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11th Intensive Course

European Master of Theoretical Chemistry and Computational Modelling

5th September 2016 - 1st October 2016

University of Porto - Faculty of Sciences - Department of Chemistry and Biochemistry, Portugal

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Foreword

Theoretical and Computational Chemistry is presently a powerful and vast field of research, which encompasses several different disciplines, having become a standard tool in the resolution of a wide range of problems. Major journals encourage the submission of manuscripts in which those disciplines are the core of the research and the application of computational methods in the study of Biology, Chemistry and Physics is widely used. Obviously, the study of these matters is complex and it requires training.

The European Master on Theoretical Chemistry and Computational Modelling (EMTCCM) was set up to train a new generation of theoretical and computational chemists, capable to address a wide range of problems centred in the molecular sciences. Coordinated by the Universidad Autónoma de Madrid, the EMTCCM was launched in 2005 already incredibly enriched by the association of 47 European institutions. Few, if any, courses in the world can count with such an involvement of expertise. In 2007 the programme was awarded accreditation by the European Chemistry Thematic Network Association (ECTNA), but it was in the summer of 2009 that the EMTCCM was officially selected for the Erasmus Mundus Action for joint master courses (http://www.emtccm.org/).

The EMTCCM is structured in two years, equivalent to 120 ECTS. Common to all participants is a one-month Intensive Course, with 24 ECTS, in which it is intended an up-to-date analysis of this rich field of research, by presenting an introduction to its current standing and in particular to its most recent developments. The course runs over four weeks and welcomes several international experts as lecturers.

In 2016, the EMTCCM intensive course took place in Porto. Included in the present publication are the timetable of the course, the abstracts of the lectures and the webpages that give access to the lecturers *cvs*. The program itself has been designed to give the students lectures in the morning and sometimes at the beginning of the afternoon too and workshops subsequently, in which hands on experience of the course material will be possible to acquire adequately designed computer labs. Evaluation took place at the end of each week.

I am deeply grateful to all the lecturers whom have so generously given their time to share their knowledge with the students of the EMTCCM and whom have patiently responded to all my organizational requests throughout the year. I very much hope that this Intensive Course was enjoyed by all.

Maria João Ramos

(Director of the Intensive Course)

ISSN: 2279-8773

Acknowledgements

We are very grateful to the University of Porto for all the invaluable administrative support that has been providing us with, along the European Master process. We would also like to thank the Department of Chemistry and Biochemistry in which the whole event took place.

The Organizing Committee

Maria João Ramos (coordinator)
Pedro Fernandes
Alexandre Magalhães

ISSN: 2279-8773

Notes

The 24 Teaching Credits of the second year of the European Master in Theoretical Chemistry and Computational Modelling correspond to an International Intensive Course and to the tutorial work the student must carry out during a period of three more months at the corresponding home Institution.

Saturday mornings were devoted to evaluation.

Further evaluation was based on a written plan of the research project/thesis to be sent to the Master Coordinator three months after the end of the Intensive Course.

Legend

ACT - Advanced Computational Techniques
AES - Advanced Electronic Structure Theory
CS - Communication skills
EC - Enzymatic Catalysis
ES - Ethics in Science
MDS - Molecular Dynamics Simulations
MDVS - Molecular Docking and Virtual Screening
MP - Metalloproteins
Nano - Nanotechnology
PD&E - Protein Dynamics and Energetics
QCMEC - Quantum Chemical Modeling of Enzymatic Catalysis
QMMM - Hybrid QM/MM Methods
SSCS - Solid State Chemistry and Surfaces

Intensive Course Web page

URL: http://www.fc.up.pt/pessoas/mjramos/EMTCCM-2016/index.html

ISSN: 2279-8773

Timetable

First week 5-10 September

	05/set	06/set	07/set	08/set	09/set	10/set
Time	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
08:30-09:00	Registration	AES Yáñez	AES Duarte	AES Bolvin	AES Dias	
09:00-10:00	Test	AES Yáñez	AES Duarte	AES Bolvin	AES Dias	
COFFEE	Introduction					
10:30-11:15	AES de Graaf	AES Yáñez	AES Wesolowsky	AES Bolvin	AES Dias	Evaluation
11:15-12:00	AES de Graaf	AES Yáñez	AES Wesolowsky	AES Bolvin	AES Dias	
LUNCH						
14:00-14:45	AES de Graaf	AES Duarte	AES Wesolowsky	AES Workshop Wesolowsky	AES Workshop Dias	
14:45-15:30	AES de Graaf	AES Duarte	AES Wesolowsky			
COFFEE					Free afternoon	
16:00-17:30	Workshop (AES) de Graaf	Workshop (AES) Yáñez	Workshop (AES) Duarte	Workshop (AES) Bolvin		

ISSN: 2279-8773

Second week 12-17 September

	12/set	13/set	14/set	15/set	16/set	17/set
Time	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
08:30-09:15	AES Biczysko	MDS Sousa	MDS Worth	SSCS Broer	SCSS Remco	
09:15-10:00	AES Biczysko	MDS Sousa	MDS Worth	SSCS Broer	SCSS Remco	
COFFEE						
10:30-11:15	AES Biczysko	MDS F. Fernandes	MDS Worth	SSCS Broer	SCSS Remco	Evaluation
11:15-12:00	AES Biczysko	MDS F. Fernandes	MDS Worth	SSCS Remco	Ethics Broer	
LUNCH						
14:00-14:45	MDS Sousa	MDS F. Fernandes	MDS Workshop Sousa	SSCS Workshop Broer	SSCS Workshop Remco	
14:45-15:30	MDS Sousa	MDS F. Fernandes				
COFFEE			Free afternoon	Free afternoon	Free afternoon	
16:00-17:30	AES Workshop Biczysko	MDS Workshop F. Fernandes				

