

PX919-7.5 Quantum Chemistry

20/21

Department

Physics

Level

Taught Postgraduate Level

Module leader

Reinhard Maurer

Credit value

7.5

Module duration

10 weeks

Assessment

60% coursework, 40% exam

Study location

University of Warwick main campus, Coventry

Description

Introductory description

N/A.

[Module web page](#)

Module aims

This module provides an in-depth overview of quantum chemistry methods to predict molecular and materials properties. These methods provide the most accurate prediction of the quantum mechanical properties of molecules and form the basis for many more approximate methods. Upon recapitulating the mathematical foundations and properties of many-body quantum systems, the lectures and workshops will establish the algorithmic properties of various quantum chemistry methods and their advantages and disadvantages. The focus will be on providing students with the necessary tools to apply quantum chemistry methods in their research, while also establishing important general concepts such as Perturbation Theory.

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. Basics (4 hrs):
 - a) Short introduction to mathematical concepts used in wave function theory: vector and functional analysis, representation theory, tensor spaces
 - b) Properties of many-body wave functions, position and momentum representation
 - c) Spin: Slater determinants, configurational state functions, spin contamination
 - d) Hartree-Fock Theory: Derivation, algorithm, properties, Coulomb and exchange integrals, ROHF and UHF variants
 - e) 2nd quantization representation, density matrices, and N-particle reduced electron density matrices, natural orbitals
 - f) Koopman's Theorem and Brillouin Theorem
2. Correlation (4 hrs)
 - a) Configuration Interaction
 - b) MCSCF wave functions
 - c) Coupled Cluster Theory
 - d) Density Matrix Renormalisation Group and modern matrix/tensor-product state wave function representations
 - e) Perturbation Theory: Moeller-Plesset and Multireference PT
3. Green's Functions, Linear Response, and Many Body perturbation Theory (2 hrs)
 - a) Rayleigh-Schrödinger Perturbation Theory and Feynman Diagrams
 - b) The One-particle Green's Function and approximative MBPT methods
 - c) The Two-particle Green's Function and approximative MBPT methods

Learning outcomes

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

- Demonstrate knowledge of wave function theory including the basic properties of many-body wave functions and their construction.
- Be aware of all major quantum chemical wave function methods, including their predictive capabilities and their limitations.
- Understand the concepts of correlation and exchange and general strategies how to address them in molecules and materials.
- Be able to differentiate between wave-function-based and quasi-particle-based quantum chemistry methods.
- Be able to follow a basic quantum chemistry algorithm and apply various computational quantum chemistry methods to calculate molecular properties.

Indicative reading list

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Attila Szabo, Neil S. Ostlund, Dover Books

Subject specific skills

Demonstrate knowledge of wave function theory including the basic properties of many-body wave functions and their construction

Be aware of all major quantum chemical wave function methods, including their predictive capabilities and their limitations

Understand the concepts of correlation and exchange and general strategies how to address them in molecules and materials

Be able to differentiate between wave-function-based and quasi-particle-based quantum chemistry methods

Be able to follow a basic quantum chemistry algorithm and apply various computational quantum chemistry methods to calculate molecular properties

Transferable skills

Scripting, use of HPC, data analysis.

Study

Study time

Type	Required
Lectures	5 sessions of 2 hours (13%)
Practical classes	2 sessions of 2 hours (5%)
Private study	39 hours (52%)
Assessment	22 hours (29%)
Total	75 hours

Private study description

Further reading, familiarisation with codes via tutorials 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 D

Weighting Study time Eligible for self-certification

Assessment component

Assessed work based on workshops 60% 12 hours No

Two pieces of assessed work based on the material of the two workshops.

Reassessment component is the same

Assessment component

Viva Voce Exam 40% 10 hours No

30 minutes.

Reassessment component is the same

Feedback on assessment

Written annotations to submitted computational notebooks
Verbal discussion during viva voce exam
Written summary of viva performance

[Past exam papers for PX919](#)

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)