理 學 院
107 學年度第一學期模組化課程

石墨烯相關系統的幾何和電子特性：化學鍵

Geometric and electronic properties of graphene-related systems: chemical bonding schemes

授課教師：

林明發

國立成功大學物理學系

課程類別	學分數	選必修	開課人數	開課日期及上課時間	上課地點
講義	1	選修	20	2018/07/09(一)-2018/07/13(五) 下午 14:00-17:00	待確認

先修課程或先備能力：

量子物理

建議修課年級：

大三、大四、碩士班

建議修課學生背景：

理學院、工學院、電資學院

教學方法：

講授 100 %

評量方式：

問題考試 30 %、科學報告 40%、出席率 30%

補充說明：

(i)每堂課程皆有問題討論，考試預計於最後一節課。

(ii)預計於最後一節課繳交書面報告，內容盡可能完整詳細。內容完整度為評分要件。

學習規範：

無

課程概述：

1. **Emergent graphene-related materials: essential properties, such as electronic properties and optical properties, and applications, such as LED, solar cells and photo-detectors.**
2. **First-principle calculations for exploring the geometry- and adatom-enriched essential properties of graphene-related systems. The critical orbital hybridizations are accurately obtained from the carbon- and adatom-dominated energy bands, the spatial charge density and the difference after chemisorption, the free carrier density/ band gap, and the atom- and orbital-decomposed densities of states (DOSs). The concise chemical pictures are very useful in fully understanding the fundamental properties, covering optimal geometric structures, electronic properties and magnetic configurations. Three kinds of spin arrangements, non-magnetism, ferromagnetism and anti-ferromagnetism, are clearly identified from the spin-split band structure, the net magnetic moment, the spatial spin distribution, and the spin-projected DOSs.**
3. **How to solve the various Hamiltonians is always one of the main-stream topics in physics science.**

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Tight-binding model is applicable for studying the emergent 2D materials, accompanied with 3D, 1D and 0D systems, which might possess the critical intrinsic properties, the lattice symmetries, planar/curved surfaces, few- or multi-layer structures, distinct dimensionalities, stacking configurations, single- or multi-orbital hybridizations, intralayer and/or interlayer hopping integrals, significant/negligible spin-orbital couplings.

課程進度：

堂次	時數	進 度 說 明
1	3	石墨烯相關材料簡介
2	3	數值方法簡介: 第一原理方法
3	3	數值方法簡介: 緊束模型
4	3	數值計算
5	3	數值計算

課程學習目標：

1. **Understanding about the geometric and essential properties of various emergent graphene-related materials**
2. **Know basically how to use numerical computations (First-principles calculations and tight-binding model)**
3. **Apply basic simulation and modelling tools to solve simple problems related to graphene materials**

課程的重要性、跨域性與時代性：

此課程進一步發展第一原理計算及廣義化緊束模型，包含更多的複雜交互作用，結合其他理論理解更廣泛的基本性質，以及推廣至任何維度的凝態系統。對於能帶的模型計算、磁量子化性質和碳相關系統的電子結構、光學性質與庫倫激發作用等的系統性完整研究。涵蓋理工學院與電資學院等跨領域範疇。

其他備註:

課程教材:

1) N. T. T. Tran, S. Y. Lin, C. Y. Lin and M. F. Lin, “Geometric and electronic properties of graphene-related systems: Chemical bondings", CRC Press, ISBN 9781138556522 (2017).

2) C. Y. Lin, R. B. Chen, Y. H. Ho and M. F. Lin, “Electronic and optical properties of graphite-related systems”, CRC Press, ISBN 9781138571068 (2017).

參考書目:

Charles Kittel, “Introduction to Solid State Physics”, John Wiley and Sons Ltd, (2004).