ISSN: 2279-8773

Third week 19-24 September

	19/set	20/set	21/set	22/set	23/set	24/set
Time	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
08:30-09:15	QMMM Sousa	MDVS Cerqueira	PD&E P. Fernandes	EC P. Fernandes	Nano Magalhães	
09:15-10:00	QMMM Sousa	MDVS Cerqueira	PD&E P. Fernandes	EC P. Fernandes	Nano Magalhães	
COFFEE						
10:30-11:15	QMMM Sousa	MDVS Cerqueira	PD&E P. Fernandes	EC P. Fernandes	Nano Magalhães	Evaluation
11:15-12:00	QMMM Sousa	MDVS Cerqueira	PD&E P.Fernandes	EC P. Fernandes	Nano Magalhães	
LUNCH						
14:00-14:45	MDVS Cerqueira	MDVS Workshop Cerqueira	Free afternoon	PD&E Workshop P. Fernandes	Nano Workshop Magalhães	
14:45-15:30	MDVS Cerqueira					
COFFEE		Free afternoon			Free afternoon	
16:00-17:30	QMMM Workshop Sousa			EC Workshop P. Fernandes		

ISSN: 2279-8773

Fourth week 26 September-01 October

	26/set	27/set	28/set	29/set	30/set	01/out
Time	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
08:30-09:15	QCMEC Himo	CS - 1	ACT Lagana	MP Russo	CS - 2	
09:15-10:00	QCMEC Himo	CS - 1	ACT Lagana	MP Russo	CS - 2	
COFFEE						
10:30-11:15	QCMEC Himo	CS - 1	ACT Lagana	MP Russo	CS - 2	Evaluation
11:15-12:00	QCMEC Himo	CS - 1	ACT Lagana	MP Russo	CS - 2	
LUNCH						
14:00-14:45	QCMEC Workshop Himo	CS - 1	ACT Workshop Lagana	MP Workshop Russo	CS - 2	
14:45-15:30						
COFFEE						
16:00-17:30	Posters & Lectures Study	Posters & Lectures Study	Free afternoon	Posters & Lectures Study	Posters & Lectures Study	

ISSN: 2279-8773

Contents and Lectures

During the Intensive Course, the following subjects have been lectured by:

ISSN: 2279-8773

ISSN: 2279-8773

Molecular Orbital Methods

Coen de Graaf [1]

University of Gröningen

An accurate inclusion of the electron correlation effects is of major importance to obtain a theoretical description of the electronic structure that can be used to interpret experimental data, predict interesting phenomena and/or develop new theoretical concepts. The inclusion of electron correlation effects in the theoretical description of the electronic structure can be done in several ways. Semi-empirical methods played an important role in the early days of quantum chemistry. This role has been gradually taken over by density functional theory, although for huge systems (several thousands of atoms) semi- empirical schemes are still applied. The correlated wave function methods form another important family of computational strategies to describe electron correlation effects. Based on the mean-field Hartree-Fock description, a hierarchy of methods has been developed that improve the approximate solutions of the Schrödinger equation in a systematic way. Wave function based methods are specially relevant for systems with near degeneracies or unpaired electrons, for the description of excited states and/or avoided crossings, among other examples. The methods can also be used to obtain highly precise results of benchmark quality for small molecules.

The course consists of four 45-minute lectures and an hands-on session. The lectures cover theoretical aspects of the different computational schemes combined with practical considerations about the application of the method and the interpretation of the results. The following aspects of correlated wave function methods are worked out: Static versus dynamic electron correlation; Configuration interaction; Perturbation theory; Coupled cluster approaches and Multiconfigurational approaches.

[1] http://www.rug.nl/staff/c.de.graaf/

ISSN: 2279-8773

Wavefunction and Bonding Analysis

Manuel Yáñez [2]

Departamento de Química, Facultad de Cinecias, Módulo 13. Universidad Autónoma de Madrid. Cantoblanco. 28049-Madrid. Spain

By solving the Schroedinger equation (approximately in most cases) one gets an approximation to the exact energy of the system investigated and to the wavefunction that describes it. Associated with the square of the latter it is possible to obtain the electron density distribution of the system under investigation. The aim of this course is to present the different methods, currently available, to get information about the properties of the system, through the analysis of the wavefunctio. In most cases the analysis is carried out on the electron density distribution function closely related to the square of the wavefunction, which, differently from the wavefunction itself has a well defined physical interpretation. The methods based on the analysis of the electron density are very much employed because, after all, chemical processes are the result of breaking and making bonds, in which a significant rearrangement of the electron density of the system takes place. Perhaps, one of the most popular is the atoms in molecules theory (AIM)[1]. This approach is based on a topological analysis of the electron density function, $\rho(\mathbf{r})$, and its Laplacian, $\nabla^2\rho(\mathbf{r})$. This topological analysis leads to the definition of the molecular graph as the ensemble of stationary points of $\rho(\mathbf{r})$, maxima (nuclei), minima (cage points) and saddle points (ring and bond critical points), and the paths connecting them. The values of the electron density at the bond critical points as well as the value of $\nabla^2\rho(\mathbf{r})$ offer important information about the strength and the nature of the interaction between two (bonded) atoms.

Alternatively, the electron density of a chemical system can also be analyzed by the so-called electron localization function (ELF)[2-4] theory. The ELF theory was originally conceived as a local measure of the Fermi hole curvature around a reference point within the Hartree-Fock approximation,[2] and therefore it measures the likelihood of finding an electron in the neighborhood space of a reference electron located at a given point and with a different spin. This implies that the value of the ELF function should be large in those regions of the space where the probability of finding an electron pair is maximum. This analysis leads to the partition of the molecular space into electronic domains, or basins. There are two types of basins: polysynaptic basins (generally disynaptic), which are formed by the contribution of two or more atomic valence shells, and which therefore accommodate bonding pairs, and monosynaptic basins, which belong to only one valence shell, and which qualitatively correspond to lone-pairs or core-electron pairs.

