UCLouvain

lphys2244

2021

Molecular physics

5.00 credits	22.5 h + 7.5 h	Q2

Teacher(s)	Lauzin Clément ;
Language :	English
Place of the course	Louvain-la-Neuve
Main themes	The teaching unit covers three themes. The first part gives an overview of the molecular Hamiltonian and the separation of variables. The second part is dedicated to group theory and the use of the symmetry in order to simplify molecular physics problems and the third focuses on different applications.
Learning outcomes	**At the end of this learning unit, the student is able to :** **a. Contribution of the teaching unit to the learning outcomes of the programme (PHYS2M and PHYS2M1)** AA 1.1, AA1.2, AA1.3, AA 1.5, AA 1.6, AA 2.1, AA2.3, AA 3.1, AA 5.2 **b. Specific learning outcomes of the teaching unit** At the end of this teaching unit the student will be able to : 1 1. determine the symmetry of a molecule and use it in order to construct symmetry adapted wavefunctions ; 2. use the symmetry and the Pauli principle to rationalize the intensity of a molecular absorption spectrum ; 3. solve a Hückel problem ; 4. understand the basic concepts of molecular dynamics calculations.
Evaluation methods	Written or oral exam or written report.
Teaching methods	Lectures and 2 laboratories (1 experimental and 1 theoretical)
Content	The teaching unit is structured as follows : 1. Structural and dynamical properties of molecules : polyatomic molecular Hamiltonians, separation of the electronic and nuclear motions, molecular coordinates, adiabatic and diabatic representations, conical intersections. 2. Group-theoretical determination of molecular structure : introduction and general theory, classification of the electronic, vibrational, rotational and nuclear spin states of molecules. 3. Introduction to quantum chemistry : molecular Hartree-Fock equations, LCAO (Linear Combination of Atomic Orbitals) method, Roothaan-Nesbet-Pople equations, electronic configurations. 4. Various applications to illustrate the lectures : molecular spectroscopy, time-dependent methods applied to molecular quantum dynamics, “hands-on” introduction to molecular dynamics codes (e.g. MCTDH). According to the interests of the audience, other selected topics could be addressed, such as e.g. photo-absorption and photo-dissociation, laser-control, time-resolved spectroscopy, molecular wavepacket propagation. It is worth stressing that, all along the lectures, the symmetry of the molecules will be used to solve molecular physics problems, thus providing at the same time an interesting and concrete scope of application of group-theoretical tools.
Bibliography	P. Bunker, P. Jensen, Molecular Symmetry and Spectroscopy ,(2006) NRC Research Press. ISBN 978-0-660-19628-2. D.J. Tannor, Introduction to Quantum Mechanics- A Time-Dependent Perspective (2007) University Science Books . F.Gatti, B.Lasorne, H.-D.Meyer, A.Nauts, Applications of Quantum Dynamics in Chemistry, (2017) Springer.
Faculty or entity in charge	PHYS

Programmes containing this learning unit (UE)				
Program title	Acronym	Credits	Prerequisite	Learning outcomes
Master [120] in Physics	PHYS2M	5		🔍
Master [60] in Physics	PHYS2M1	5		🔍