice

10. **教学内容**
Course Contents

（如面向本科生开放，请注明区分内容。 If the course is open to undergraduates, please indicate the difference.）

Section 1	晶体结构基础 Fundamentals of crystalline structures
Section 2	化学键基础 Fundamentals of chemical bonds
Section 3	能带结构中的化学键特征 From chemical bonds to band structures
Section 4	能带结构中的物理和化学性质 Physical and Chemical properties from band structures
Section 5	密度泛函理论与能带结构计算 Density Functional Theory and band structure calculations
Section 6	密度泛函理论基础及其应用 Fundamentals of Density-Functional Theory and its application
Section 7	表面与界面 Interfaces and surfaces
Section 8	含时过程和从头计算分子动力学 Time-dependent process and Ab Initio molecular dynamics
Section 9	相关的应用专题 Selected application topics

11. 课程考核
Course Assessment

（①考核形式 Form of examination；②.分数构成 grading policy；③如面向本科生开放，请注明区分内容。If the course is open to undergraduates, please indicate the difference.）

主题科学报告（50%）+小组报告（50%）

Scientific report（50%）+ Group project（50%）

12. 教材及其它参考资料
Textbook and Supplementary Readings

1.Roald Hoffmann, Solids and Surfaces: A Chemist's View of Bonding in Extended Structures
2.Walter Harrison, Elementary Electronic Structure
3.Richard M. Martin Electronic Structure: Electronic Structure Basic Theory and Practical Density Functional Approaches