PX919-10 Quantum Chemistry

24/25

Department
Physics
Level
Taught Postgraduate Level
Module leader
Reinhard Maurer
Credit value
10
Module duration
10 weeks
Assessment
60% coursework, 40% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

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.

Module web page

Module aims

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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.

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
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
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

Teaching split

Provider	Weighting
Chemistry	50%
Physics	50%

Study time

Type	Required
Lectures	5 sessions of 2 hours (10%)
Practical classes	2 sessions of 2 hours (4%)
Private study	64 hours (64%)
Assessment	22 hours (22%)
Total	100 hours

Private study description

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 D1

	Weighting	Study time	Eligible for self-certification
Assessed work based on workshops	60%	12 hours	Yes (extension)
Two pieces of assessed work based on the material of the two workshops.			
Viva voce Exam	40%	10 hours	No

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

There is currently no information about the courses for which this module is core or optional.