R O M Â N I A
MINISTERUL EDUCAȚIEI ȘI CERCETĂRII
Universitatea din Craiova
FACULTATEA DE ȘTIINȚE/ DEPARTAMENTUL DE CHIMIE
Craiova, Str. Calea București, nr. 107I
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Subject Description

1. Program information

1.1. Institution	University of Craiova
1.2. Faculty	Science
1.3. Department	Chemistry
1.4. Study field	Chemistry
1.5. Study level	Master
1.6. Type of education	full-time
1.7. Study program	Advanced Chemistry

2. Subject information

2.1. Subject			**Advanced computational chemistry**				
2.2. Course coordinator			Lect.dr. Aurelian Dobrițescu				
2.3. Application coordinator			Lect.dr. Aurelian Dobrițescu				
2.4. Year of study	II	2.5. Semester	3	2.6. Type of evaluation	V	2.7. Subject type	DS/DOP

3. Total estimated type (hours/semester)

3.1. Number of hours per week	4	from which: 3.2 course	2	3.3. lab	2
3.4. Total hours in curriculum	56	from which: 3.5 course	28	3.6. lab	28
Time allocation – hours/week					
Study using textbooks, course materials, bibliographies, and notes					30
Additional documentation in the library, on specialized electronic platforms, and in the field					28
Preparation of seminars/labs, assignments, reports, portfolios, and essays					25
Tutoring					5
Examinations					4
Other activities (individual research, problem solving, independent computational work)					2
3.7. Total hours of individual study					94
3.8. Total hours per semester					150
3.9. Number of ECTS					6

4. Preconditions (if the case)

4.1. of curriculum	• Quantum Chemistry I, Mathematical Methods in Chemistry, Linear Algebra, Statistical Thermodynamics
4.2. of competences	• Fundamental and advanced knowledge of quantum mechanics, Core competences in quantum chemistry, Solid background in mathematical methods, Basic understanding of statistical thermodynamics, Analytical skills

5. Conditions (if the case)

5.1. for course	• Appropriate lecture facilities equipped with standard teaching infrastructure, access to specialized bibliographic resources and electronic scientific databases
5.2. for labs	• Computer laboratory with adequate hardware resources, Availability of specialized computational chemistry software, Technical infrastructure ensuring reliable operation and data management

6. Course objectives - expected learning outcomes achieved by completing and passing the course

Knowledge	1. Graduates define, understand, explain, and apply advanced knowledge of chemistry from specialized literature in practice. 2. Graduates write analysis and scientific reports, presenting the results of their research and experiments, in line with professional ethics and standards.
Skills	1. Graduates apply major concepts in analytical, inorganic, organic, and physical chemistry to chemical practice. 2. Graduates apply critical thinking, following the structure and principles of scientific writing to develop and present scientific reports.
Responsibility and autonomy	1. Graduates are able to adapt major scientific concepts in the field of chemistry to conduct research, improve or develop new concepts, knowledge, theories, and operational methods, products, and services in order to apply them in specific activities for product and process quality control. 2. Graduates prepare and present scientific reports in line with ethical standards for collecting and interpreting results.

7. Table of contents

7.1. COURSE	Mode of operation	Teaching methods	Allocated time (hours)
1. Scope and Formal Structure of Computational Chemistry • Computational chemistry as applied mathematical physics • Exact vs. approximate solutions of the electronic Schrödinger equation • Variational principles and upper-bound theorems • Determinism, numerical error, and epistemic limits	On site (week 1)	Expository lecture; conceptual and comparative analysis; guided theoretical discussion	2
2. Mathematical Foundations of Quantum Chemistry • Hilbert spaces and inner products • Linear operators and spectra • Hermiticity, commutators, and expectation values • Functional analysis in quantum chemistry	On site (week 2)	Lecture with formal derivations; proof-based instruction; seminar-style discussion	2
3. Basis Sets and Mathematical Approximations • Atomic orbitals vs. basis functions • Gaussian-type orbitals (GTOs) and Slater-type orbitals (STOs) • Minimal, split-valence, polarized, and diffuse basis sets • Basis set superposition error (BSSE) (CVD)	On site (week 3)	Comparative theoretical analysis; concept-based explanation of basis truncation	2

4. Hartree–Fock Theory • Self-consistent field (SCF) procedure • Restricted, unrestricted, and ROHF methods • Physical interpretation of Hartree–Fock orbitals • Limitations of Hartree–Fock theory	On site (weeks 4)	Step-by-step derivation of SCF equations; conceptual modeling of mean-field approximation	2
5. Electron Correlation and Post-Hartree–Fock Methods • Nature of electron correlation • Møller–Plesset perturbation theory (MP2, MP3) • Configuration Interaction (CI) • Coupled Cluster methods (CCSD, CCSD(T))	On site (week 5)	Formal classification of correlation effects; comparative method analysis (MP, CI, CC)	2
6. Density Functional Theory (DFT): Fundamentals • Hohenberg–Kohn theorems • Kohn–Sham equations • Exchange–correlation functionals • Local, semi-local, hybrid, and meta-GGA functionals	On site (weeks 6)	Theorem-based instruction; formal derivation of Kohn–Sham equations	2
7. Advanced Topics in DFT • Dispersion corrections (DFT-D, vdW methods) • Limitations and common pitfalls of DFT • Choosing the “right” functional	On site (week 7)	Constraint-based functional analysis; guided discussion of DFT limitations	2
8. Geometry Optimization and Potential Energy Surfaces • Molecular geometry optimization algorithms • Transition states and reaction pathways • Potential energy surfaces (PES) • Intrinsic reaction coordinate (IRC) calculations	On site (week 8)	Mathematical explanation of optimization algorithms; PES topology analysis	2
9. Molecular Properties and Spectroscopy • Calculation of molecular properties • Vibrational frequencies and IR/Raman spectra • Electronic excitations (TD-DFT) • NMR chemical shifts and spin–spin couplings	On site (week 9)	Operator-based derivation of molecular properties; linear response theory exposition	2