A third complementary procedure to analyze bonding, but not related directly with a direct analysis of the electron density is the natural bond orbital (NBO) method.[5] The NBO approach[5] describes the bonding in terms of localized hybrids and lone pairs obtained as local block eigenvectors of the one-particle density matrix. Besides, a second-order perturbation analysis of the Fock matrix permits to quantify the interactions between occupied MOs of the Lewis base

[2] http://www.uam.es/departamentos/ciencias/quimica/estruct/manuel/

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and unoccupied MOs of the Lewis acid, in a typical electron transfer process from the former towards the latter.

Some times very simple models may provide qualitative useful information on reactivity trends or to determine the most reactive site of a molecular system. This is the case for instance, for many electrophilic or nucleophilic additions, in which one of the reactants is an ionic species. In such cases the molecular electrostatic potentials,[6] defined as the potential (attractive or repulsive) that a unit positive charge experiences in the surroundings of a molecular system, usually yield reliable information to locate the most active site of the neutral reactant, information which is particularly useful when the reactant have several active sites susceptible of undergoing an electrophilic or nucleophilic attack. We will discuss different examples. The limitation of these models and others based exclusively in a static description of the reactants will be also analyzed.[7]

We will show how these different techniques are complementary by discussing some critical cases in which not all the available techniques offer an unambiguous description of the bonding pattern of systems.

A particularly interesting and challenging case is that of the non-covalent interactions, which in most cases are weak or very weak and difficult to describe accurately by the aforementioned approaches. Hence, the last part of the course will be devoted to present the so-called Non-Covalent Interaction (NCI) method specifically designed to describe these kinds of interactions.[8]

References

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ISSN: 2279-8773

Valence Bond Theory

Fernanda Duarte [3]

University of Oxford

In these lectures we will discuss the basic ideas and concepts of Valence Bond (VB) theory in the context of molecular modeling. We will start with a historical overview of both Molecular Orbital (MO) and Valence Bond (VB) theory, analyzing their similarities and differences. Through illustrative examples, we will show how both *ab initio* and empirical VB theory can be used for studying challenging chemical processes both in the condensed phase and in enzymes. We will also discuss some technical aspects of the EVB framework, as well as recent developments and extensions of this approach. The lectures will be also combined with a practical tutorial, where the students will use a software to model a simple S_N2 reaction process in gas phase and solution using the EVB approach.

[3] https://fduarteg.wordpress.com/

ISSN: 2279-8773

Density Functional Theory based methods for Chemistry

T.A. Wesolowski [4]

Department of Physical Chemistry, University of Geneva

- Introduction: Elements of variational calculus
- Introduction: Hohenberg-Kohn theorems
- Kohn-Sham DFT: the formalism
- Kohn-Sham DFT : ”Exact” calculations
- Kohn_Sham DFT: Approximations for density functional for exchange-correlation energy in Kohn-Sham equation:
    - LDA, GGA, and beyond
- Beyond Kohn-Sham DFT (a): adiabatic connection and generalised Kohn-Sham formalism
- Beyond Kohn-Sham DFT (b): multiconfigurational DFT and range-separated functionals
- Beyond Ground-State: excited states from Linear-Response Time-Dependent DFT

[4] https://www.unige.ch/sciences/chifi/wesolowski/

ISSN: 2279-8773

Relativistic effects

Hélène Bolvin [5]

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The aim of these lectures is to give the basics for understanding the equations of relativistic quantum chemistry and to show in which cases relativistic effects must be included in the calculations.

Lecture 1: Introduction to relativistic quantum chemistry

• the Dirac equation

• the hydrogen-like solutions to the Dirac equation

• the two-electron interaction in relativistic quantum chemistry

• from 4 to 2-components, decoupling from the large and the small components

• scalar relativistic effects, spin, spin-orbit coupling

Lecture 2 : Relativistic effects in quantum chemistry

• relativistic effects on the atomic structure
atomic spinors, electronic configuration, spin-orbit

• relativistic effects on the chemical bonding
scalar and spin-orbit effects

• relativistic effects on spectroscopy
absorption spectra, phosphorescence, EPR parameters, NMR parameters

Lecture 3 : Tutorials : Study of the AmO_2^{3+} cation

[5] http://www.lcpq.ups-tlse.fr/spip.php?article928&lang=en

ISSN: 2279-8773

Spectroscopy

Teixeira Dias [6]

University of Aveiro

These lectures addressed the following main topics: 1) Perturbation Theory, 2) Time-Dependent Perturbation Theory, 3) Absorption and Emission of Radiation, and 4) Raman Scattering. An application of the variation perturbation method that provides an upper bound to the second order energy was presented to the students as a work to take home after the EMTCCM-2016 to be solved using Mathematica. In the workshop, the students used Mathematica to deal with Lorentzian and Gaussian band shapes, and to hands-on approach the concept of convolution of an ideal spectral band with a spectrometer response function.

