CH274-15 Electrons in Molecules and Solids

23/24

Department
    Chemistry
Level
    Undergraduate Level 2
Module leader
    Ross Hatton
Credit value
    15
Module duration
    10 weeks
Assessment
    20% coursework, 80% exam
Study location
    University of Warwick main campus, Coventry

Description

Introductory description

N/A

Module web page

Module aims

This module introduces students to several fundamental aspects of physical chemistry.

The first part will introduce the fundamental concepts of solid state chemistry that relate to crystal structure, chemical bonding in solids and to the electronic properties of solids. This will establish to students how quantum and statistical mechanics applied to solid materials can be used to derive various condensed matter properties such as electrical conduction and opto-electronic characteristics. Special emphasis will be given to directly connecting quantum mechanical properties to examples from modern electronics applications.

The second part will develop students' knowledge of symmetry and group theory and its role in molecular structure and bonding and the interpretation of electronic and vibrational spectra. It will provide students with working knowledge of the various relaxation pathways available to electronically excited molecules.

As part of the key skills training in the 2nd year of the chemistry programme, students will be introduced to advanced practices of scientific computing, data analysis, and visualization in the context of chemistry.

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.

- Review of QM: the free particle, the particle in a box
- Molecular Orbital and Hückel theory
- Review of crystal structure: unit cells, Bravais lattices, the Wigner-Seitz cell, reciprocal lattice, examples of different crystals and their corresponding reciprocal counterparts
- The dispersion relation and the concept of momentum as quantum number in solids
- Molecular orbital theory for solids: Hückel model for 1D periodic system, the tight-binding approximation
- Electronic band structures and density of states, the Fermi-Dirac distribution, density of occupied states
- Metals: position of Fermi level, density electrons participation in conduction, optical properties, work function, contact potential
- Intrinsic semiconductors: position of Fermi level, density of electrons participation in conduction, effect of temperature and magnitude of band gap, optical properties, conduction by holes
- Doped semiconductors: position of Fermi level, density electrons participation in conduction, extrinsic, saturation, and intrinsic temperature regimes
- Introduction to semiconductor devices: p-n junction, photovoltaic cell, light emitting diode, logic gates
- Scientific Computing using the Python scripting language
- Symmetry and group theory recap
- Applications of symmetry and group theory to polyatomic chemical bonding, such as symmetry of molecular orbitals and constructing molecular orbitals from atomic orbitals, and orbitals in high symmetry complexes (square planar, etc.)
- Applications of symmetry and group theory to molecular vibrations and IR/Raman spectroscopy; symmetry of vibrations and selection rules
- Applications of symmetry and group theory to polyatomic electronic spectroscopy
- Term symbols, selection rules, and Franck-Condon factors for diatomic molecules
- Jablonski diagrams and the fate of electronically excited states; quantum yields for photochemical processes and their link to first-order rate coefficients, photochemical reactivity

Learning outcomes

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

- Understand the essential differences in the electronic properties of metals, semiconductors and insulators, their connection to the quantum mechanical properties of solids and their

influence on the electrical conductivity and its temperature dependence
- Describe the quantum-mechanical origin of extended electronic states (bands) in condensed matter
- Apply their knowledge of molecular and solid-state bonding concepts to construct simplified quantum mechanical model systems such as Hückel and tight-binding models
- Understand the relation between optical properties and electronic structure of materials
- Appreciate the concept of doping and the mechanisms of hole conduction in semiconductor materials
- Have a basic knowledge of the characteristic and basic electronic properties of p-n junctions
- Carry out linear combinations of orbitals to form molecular orbitals and apply this to polyatomic systems (e.g., square planar, octahedral)
- Find symmetry species of normal modes of vibrations and deduce which modes are IR/Raman active
- Understand the role of symmetry in electronic spectroscopy (vibronic transitions, selection rules) and discuss how the intensities of vibronic transitions are explained by the Franck-Condon principle
- Construct a Jablonski diagram showing all the relaxation pathways available to electronically excited molecules and relate the quantum yields of photochemical processes to first-order rate equations
- Use the Python programming language to write code capable of performing important scientific tasks including spectral data fitting (including simultaneous fits of multiple datasets), solving quantum mechanical equations and graphical visualization of the results.

