DIPARTIMENTO DI SCIENZE

COURSE: Quantum Chemistry and Molecular Modeling			
ACADEMIC YEAR: **2019-2020**			
TYPE OF EDUCATIONAL ACTIVITY: Free choice			
TEACHER: **Camilla Minichino**			
e-mail: **camilla.minichino@unibas.it**		website: http://scienze.unibas.it/site/home.html	
phone: **0971-206158**		mobile (optional):	
Language: ITALIAN			
ECTS: (lessons e tutorials/practice) **6**	n. of hours: (lessons e tutorials/practice) **48**	Campus: Potenza Dept./School: **Dipartimento di Scienze** Program: : **Scienze Chimiche (LM54)**	Semester: **II** From **02.03.2020** to **31.05- 20.06 2020**

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

The course has the purpose of i) providing an overview of the methods of theoretical chemistry with particular reference to the aspects of the determination of the molecular electronic structure ii) showing how these methods may be used for the atomistic modeling of chemical systems and for computing molecular properties.

After completing the course the student i) knows the theoretical foundations, the potential and limitations of the methods of quantum chemistry; ii) is able to set up and develop a simple computational chemistry project; iii) • understands the language of molecular modeling (acronyms and abbreviations); iv) is able to deal with the vast literature on the subject.

PRE-REQUIREMENTS

Basic knowledge of molecular quantum mechanics

SYLLABUS

Separation of motions in quantum mechanics. **(6 h)**

Separation between electronic and nuclear motions: adiabatic and Born-Oppenheimer approximation. Comparing adiabatic, diabatic and non-adiabatic approach. Non-crossing rule and conical intersections. Separation between internal and external nuclear motions. Coordinate systems and vibrational modes.

Potential energy surfaces and their exploration. **(8 h)**

Methods for finding local extrema on the potential energy surfaces. Reaction pathways. Molecular force fields. Brief overview of classical molecular dynamics and Monte Carlo simulations and their use in the global optimization problems.

Theoretical methods for molecular electronic structure. **(20 h)**

General aspects of the molecular orbital model. HF method. Basis sets. Electron correlation. Density functional theory. Molecular properties, descriptors of the electronic wave function and the charge distributions. Methods for describing electronic excited states. Solvation and continuum models.

Computational aspects. **(6 h)**

Presentation of some quantum chemistry software packages, input preparation and output reading, calculation examples, analysis of the key information, strategies for solving problems related to the optimization of molecular structures and the SCF convergence, visualization and analysis of the results using molecular graphics programs.

Additional topics *(8 h)

Some theoretical approaches in the study of elementary chemical processes, modulation effect of nuclear motions on molecular observables, valence bond theory, relativistic quantum chemistry, description of condensed phase systems in the framework of DFT theory, hybrid models of molecular mechanics / quantum mechanics, elements of quantum dynamics.

**Only some of these topics, depending on students' interests, will be covered.*

TEACHING METHODS

Theoretical lessons and tutorials on some quantum chemistry software packages.

EVALUATION METHODS

Oral examination, with the possibility of discussing a short written report on a modeling project or on a depth study of a specific topic (agreed with the instructor).

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

Lecture notes and presentation slides (https://cloud.unibas.it/index.php/s/vsLvO06oK1cXVjQ e/o https://elearning.unibas.it/)

- *Texbooks*

  L. Piela. *Ideas of Quantum Chemistry, II Edition, Elsevier, 2013.*

  A. Szabo and N.S. Ostlund. *Modern Quantum Chemistry – Introduction to Advanced Electronic Structure Theory, Dover, 1996.*

  C. J. Cramer. *Essentials of Computational Chemistry Theories and Models, II Edition, Wiley, 2004.*

  F. Jensen. *Introduction To Computational Chemistry, III Edition, Wiley, 2017.*

- *Additional Readings::*

  R. Mc Weeny. *Methods of Molecular Quantum Mechanics, II Edition, Academic Press, 1992.*

  W. Koch and M.C. Holthausen. *A Chemist's Guide to Density Functional Theory. II Edition, Wiley-VCH, 2001.*

  D. C. Young. *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, Wiley, 2001.*

  A. Leach. *Molecular Modelling: Principles and Application, II Edition, Prentice Hall, 2001.*

  J.B. Foresman and A. Frisch. Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian, III Edition, Gaussian Inc., 2015.

  T. Helgaker, P. Jørgensen, and J. Olsen. *Molecular Electronic Structure Theory, Wiley, 2000.*

  P. Norman, K. Ruud, and T.Saue. *Principles and Practices of Molecular Properties: Theory, Modeling, and Simulations, Wiley, 2018.*

  F. Gatti, B. Lasorne, H.-D. Meyer,and A. Nauts. *Applications of Quantum Dynamics in Chemistry, Springer, 2018.*

INTERACTION WITH STUDENTS

At the beginning of the course the instructor, after describing goals, learning objectives, detailed course topics, evaluation method, gives the password for accessing the link where the course material is stored. The lecturer also collects a list of students together with name, family name, e-mail and possibly cell phone number and reminds to be always available for providing help and assistance.

Office hours are normally on Tuesdays and Wednesdays 11 am : 1 pm in room 3D-103B (changes in the schedule may occur, due to official and institutional duties, therefore send an e-mail in advance) or in different hours/days by appointment.

EXAMINATION SESSIONS (FORECAST)[1]

21/01/2020, 04/02/2020, 20/02/2020, 03/03/2020, 26/05/2020, 09/06/2020, 07/07/2020, 21/07/2020, 15/09/2020, 06/10/2020, 15/12/2020.

SEMINARS BY EXTERNAL EXPERTS YES □ NO ■

FURTHER INFORMATION

[1] Subject to possible changes: check the web site of the Teacher or the Department/School for updates.