[6] http://www.ciceco.ua.pt/JoseTDias

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Excited states, photochemistry

Malgorzata Biczysko [7]

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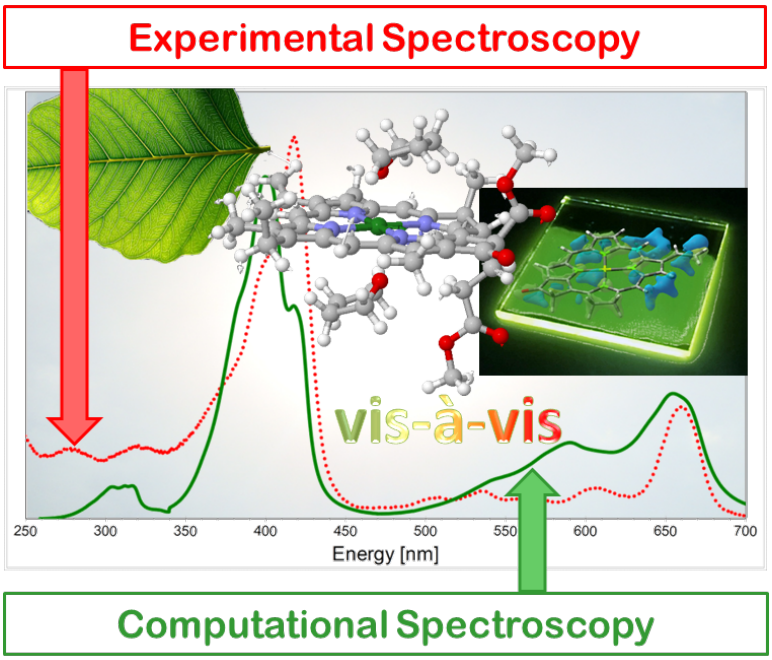
Most of the real-world processes takes place in 'bright' environments, i.e. the molecular system are exposed to solar irradiation, which manifests in photophysical and photochemical processes which are continuously happening not only in the laboratories but in the 'normal' every-day life [1-7]. Thus, the absorption and the emission of light in the UltraViolet-Visible (UV-vis) energy range (200-750 nm, 6.2-1.6 eV) is the most well-known and omnipotent spectroscopic phenomena. As the most natural examples one can mention the existence of colors and the visual abilities of human beings [2]. On the other hand, relatively high energy provided by UV photons leads to destructive processes. In this regard DNA strong absorbtion of UV light is a phenomenon of key biological interest, since a cascade of photochemical events can start from the DNA singlet excited electronic states, leading to the damage of the genetic code, and, eventually, to mutagenesis and carcinogenesis [3,4]. However, these undesired processes can be compensated by the possibility of fast and efficient non-radiative excited state decay channels. Another key issue of current interest are related to the natural and artificial light harvesting systems, such as identification of the most interesting chromophores among a large number of potential candidates for the design of new solar cells [5], or unraveling the many effects contributing to the complex light harvesting processes in natural photosystems [6].



Understanding of optical properties as well as photochemical and photophysical processes is provided through spectroscopic studies, either standard state-to-state one photon absorption and emission (OPA and OPE), their chiroptical couterparts: electronic circular dichroism (ECD) and circularly polarized luminescence (CPL); two-photon processes (TP) as well as pump-probe time-resolved experiments providing insights on excited states dynamics. Moreover, electronic spectra are often used to study the interactions between a molecule and its environment, being the first and key investigations in many different areas of the molecular, biological and nanotechnology sciences. However, spectroscopic results do not provide direct access to

[7] http://icqms.shu.edu.cn/?page_id=26

ISSN: 2279-8773

molecular structure and dynamics, and interpretation of the indirect information that can be inferred from analysis of the experimental data is seldom straightforward. Typically these complications arise from the fact that spectroscopic properties depend on the subtle interplay of several different effects, whose specific roles are not easy to separate and evaluate. In this context, computational studies can be extremely helpful, essentially at three different levels: (i) supporting and complementing the experimental results to determine structural, electronic and dynamical features of target molecule(s) starting from spectral properties; (ii) dissecting and quantifying the role of different effects in determining the spectroscopic properties of a given molecular / supra-molecular system; (iii) predicting electronic, molecular and spectroscopic properties for novel/modified systems. In such a way computational studies allow the assignment of experimental spectra and their interpretation in terms of basic physical-chemical processes.

These lectures and exercises are intended to give a general overview about computational approaches for modelling excited electronic states, while only essential aspects of the underlying theoretical models will be discussed. I will particularly concentrate on computational approaches related to the simulation and interpretation of state-to-state electronic spectra: one photon absorption and emission, as well as their chiroptical counterparts.

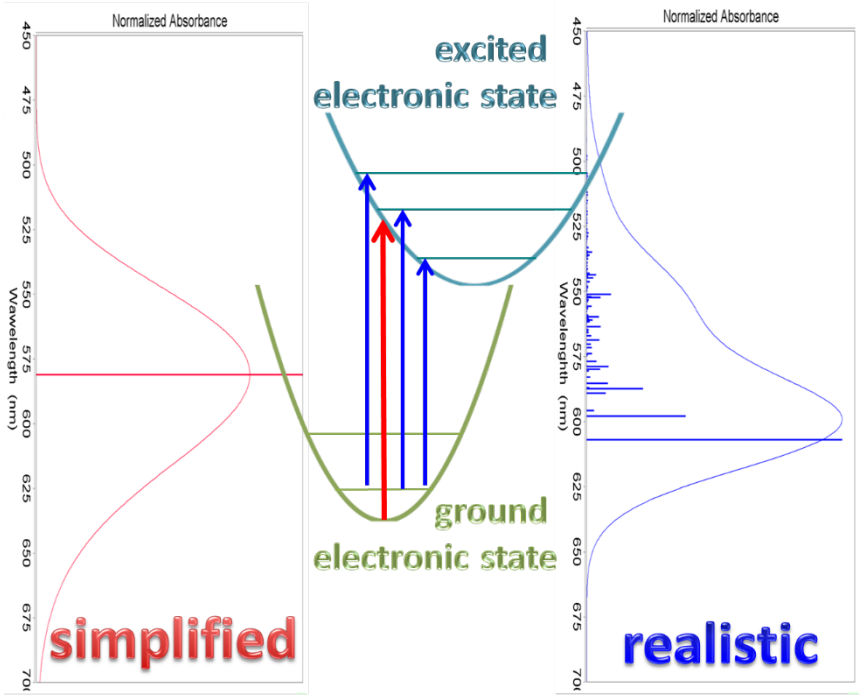


Figure 1. Simulation of electronic spectra: simplified model with only vertical electronic transition vs realistic model where transitions between vibrational levels of the two electronic states are taken into account.

