Quantum Mechanics and Modelling II

Niveau d'étude
BAC +4

Composante
Faculté des Sciences

En bref

- **Date de début des cours:** 1 sept. 2021
- **Langue(s) d'enseignement:** Anglais
- **Méthode d'enseignement:** En présence
- **Organisation de l'enseignement:** Formation initiale
- **Ouvert aux étudiants en échange:** Non

Présentation

Description

In this course a complete description of the structural, electronic and vibrational properties of molecules is given together with the quantum treatment of these properties in computer simulations.

In parallel the structural and electronic properties of solids is addressed with an emphasis on the properties of metals and semiconductors.

Volumes horaires* :

CM : **42H**

TD : **21H**

Objectifs

1) Understand the peculiarities of the electronic properties of molecules

2) Understand the peculiarities of the vibrational properties of molecules

3) Be able to describe the excited states of molecules

4) Apprehend and be able to determine the electronic properties of a crystal (1D, 2D, 3D)

5) Determine from first principles the transport and thermal properties of solids

Pré-requis nécessaires

Differential calculus. Matrix algebra.

Contrôle des connaissances

Final exam (1)

Syllabus

7 Molecular Structure: WF methods 9h (6h CM, 3h TD)

7.1 Adiabatic Hypothesis and Born-Oppenheimer Approximation

7.2 SCF MO Treatment of Polyatomic Molecules

7.3 Electron-Correlation Methods: CI

7.4 Electron-Correlation Methods: (RS) Perturbation Theory (Mpn)

7.5 Electron-Correlation Methods: CC and MR

8 Molecular Structure: Density Functional Theory 4.5h (4.5h CM)

8.1 Hohenberg-Kohn Theorems

8.2 The Kohn-Sham Approach

8.3 Exchange-Correlation Functionals

9 Molecular Rotational and Vibrational Motion 9h (6h CM, 3h TD)

9.1 Rotation of Molecules

9.2 Vibration of Molecules

9.3 Rotation-vibration spectra of Diatomic Molecules

9.4 Vibrations of Polyatomic Molecules – IR and Raman selection rules

9.5 Anharmonicities and Coriolis forces

10 Molecular Electronic Excited States 4.5h (4.5h CM)

10.1 Franck-Condon Principle and Vibronic Transitions

10.2 The Electronic Spectra of Molecules

10.3 Spin-Forbidden Transitions

10.4 Decay of Excitations

11 Molecular Electronic Excited States Structure 4.5h (4.5h TD)

11.1 Linear Response Methods

11.2 MR Methods

12 Electronic Structure of Solids 31.5h (21h CM, 10.5h TD)

12.1 Direct and Reciprocal Lattices

12.2 1D - Electronic Structure of the model chain (H)n

12.3 1D - Electronic Structure of the dimerised model chain (H2)n

12.4 1st Order Peierls Distortions in 1D periodic systems

12.5 2D – Electronic structure of the square lattice (H)n

12.6 Notion of Fermi surface

12.7 Bloch and Crystals Orbitals

12.8 Electronic structure of metals

12.9 Electronic structure of semiconductors

12.10 Transport Properties of solids

12.11 Thermal properties of solids

Infos pratiques

Contacts

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Lieu(x)

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