Indicative reading list

P. W. Atkins & J. de Paula, Physical Chemistry
D. C. Harris & M. D. Bertolucci, Symmetry and Spectroscopy: An introduction to Vibrational and Electronic Spectroscopy
A. Vincent, Molecular Symmetry and Group Theory
R. Turton, The Physics of Solids
P.A. Cox, The Electronic Structure and Chemistry of Solids
H. Ibach & H. Lüth, Solid-State Physics: An Introduction to Principles of Materials Science
P. Atkins & R. Friedman, Molecular Quantum Mechanics
J. Singleton, Band Theory and Electronic Properties of Solids

Research element

e.g. essay, dissertation, individual or group research, research skills activity, etc.

Subject specific skills

Numeracy
Problem solving
Critical thinking
Organisation and time management
Information literacy and research skills

Digital skills and literacy

Transferable skills

Numeracy
Problem solving
Critical thinking
Organisation and time management
Information literacy and research skills
Digital skills and literacy

Study

Study time

Type	Required
Lectures	32 sessions of 1 hour (21%)
Other activity	12 hours (8%)
Private study	106 hours (71%)
Total	150 hours

Private study description

N/A

Other activity description

Chemical Bonding in Molecules and Solids (RJM)
-1 Vevox seminar (whole class)
-3 Q&A sessions (whole class)
-2 Pen & Paper exercise workshops (medium size, 20-25 students per group)
-2-3 Homework exercises in each lecture handout with the option of receiving feedback when handing in homework
-Moodle/Teams Forum
-1 revision session in Term 3

Electrons in Solids and Materials (RH)
-3 Q&A sessions (whole class).
-2 Pen&Paper Exercise Workshop (medium size groups, 5). Students to sign up for a session and attendance monitored to ensure good attendance.
-8 exercises with detailed model answers and video recordings of pen&paper solving.
-Question Forum.
-1 Q&A revision sessions (whole class).
-1 Revision Exercise Workshop (whole class).

Symmetry and Group Theory (VS)
-1 Vevox Seminar (entire cohort).
-2 Q&A sessions (entire cohort).
-8 Online self-tests.

- 20 Questions embedded within lectures.
  2 workshop repeated 5 times (group size 25).
  1 Q&A revision sessions (entire cohort).
  5 office hours starting from week 6 of term 2.

  Electronic Spectroscopy & Photochemistry (DM)
  -2 online Q&A sessions (entire cohort).
  -Questions embedded within lecture (detailed walkthrough videos available online).
  -2 pen and paper workshops repeated 5 times (group size ~25) - face-to-face ideally, run in weeks 9 and 10 of term.
  -2 computational workshops, with detailed video walkthroughs available online.
  -1 Q&A revision session in term 3 (entire cohort).

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 D4

	Weighting	Study time
Assessed coding workshop 1	10%	
Python notebook associated with Professor Maurer's part of course		
Assessed coding workshop 2	10%	
Python notebook associated with Dr Murdock's part of course		
In-person Examination	80%	

- Answerbook Green (8 page)
- Students may use a calculator
- Graph paper
- Periodic Tables

Feedback on assessment

Oral and written feedback on assessed work from module leader/ tutors. Cohort level examination feedback provided via Moodle.

Past exam papers for CH274

Availability

Post-requisite modules

If you pass this module, you can take:

- CH3G3-30 Advanced Chemistry (Organic, Inorganic and Physical) Industrial Placement
- CH3F1-15 Advanced Physical Chemistry and Laboratory
- CH3F3-30 Advanced Chemistry (Organic, Inorganic and Physical)

Courses

This module is Core for:

- UCHA-4 Undergraduate Chemistry (with Intercalated Year) Variants
  - Year 2 of F101 Chemistry (with Intercalated Year)
  - Year 2 of F122 Chemistry with Medicinal Chemistry (with Intercalated Year)
- UCHA-3 Undergraduate Chemistry 3 Year Variants
  - Year 2 of F100 Chemistry
  - Year 2 of F100 Chemistry
  - Year 2 of F121 Chemistry with Medicinal Chemistry
- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 2 of F100 Chemistry
  - Year 2 of F110 MChem Chemistry (with Industrial Placement)
  - Year 2 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement
- Year 2 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 2 of F109 MChem Chemistry (with International Placement)
  - Year 2 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 2 of F100 Chemistry
  - Year 2 of F105 Chemistry
  - Year 2 of F110 MChem Chemistry (with Industrial Placement)
  - Year 2 of F109 MChem Chemistry (with International Placement)
  - Year 2 of F125 MChem Chemistry with Medicinal Chemistry
- Year 2 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)