Currently, most computations are limited to excitation energy and electronic transition moments, which are in turn convoluted to simulate the natural broadening in real conditions. In doing so, the experimental asymmetry of the band-shape, due to the vibronic structure is lost, leading to an incorrect estimate of the absorption and emission maxima and their relative intensities (Fig.1). Moving from the common practice of extracting numerical data from experiment to be compared with quantum mechanical (QM) results toward a direct *vis-`a-vis* comparison of experimental and simulated spectra strongly reduce any arbitrariness in the

ISSN: 2279-8773

analysis of complex experimental outcomes and allow a proper account of the information connected to both position and shape of spectral bands. Simulation of vibrationally-resolved electronic spectra [3-12], including environment and temperature effects, can be routinely done nowadays even for medium-to-large systems. Moreover, multiple electronic states can be taken into account, making possible the full characterization of the photophysical properties of natural compounds, with all analysis further facilitated thanks to user-friendly graphical tools [13].

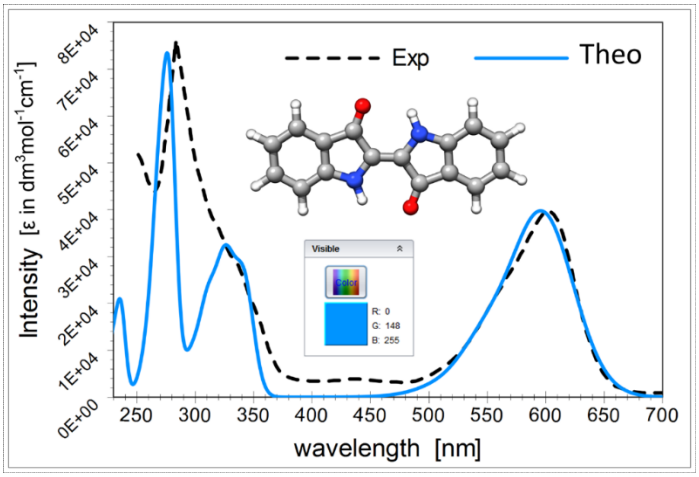


Figure 2. Simulated and experimental spectra of indigo, along with color prediction.

I. Unified and general theoretical model

Presented theoretical model [3-12] is developed for systems and phenomena localized on a limited space region, but possibly tuned by the more distant environment. Furthermore, it is assumed that the Born-Oppenheimer approximation is satisfied and that quantization of molecular rotation can be neglected. Under such circumstances the physical-chemical properties of a molecular system are governed by a potential energy surfaces (PESs) and by the corresponding property surfaces (PSs) for each electronic state, together with the needed transition moments.

Electronic spectra involve transitions between vibrational energy levels of two different electronic states, the upper state being neutral or ionic, and deriving from valence or core electron excitation. Electronic spectra line shapes, based on the underlying vibrational pattern, can be simulated by assuming that the electronic transition takes place in such a short time that the position of the nuclei remains almost unchanged. Then, the vibrational pattern of electronic spectra can be obtained from the computation of the overlap integrals, also known as Franck-Condon (FC) integrals, between the vibrational wavefunctions of the electronic states involved in the transition. In this frame, the theoretical models are defined according to the description of the PES for the electronic states involved and the approximation used for the evaluation of the transition dipole moment. This general procedure relies (so far) on the harmonic approximation, however anharmonic effects on excited electronic state frequencies can be taken into account by applying mode-specific anharmonic corrections. Finally, the issue of the infinite number of vibronic transitions can been overcome by the development of pre-screening black-box procedures and time-dependent path-integral models. The latter are characterized by an automatic inclusion of all vibrational states, while the former procedures allow to identify and assign single vibronic transitions; both approaches can be effectively combined in order to take into account their respective advantages.

II. Computational strategy: accuracy and feasibility

ISSN: 2279-8773

In many practical cases, a detailed analysis of the experimental electronic spectra is quite difficult due, for example, to the often non-trivial identification of the electronic band origin, multi-mode effects, possible overlaps of several electronic transitions and non-adiabatic and/or anharmonic effects. Although such complications are challenging also for the theoretical approaches, examples clearly show how theoretical simulations can provide a valuable tool with remarkable interpretative potential. When choosing the most proper model for a specific system, it should be realized that it is in general unknown *a priori* whether non-adiabatic effects exist in the region of the coordinate space relevant for the spectral features. In this respect, a particular care need to be taken while applying approaches, like the vertical ones, which may be operated with a minimal exploration of the final state PES. On the other side, more extended examinations of PES, such as those necessary to locate the excited state minima can bring to light issues that may otherwise remain unobserved. After that, for cases where relevant non-adiabatic effects exist, a proper modeling of the spectroscopy of the system under investigation cannot be done without a multi-electronic state treatment. On the other hand a disagreement between simulations and experiment may indicate existence of significant non-adiabatic couplings and can be used as a 'finger-print' of such effects. However, one should be aware that the disagreement between experimental and simulated spectra should not be attributed to non-adiabatic effects prior to exploring in detail the possible features of ``single-state'' vibronic models (e.g. full dimensionality). Beyond the possible non-adiabatic interactions, anharmonicity stands as an additional general factor to be taken into account in the spectroscopy of real systems. While a general route to its full treatment is out of reach for sizeable systems, it can be accounted for in a simplified manner in semi-rigid systems with nearly ``diagonal'' normal modes of the reference state leading, nonetheless, to significant improvement of the simulated spectra accuracy.

