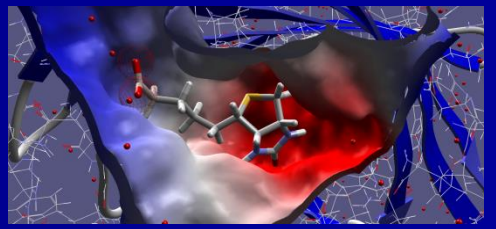
Modelarea sistemelor biomoleculare

Master BFM, an I/ an II



Vasile CHIŞ

Babeş-Bolyai University
Faculty of Physics
Kogălniceanu 1, RO-400084 Cluj-Napoca, Romania

Course details

SEMESTRUL II

COD	DENUMIREA DISCIPLINELOR	Credite ECTS	Ore fizice săptămânale			Ore convenționale săptămânale			Forma de evaluare			Fel disciplină
			C	S	LP	FF	I	T	Ex	C	VP	
FMR2201	Radioizotopi si radioterapie	5	2	0	1	6.5	2.5	9	X	-	-	DS
FMR2202	Imagistică medicală	5	2	0	2	8	1	9	X	-	-	DS
FMR2203	Modelarea sistemelor biomoleculare	5	2	0	2	8	1	9	X	-	-	DS
FMR2204	Nanobiofotonică	5	2	0	2	8	1	9	X	-	-	DS
FMR2206	Biofizica moleculara si celulara	5	2	0	2	8	1	9	X	-	-	DS
FMX2205	Curs opțional 1	5	2	0	2	8	1	9	X	-	-	DC
	TOTAL CREDITE =	**30**										
	TOTAL ORE PE SĂPTĂMÂNĂ =		**12**	**0**	**11**	**46.5**	**7.5**	**54**				
			23									
	TOTAL ORE FIZICE / CONVENȚIONALE PE SEMESTRU =		**322**			**756**						
	TOTAL EVALUĂRI =								**6**	**0**	**0**	

Schedule

Course: Thursday, 12-14, “Victor Mercea” Amphitheater

Lab:

1-st year students: Tuesday, 14-16, room 233 - C. Craciun

2-nd year students: Tuesday, 16-18, room 233 – C. Craciun

Syllabus **FMR2203**

Course details

Assignment

3.5 p – written test

4.0 p – practical test

1.5 p – research paper analysis (optional)

- oral presentation

1.0 p – Bonus

Computational Chemistry (Quantum chemical calculations)

- a branch of theoretical chemistry (molecular physics)
- the overlap area between computer science and chemical-physics

major goals

- to create efficient **mathematical approximations** and **computer programs**

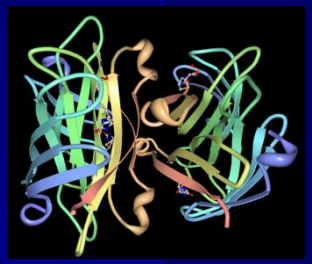
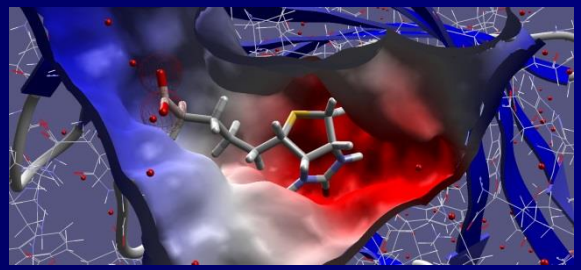
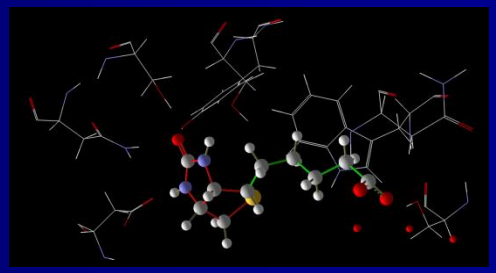
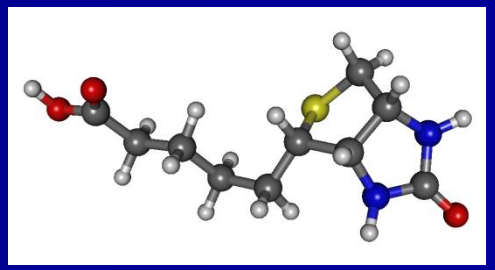
  to calculate the **properties of molecules** (such as total energy, dipole and quadrupole moment, vibrational frequencies, reactivity and other diverse spectroscopic quantitities and cross sections for collision of molecules with different atomic or subatomic projectiles)

- to apply these programs to concrete physico-chemical systems

Why “Molecular modeling” ?

