



Universidade do Minho



## Curricular Unit

Advanced Physics Topics 1

## Module

Modelling Electronic Structure of Layered Materials

## Type

Lecture course

## Contact hours

18

## Professor/Researcher in charge

Nuno Peres, João Lopes dos Santos, Ricardo Ribeiro

## Summary of Contents

Tight binding models. General Concepts. Wannier States, Slater-Koster parameters.

Modelling band Structure of graphite. Slonczewski-Weiss-McClure parameters

Graphene. Tight binding description. Continuum Models. Edge states and defects. Optical properties. Tight binding models and Stress.

Bilayers and Multilayers. Variations in stacking. Twisted bilayer.

Layered Transition metal dichalcogenides

Ab-initio methods. Principles and practical approaches.

## References

Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond, W. Harrison, Dover 2011

Castro Neto, A. H.; Guinea, F.; Peres, N. M. R.; Novoselov, K. S. & Geim, A. K.

The electronic properties of graphene *Rev. Mod. Phys., American Physical Society*, 2009, 81, 109-162,

Peres, N. M. R., *Colloquium* : The transport properties of graphene: An introduction *Rev. Mod. Phys., American Physical Society*, 2010, 82, 2673-2700.

Electronic Structure Calculations for Solids and Molecules Jorge Kohanoff, Cambridge University Press, 2006.



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## Evaluation

Homework Problems

## Jury

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