CH-704

Computation of molecular properties

Rotzinger François

Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.

Language of teaching	English
Credits	2
Session	
Exam	Oral
Workload	60h
Hours	**28**
Courses	20
TP	8
Number of positions	

Frequency

Every 2 years

Remark

This course is cancelled

Summary

Introduction to methods for the numerical solution of Schrödinger's equation. Application of these techniques to the computation of geometries, vibrational frequencies and electronic transitions.

Content

Molecular properties - Self-consistent field (SCF) calculations - Basis functions - Basis set superposition error (BSSE) - Electron correlation - Interative natural orbital method (INO) - Geometry - Vibrational frequencies - Electronic transi-tions/excited states - Performance and comparision of computational methods - Solvation

Note

Next session Spring semester 2018

Keywords

ab initio molecular orbital methods, density functional theory

Learning Prerequisites

Important concepts to start the course

Basic items in quantum chemistry and group theory