All the above mentioned issues will be illustrated with examples showing the advantages of modern computational spectroscopy approaches with respect to traditional models. Applications will be selected to highlight their flexibility, expected accuracy and interpretative capability, and to provide some guidelines for the choice of the most suitable models for a given problem, taking into proper account their computational feasibility.

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Classical Molecular Dynamics

Sérgio Filipe Sousa [8]

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Molecular Dynamics (MD) simulations are currently a powerful tool in the study of biomolecules, being routinely applied to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. MD simulations allow the study of the dynamic properties of a system. They enable the complex and dynamic processes that take place in biological systems to be analyzed and provide the ultimate detail concerning the individual particle motion as a function of time.

In this lecture an introduction to the MD field is presented. First, an introduction to Molecular Mechanical Methods and to the most common biomolecular force fields (AMBER, CHARMM, OPLS, GROMOS) is given. This section will be followed by a presentation on the basic principles behind MD simulations, giving particular attention to four critical aspects in MD simulations: the selection of the time step; the use of cut-offs; the use of boundary conditions; and the treatment of long-range interactions. This section will also introduce the strengths and limitation of the method, time scales in biomolecular simulations, and the different types of MD simulations. Special emphasis will be given to the several steps required for performing an MD simulation on a Biomolecular System.

This module will continue with a discussion on the range of application of the commonly available biomolecular force fields, and on the use of common strategies for force field parameterization for specific groups of compounds of relevance in biomolecular systems: metal complexes, biomembrane components, and drug like compounds.

Finally, some examples of application will be given focusing on the calculation of relevant properties from MD simulations. Examples will include the calculation of the Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF), Radial Distribution Functions (RDFs), Hydrogen Bonding Analysis, Interacting Distances and Angles, and Solvent Acessible Surface Areas (SASAs).

The outline of this lectures will be as follows:

I. Molecular Mechanics and Force Fields
  A. Basic Principles and Motivation
  B. General Aspects of MM Force Fields
  C. Biomolecular Force Fields
    C1. AMBER
    C2. CHARMM
    C3. OPLS
    C4. GROMOS

[8] http://www.fc.up.pt/pessoas/sergio.sousa/

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II. Molecular Dynamics Simulations
  A. Introduction and Motivation
  B. Basic Principles
    B1. Purpose and Limitations
    B2. Time Scales in Biomolecular Simulation
    B3. Types of Molecular Dynamic Simulations
    B4. Steps for performing an MD simulation of a Biomolecular System
  C. Technical Aspects in MD simulations
    C1. The time step
    C2. Boundary Conditions
    C3. The Cut-off for the Non-bonded Interactions
    C4. Long-Range interaction algorithms

III. Force Field Parameterization for Biomolecular Simulations
  A. Range of Application of common Biomolecular Force Fields and their parameterization
  B. Challenging Systems for Biomolecular Simulations
    B1. Metalloproteins
    B2. Biomembrane componentes
    B3. Drug-like compounds
  C. Parameterization Strategies

IV. Calculation of Useful Properties from MD simulations
  A. Determination of Properties from MD simulation and their significance
    A1. Root Mean Square Deviation (RMSD)
    A2. Root Mean Square Fluctuation (RMSF)
    A3. Radial Distribution Functions (RDFs)
    A4. Hydrogen Bonding Analysis
    A5. Determination of Interacting Distances and Angles
    A6. Calculation of Solvent Accessible Surface Areas (SASAs)
  B. Examples of Application

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Accelerated sampling strategies, Free energy calculations

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1) Accelerated sampling strategies

- Cavity and configurational bias; umbrella sampling
- Wang and Landau algorithm
- Genetic algorithms

2) Free energy calculations

- Thermodynamic integration method
- Windowing procedure
- Gibbs ensembles
- Integration of Gibbs-Duhem equation

3) Workshop

- The joy of Easy Java Simulations: programing and graphical user interfaces

[9] http://webpages.fc.ul.pt/~fmfernandes/index.htm

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Quantum and Classical Molecular Dynamics

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Molecular dynamics (MD) simulations have become an essential tool to help interpret experimental data in terms of the underlying molecular motion. In these lectures we will look at the basic theory of MD and how it is applied to fundamental processes.

The following topics will be covered in the 4 sessions:

1. Introduction to chemical physics (elementary processes, spectroscopy and electronic transitions, molecular collisions and chemical reactivity)

2. Born-Oppenheimer approximation and beyond

3. Quantum methods using wavepacket propagation

4. Classical methods based on swarms of trajectories

5. Examples of application

The introduction will give an overview of fundamental chemical processes and how information on these can be obtained by experiment. The following parts will develop the theory.

The starting point for a description of a molecular system is the time-dependent Schr□odinger equation (TDSE). Using the Born-Oppenheimer approximation we are able to integrate out the electronic motion and focus on the nuclei. The validity of this approximation and what to do when it breaks down will be discussed in part 2. In part 3 methods will be developed to solve the TDSE directly. These are known as wavepacket dynamics and in addition to standard methods, a particularly powerful algorithm, the multi-congurational time-dependent Hartree (MCTDH) method.

Unfortunately wavepacket dynamics can only treat very small systems (typically 3-4 atoms). For this reason approximate methods based on classical trajectories have been developed. In part 4 it will be shown how trajectory simulations relate to the full quantum mechanical solution.