- **Understanding**, **explaining**, **predicting** (bio)molecular properties
- Get information that is complementary information to experimental data
- Research in the (bio)molecular field
- Secure a job

  -> pharmaceutical companies

Biotin (vitamin B7 or H) - a water-soluble vitamin involved in the metabolism of amino acids and carbohydrates

Streptavidin – tetramer protein

- used in biotechnolog for the purification or detection of various biomolecules

Biotin - streptavidin - one of the strongest non-covalent interactions known in nature

- shape complementary, extensive H-bonding interactions

Research paper projects

Hydrogen bonding by QM electronic structure methods
Biomolecules on surfaces
Calculation of NMR spectra: the influence of the method and basis set
TD-DFT for absorption spectra of dyes
Scaling vibrational wave-numbers
Basis set effects on molecular properties
DFT and HF for guest-host interactions
Reactivity indices from QC calculations
QC calculations on molecules in an external electric field
Ionic liquids modeled by QC methods
Anticancer drugs: is DFT helpful?
QM/MM approach for biomolecular systems
Weak (non-covalent) intermolecular interactions
DFT applied for biomaterials
pKa calculations and pH dependent molecular structures
Computational recipes for large molecules: the ONIOM method
Adsorbed molecules on metallic surfaces
Calculation of ESR spectra for paramagnetic compounds

… (your choice)

What to follow?

Subject
Aim
Computational Methodology
Usefulness of the theoretical data
Main results
Conclusions
Comments

HOME

- CV
- Research
- List of Publications
- Books
- Lectures
- Grants
- Links
- Group

Contact:

Prof. dr. Vasile Chis
Babes-Bolyai University
Faculty of Physics

Lecture Notes

Seminar.ppt
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course8.pdf
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IR_Raman.pdf
NMR_ESR.pdf

Paper projects
Questions and problems
Final Results

cap1.pdf

lab1

Bibliography
Books

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3. W.J. Hehre, L.Radom, P.v.R.Schleyer, J.A.Pople, *Ab Initio Molecular Orbital Theory*, John Willey & Sons, New York, 1986
. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons, New York, 2001.
4. D.C. Young, *Computational Chemistry*, John Wiley and Sons, 2001
5. A. Szabo, N.S. Ostlund, *Modern Quantum Chemistry; Introduction to Advanced Electronic Structure Theory*, McGraw-Hill Publishing Company, New York, 1989
6. R.G. Parr, W.Yang, *Density Functional Theory of Atoms and*

Gaussian and GaussView References

A. Frisch, Gaussian 09W Reference, http
/g_ur/g09w_ref_toc.htm

J.B. Foresman, A. Frisch, Exploring Chem
edition, 2015, http://expchem3.com/

Æleen Frisch, Hrant P. Hratchian, Roy D.
GaussView reference, http://www.gaus
(http://www.gaussian.com/g_dl/gv5re

Web resources:

A mathematical and computational revi
chemistry by P. Echenique and J.L. Alon
Quantum Chemistry-Computational Che

1. Why computing molecules?

electronic structure calculations

- electronic structure theory can be used as a very useful tool in the experimental research, providing new insights into physico-chemical problems.
- useful results for those involved in experimental research.
- interpret the properties of the novel developed materials
- modelling the biochemical compounds
- modelling the intermolecular interactions
- …

2. What shall we learn?

- the theory behind "molecular modeling"
- to use some molecular visualization packages
- to use program packages designed for molecular electronic structure theory
- to do calculations at different levels of theory and to interpret the results
- to make correlations between the experimental and theoretical data

3. Contents of this course

Hartree-Fock Theory
Basis sets
Electron Correlation Methods
Basis set superposition error
Density Functional Theory
Geometry optimizations
Calculation of vibrational spectra
Calculation of NMR and ESR spectra
Calculation of UV-VIS spectra

4. Can we do research?

pure theoretical studies
coupled experimental and theoretical investigation on the structure and properties of molecular systems

5. References

1. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons, New York, 2001
2. W. Koch M.C. Holthausen, *A chemist's guide to DFT*, Wiley-VCH, 2001
3. D.C. Young *Computational chemistry*, Wiley, 2001
4. A. Leach, Molecular *Modelling - principles and applications*, Prentice Hall, 2001
5. C. J. Cramer, *Essentials of Computational Chemistry*, John Wiley & Sons (2002)
6. V. Barone, P. Cimino, O. Crescenzi, M. Pavone, Ab Initio computation of spectroscopic parameters as a tool for the structural elucidation of organic systems, J. Mol. Struct., (Theochem), 811, 323-335 (2007)
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9. H. Zipse, Overview of Topics in "Computational Chemistry 1", http://www.cup.uni-muenchen.de/oc/zipse/contents-table-of-contents.html

