PX918-15 Electronic structure theory for experiments and models

22/23

Department
Physics
Level
Taught Postgraduate Level
Module leader
Julie Staunton
Credit value
15
Module duration
10 weeks
Assessment
50% coursework, 50% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A.

Module web page

Module aims

To provide students with an understanding of how properties measured experimentally can be described from an ab-initio electronic structure theory and an appreciation of successes and current shortcomings. To show how parameters for alloys and magnets can be calculated, tested against experiment and used in modelling properties at finite temperatures. This will be conveyed via lectures, tutorial workshops, guest seminars and web-pages.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

1. Overview of the quantum many body problem of the interacting electrons and nuclei in

materials
a) introduction to 2nd quantisation and 1- and 2-electron Green functions
b) excitation spectra, quasiparticles and spectroscopy measurements
c) Fermi surface, electron momentum density

2. Recap of electron Density Functional Theory - relationship of Kohn-Sham electronic structure to spectroscopy measurements. Starting point for many body Green function descriptions.
3. Description of transport properties ab-initio
   a) Sommerfeld theory
   b) Beyond the relaxation time approximation
4. Linear response and collective electron effects
   a) dielectric response
   b) spin susceptibility and spin waves
   c) X-ray and neutron scattering experiments
   d) DFT-based calculations
5. DFT and finite temperatures
   a) time scale separation of electronic and nuclear motion, phonons, electron-phonon effects.
   b) atom-atom interchange parameters from DFT for Bragg-Williams models of alloys, CALPHAD database
   c) identification of 'local moment' degrees of freedom in magnetic materials and spin model construction
   d) atom and spin correlation functions - tested against X-ray and neutron scattering data
   e) modelling alloy and magnetic phase diagrams ab-initio and T-dependent electronic structure
6. 1. Strong electron correlation effects
      a) Self-interaction correlation, DFT+U and brief overview of Dynamical Mean Field Theory
      b) Examples
      c) Outstanding challenges.

Learning outcomes

By the end of the module, students should be able to:

- It is expected that by the end of this module students will be able to understand the basis to quantum many body theory and the context for Density Functional Theory.
- It is expected that by the end of this module students will be able to appreciate what in principle needs to be calculated to test theory with and interpret spectroscopy, scattering and transport measurements.
- It is expected that by the end of this module students will be able to understand some collective electron effects and how they are explored experimentally and modelled computationally.
- It is expected that by the end of this module students will be able to appreciate how temperature dependent materials properties can be described by the identification and calculation of ab-initio parameters and used in appropriate models; examples of alloy and magnetic phase diagrams.
- It is expected that by the end of this module students will be able to engage with cutting-

edge topics in the study of strongly correlated electron materials.

Indicative reading list

‘Electronic Structure’ by Richard Martin (C.U.P)
‘Principles of Condensed Matter Physics’ by P.M. Chaikin and T.C. Lubensky

Subject specific skills

understand the basis to quantum many body theory and the context for Density Functional Theory.
appreciate what in principle needs to be calculated to test theory with and interpret spectroscopy, scattering and transport measurements
understand some collective electron effects and how they are explored experimentally and modelled computationally
appreciate how temperature dependent materials properties can be described by the identification and calculation of ab-initio parameters and used in appropriate models; examples of alloy and magnetic phase diagrams
engage with cutting-edge topics in the study of strongly correlated electron materials

Transferable skills

Mathematical Model-building, comparison to experiment, mathematics, programming and scripting.

Study

Study time

Type	Required
Lectures	20 sessions of 1 hour (13%)
Seminars	5 sessions of 1 hour (3%)
Tutorials	5 sessions of 1 hour (3%)
Private study	100 hours (67%)
Assessment	20 hours (13%)
Total	150 hours

Private study description

Further reading etc

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group C

	Weighting	Study time
Presentation	50%	10 hours
Oral presentation of key findings from 2 scientific journals articles in 20 minute presentation followed by 5 minutes of questions on material from audience.		
Viva	50%	10 hours
Viva examination of 30 minutes on module material.		

Feedback on assessment

Oral presentations will be double marked during the oral assessment day (by Teaching Fellow and Module Leader) and feedback in the form of written comments within 1 week of the assessment day.\r\nViva examination will be conducted by Module Leader and Teaching Fellow. \r\nOral feedback will be given shortly after the viva.\r\n

Past exam papers for PX918

Availability

Courses

This module is Core optional for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems

This module is Core option list A for:

- Year 2 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)