Throughout the lectures examples will be given of calculations to show problems and limitations. In the associated workshops there will be a chance to run some simple simulations.

While there are many textbooks on classical mechanics and on quantum mechanics, few books are based on the TDSE. Ref. [1, 2] are 2 general textbooks that do just that. Ref. [3] details the MCTDH method with applications of wavepacket dynamics calculations. Ref. [4] is a review article which covers the swarm of trajectory approach. Ref. [5] is a recent book on describing reactivity.

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Electronic Structure of Solids

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This course considers the theoretical treatment of the geometrical and electronic structure of solids and surfaces and of molecule-surface interactions. For molecules a much-used approximation is molecular orbital (MO) theory, similarly, for crystalline solids and surfaces a widely used approximation is band theory. For molecules point group symmetry can be used to make the computations easier and also to label the MO's en their energies. Likewise, for crystals one can use translational symmetry to make the computations feasible and to label the crystal orbitals and their energies. Concepts like Bloch orbitals, bands and densities of states, will be introduced and explained.

We will discuss the bulk properties of some interesting materials, like graphene, diamond and rock salt in the frameworks of Hartree-Fock and density functional band theory. Chemisortion on surfaces will also be considered. Finally, theoretical descriptions based on embedded cluster models will be discussed. The latter material models can be used for the study of local excitations in solids and on surfaces. They are also well suited for the study of solids with strong electron correlation, since for such systems the one-electron band models are too approximate.

The concepts presented will be illustrated with hands-on calculations.

The following books can been used for further reading:

Molecular Quantum Mechanics, by P.W. Atkins and R. Friedman
Solid State Physics, by N.W. Ashcroft and N. D. Mermin
Quantum Mechanics in Chemistry, by G.C. Schatz and M.A. Ratner (Dover)
Solids and Surfaces: A Chemist's View on Bonding in Extended Structures, by R. Hoffmann

[11] http://theochem.chem.rug.nl/~broer/
[12] http://www.rug.nl/staff/r.w.a.havenith/

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Ethics in Science

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This short course is concerned with ethics and integrity in science, in the planning, conducting and reporting of research. An important issue is how to recognize (and avoid) scientific misconduct.

In the planning of research conflicts of interest can easily occur. In the conduction of research it is important to have a clear distinction between the responsibilities of trainee, mentors and collaborators.

Proper data collection, selection, storage and sharing will also be discussed. With regards to reporting and publication of research, authorship, ownership and (fair) reviewing are important issues.

[13] http://theochem.chem.rug.nl/~broer/

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Hybrid QM/MM Methods

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Hybrid QM/MM Methods combine the strengths of quantum mechanics with those of molecular mechanics, enabling an accurate description of localized chemical reactions in system comprised by several thousands of atoms.

In this lecture, an introduction to hybrid QM/MM methods is presented. First, an introduction to QM/MM methods and to the advantages and limitations of this class of methods is given. Common alternatives for the treatment of the QM and MM regions are presented and discussed. This section will be followed a presentation on several technical aspects surrounding QM/MM calculations: Additive vs Substractive QM/MM schemes; Region partitioning; Treatment of the interface region; and the Treatment of the interactions between the QM and MM regions; The typical steps in QM/MM modeling will be the subject of an additional section. Finally, a discussion on alternative strategies to standard QM/MM calculations, beyond the single conformation approach, will be presented.

[14] http://www.fc.up.pt/pessoas/sergio.sousa/

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Molecular Docking and Virtual Screening

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Fueled by the advances in computational methodologies, molecular docking has become a key tool in structural molecular biology and computer-assisted drug design[1]. The goal of protein-ligand docking is to predict the predominant binding mode(s) of a ligand with a protein of known three-dimensional structure[2]. Currently, this approach represents a significant step towards understanding the principles whereby molecules bind to the receptors in their biological environment[3].

Molecular Docking is presently being used in the rapid in silico assessment of large libraries of chemical structures (available or virtual products) in order to identify those structures that are most likely to bind to a drug target, typically a protein receptor or an enzyme. These computational techniques are commonly referred as virtual screening methodologies and their application is expected to enhance the discovery of new hit- and lead-compounds in the next years[3]. Moreover, as the number of pharmaceutical targets is predicted to dramatically increase in the coming years, these methods will undoubtedly play a major role in drug design.

In this module, the key concepts and specific features of protein-ligand docking methods and structure-based virtual screening are presented. The general strengths and weaknesses that presently characterise these methodologies will be highlighted and recent successful applications of docking-based tools for hit discovery and lead optimisation will be presented.

To illustrate the above content, some particular examples will be analysed in the hands-on classes[4]. In these sessions, we will outline the computational challenges behind these methodologies as well as the interpretation of the results and comparison with the available experimental data.

References:

(1) Cerqueira NMFSA, Sousa S. F., P.A Fernandes, M. J. Ramos, "Virtual screening in Drug Design and Development", Chapter 4, 2010, Ligand-Macromolecular Interactions in Drug Discovery, Methods and Protocols, Vol. 572 .Roque, Ana Cecília A. (Ed.), ISBN: 978-1-60761- 243-8
(2) Cerqueira NMFSA, Bras NF, Fernandes PA, Ramos MJ., "MADAMM: a multistaged docking with an automated molecular modeling protocol.", Proteins. 2009 Jan;74(1):192-206.
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[15] http://web.fc.up.pt/pessoas/nscerque/doku.php/home

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Protein Dynamics and Energetics

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At the present stage of the Intensive Course the students are familiar with molecular dynamics and with importance sampling techniques. This course will focus on applications of the previously gained knowledge to the field of proteomics. To course begins with a discussion of the particular aspects of the simulation of proteins, focusing the discussion on the force fields, on the timescales of their movements and on the difficulties on obtained converged properties within reasonable simulation times. Applications will be discussed and their relevance within the broad field of proteomics will be dissected. Examples include protein folding, membrane permeation, computational mutagenesis, protein:protein docking, among others.