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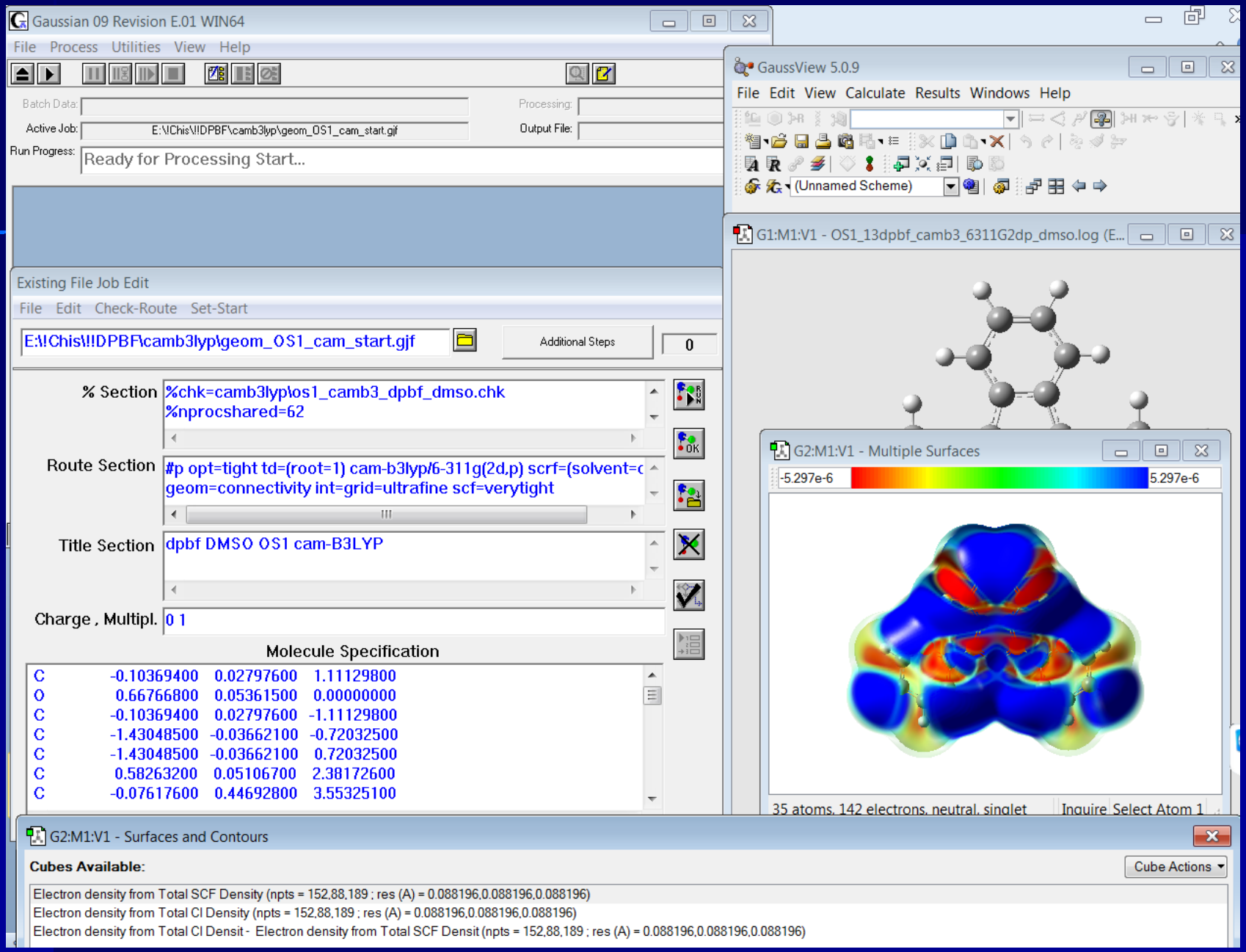
11. J.B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd edition, 2015, http://expchem3.com/ (http://www.gaussian.com/g_pix/e3_cover.jpg)

12. Æleen Frisch, Hrant P. Hratchian, Roy D. Dennington II, Todd A. Keith, John Millam, GaussView reference, http://www.gaussian.com/g_tech/gv5ref.htm (http://www.gaussian.com/g_dl/gv5ref_nav.pdf.zip)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File Process Utilities View Help
Batch Data:
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Output File:
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5.297e-6
35 atoms, 142 electrons, neutral, singlet
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G2:M1:V1 - Surfaces and Contours
Cubes Available:
Cube Actions
Electron density from Total SCF Density (npts = 152,88,189 ; res (A) = 0.088196,0.088196,0.088196)
Electron density from Total CI Density (npts = 152,88,189 ; res (A) = 0.088196,0.088196,0.088196)
Electron density from Total CI Densit - Electron density from Total SCF Densit (npts = 152,88,189 ; res (A) = 0.088196,0.088196,0.088196)

DFT as a "computational spectroscopy" tool