

Quantum Modeling in molecular and material sciences

Niveau d'étude
Bac +5

ECTS
3 crédits

Composante
**Sciences Fondamentales
et Appliquées**

Présentation

Description

This course deals with the geometric and electronic structure of molecular and solid-state compounds and the solid state. The principles of the theory of molecular and crystalline orbitals will be presented. The classic rules to rationalize the structural arrangements will be discussed (Zintl-Klemm concept, VSEPR, Wade-Mingos,...), in particular, the families of materials will be studied from chemical bonds point of view. The visualization and the structural study of crystalline compounds will be carried out using the computer graphics software VESTA (simulation of the peaks of a diffractogram). The analysis of the density of states, chemical bonds and surface reactivity will be studied for several crystalline systems of interest in materials science and heterogeneous catalysis.

Programme détaillé

Program overview:

Geometric and electronic structures of materials, surfaces and molecular systems (basic knowledges in crystal structures; theory of molecular and crystal orbitals).

Study of the elements required for structural determination (powder diffractometry) and the theory of crystalline orbitals

Study of the concept Zintl-Klemm, VSEPR, Wade-Mingos,...).

Analysis of the density of states, chemical bonds and surface reactivity for several crystalline systems of interest in materials science and heterogeneous catalysis.

Compétences visées

Rationalize the structural and electronic properties of molecular and solid state compounds.

Analyze the electronic density of a compound using quantum chemical tools (OM, bands, DOS, COHP).

Correlate surface reactivity to surface properties.

Know how to write a project

Liste des enseignements

	Nature	CM	TD	TP	Crédits
Quantum modeling in molecular and materials sciences/Modélisation quantique en sciences moléculaires et des matériaux	UE			25h	3 crédits

UE = Unité d'enseignement

EC = Élément Constitutif