[16] http://www.fc.up.pt/pessoas/pafernan/

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Enzymatic Catalysis

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This course will address the most relevant aspects for the computer simulation of enzymatic reactions. A first, broad overview about general enzyme catalysis will be presented. Then the course will focus on strategies to simulate enzymes, emphasizing the most relevant difficulties and peculiarities associated to these so complex molecules. Finally the course will explain in detail a step-by-step procedure to computationally predict the chemical mechanism of a given enzyme. A set of examples will then illustrate the concepts.

[17] http://www.fc.up.pt/pessoas/pafernan/

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Nanoscience

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In this course, a very general overview of basic concepts in nanoscience will be given, in particular the dependence of electronic structure of materials on their size and the emergence of quantum effects at nanoscale. The special case of carbon nanotubes will be presented. We will analyze the advantages and limitations of popular quantum methods to model nanostructures, with special emphasis on semiemepirical methods which are able to provide a good compromisse between accuracy and time of computation.

At the hands-on session, the energetics of a particular S_N2 reaction will be analyzed inside the environment of a series of armchair carbon nanonotubes, using a semiempirical method. The students will have to prepare molecular models, input files for calculations and, finally, compare the results with data in literature.

References

Masaru Kuno, *Introductory Nanoscience*, Garland Science-Taylor & Francis Group, London, 2012.

[18] http://www.fc.up.pt/pessoas/almagalh/

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The Quantum Chemical Cluster Approach for Enzyme Modelling

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The lectures give a brief account of the methods and models used to study enzyme active sites and reaction mechanisms using quantum chemical methods. With density functional theory, it is today possible to routinely and quite accurately treat systems consisting of ca 300 atoms. This has made it possible to model enzyme active sites in a more realistic way. The calculated energies can be used to rule out or substantiate reaction mechanisms and have also been shown to be sufficiently accurate to satisfactorily reproduce various kinds of selectivities. Indeed, many mechanistic problems have been solved for a wide variety of enzymatic systems. Recent advancements of this methodology are discussed and a number of relevant applications are given.

[19] http://www.organ.su.se/himo/?page=about

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Enzyme promiscuity: the case of carbonic anhydrase

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Metal ions are fundamental for the life owing to indispensable components of the cellular machinery. They are involved in numerous essential functions going from nucleic acid and protein stabilization to enzyme catalysis. Thousands of known enzymes are characterized by the presence of one or more metal ions in the catalytic active site.

In these enzymes metal cations have various distinctive properties acting in different mechanisms of substrate/cofactor activation in both non-redox and redox catalysis and often play other roles not well established.

The presented cases will concern metalloenzymes afferent to enzymatic family of carbonic anhydrases (CAs). In particular, substrate promiscuity due to native and promiscuous substrates and enzymatic promiscuity due to the native metal ion substitution will be the examined aspects of the catalytic activity of CA. The calculations have been performed by cluster as well as by hybrid QM/MM approaches by using in both cases the density functional theory as quantum mechanical tool.

After elucidating the catalytic prosmicuity phenomenon, a deeper insight on the catalytic mechanisms of every studied case will be given.

References

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[21] http://www.unical.it/portale/portaltemplates/moduli/show_scheda_persone.cfm?11052 https://scholar.google.it/citations?user=0cghFGwAAAAJ&hl=it&oi=ao

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Advanced Computational Techniques

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First part: CONCURRENT COMPUTING ARCHITECTURES

Circuitry evolution to high performance computing (speed, storage, networks,..)
Duty cycle, Moore limit and concurrency
Multiprogramming, time-sharing, look ahead, instruction rescheduling
Components' parallelism I/O processors, Memory hierarchy, memory banques
Cache memory and mapping
Reduced sets of instructions
Multiple functional units and pipelining (instruction, data)
Vector computing, Super-scalarity and multi-scalarity
Stream taxonomy (SIMD, SIMD, MIMD)
Memory taxonomy (shared and distributed)
Networking taxonomy
Distributed computing and grids

Second part: PARALLEL COMPUTING PARADIGMS AND MODELS

Approaches to parallelism and parallelization schemes
Partitioning
Communications
Granularity
Domain and functional decomposition
Parallel programming paradigms (shared memory, threads, message passing, data parallel)
Models of parallelism (sequential, farm, pipe, loop)
examples (Matrix operations, π calculation)
MPI history and related programming model
MPI functions
Examples
Communications
Examples
Main MPI routines
Collective operations

[22] http://www.chm.unipg.it/antonio

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Communication skills

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Communication in Science is a fundamental topic to modern and democratic societies. Therefore, a competitive scientific curriculum of a young researcher has to take into account communication skills, in order to be able to disseminate the results of her/his work towards peers, other experts and general public.

In this practical course, all students have to do a short oral presentation to the classroom that summarizes the results of a recent published paper on a subject related to the topics of the Intensive Course in TCCM. The objective of this activity is to develop several transferable skills such as: read and interpret a new published paper (the papers are randomly distributed among students); synthesize the work into a few main ideas; prepare a short communication (up to 12 minutes) with an appropriate presentation software program; speak to an expert audience.

In the first day of this module, CS-1, the students have to prepare their works. The last day, CS-2, is assigned to communications and to the evaluation by a juri formed by two professor (this year Professors José Ferreira Gomes and Alexandre Magalhães).

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