10. Molecular Mechanics and Force Fields • Classical mechanics approximation • Force field components and parametrization • Common force fields (AMBER, CHARMM, OPLS) • Applicability and limitations	On site (week 10)	Conceptual contrast between classical and quantum descriptions; analytical decomposition of force fields	2
11. Molecular Dynamics Simulations • Newtonian equations of motion • Integration algorithms (Verlet, leap-frog) • Ensembles (NVE, NVT, NPT) • Temperature and pressure control	On site (weeks 11)	Mathematical derivation of equations of motion; ensemble theory lectures	2
12. Monte Carlo Methods and Statistical Sampling • Statistical mechanics background • Monte Carlo algorithms • Metropolis method • Applications in adsorption and phase equilibria	On site (week 12)	Probability-based instruction; formal justification of Monte Carlo algorithms	2
13. Computational Chemistry in Materials and Biochemistry • Periodic systems and solid-state calculations • Introduction to plane-wave DFT • Modeling surfaces and interfaces • Computational drug design and docking (overview)	On site (week 13)	Formal introduction to periodic systems; conceptual modeling of surfaces and interfaces	2
14. Emerging Trends and Student Presentations • Machine learning in computational chemistry • High-throughput screening • Multiscale modeling • Ethical use, limitations, and future perspectives	On site (week 14)	Research-oriented seminars; instructor-led synthesis of emerging theoretical directions	2

References:

1. **Cramer, C. J.** (2024). *Essentials of computational chemistry: Theories and models* (3rd ed.). Wiley.
2. **Jensen, F.** (2022). *Introduction to computational chemistry* (4th ed.). Wiley.
3. **Burke, K.** (2023). Perspective on density functional theory. *The Journal of Chemical Physics, 158*(15), 150901. https://doi.org/10.1063/5.0141394.
4. **Neese, F., Wennmohs, F., Becker, U., & Riplinger, C.** (2022). The ORCA quantum chemistry program package. *The Journal of Chemical Physics, 152*(22), 224108. https://doi.org/10.1063/5.0004608.
5. Lecture notes, 2025.

7.2. Lab	Mode of operation	Teaching methods	Allocated time (hours)
1. Introduction to computational chemistry software (Gaussian, ORCA, GAMESS, VASP – overview).	On site (week 1)	Conceptual computational illustration of exact vs. approximate solutions; numerical error analysis	2
2. Solving simple quantum systems numerically. Visualization of wavefunctions and probability densities.	On site (week 2)	Symbolic and numerical representation of operators and spectra; visualization of eigenfunctions	2
3. Basis set convergence studies. Effect of basis set choice on molecular properties	On site (week 3)	Computational illustration of basis set convergence and BSSE effects	2
4. Hartree–Fock calculations on small molecules. Analysis of orbital energies and electron density.	On site (weeks 4)	Implementation and analysis of restricted and unrestricted HF calculations	2
5. Comparison between HF and correlated methods. Correlation energy evaluation.	On site (week 5)	Computational comparison of HF and correlated methods on model systems	2
6. DFT calculations with different functionals. Benchmarking DFT results against higher-level methods.	On site (weeks 6)	Comparative DFT calculations using different exchange–correlation functionals	2
7. Non-covalent interaction analysis. Energy decomposition approaches.	On site (week 7)	Computational illustration of dispersion corrections and functional-dependent results	2
8. Geometry optimization and transition state search. Reaction pathway modeling.	On site (week 8)	Geometry optimization, transition state search, and IRC calculations	2
9. Simulation of IR, UV-Vis, and NMR spectra. Comparison with experimental data.	On site (week 9)	Simulation and interpretation of IR, Raman, UV–Vis, and NMR spectra	2
10. Energy minimization using molecular mechanics. Comparison between MM and QM descriptions.	On site (week 10)	Energy minimization and force field parameter exploration	2
11. Molecular dynamics simulations of liquids or biomolecules. Trajectory analysis and visualization.	On site (weeks 11)	Molecular dynamics simulations; trajectory and ensemble analysis	2
12. Monte Carlo simulations. Adsorption and equilibrium property calculations.	On site (week 12)	Monte Carlo simulations and statistical sampling of equilibrium properties	2
13. Surface or solid-state calculation. Protein–ligand interaction modeling (introductory).	On site (week 13)	Plane-wave DFT calculations and introductory docking simulations	2

14. Student project presentations. Critical discussion of computational results.	On site (week 14)	Student-led presentations; computational or theoretical mini-projects	2

References:

1. **Jensen, F.** (2022). *Introduction to computational chemistry* (4th ed.). Wiley.
2. **Neese, F., Wennmohs, F., Becker, U., & Riplinger, C.** (2022). The ORCA quantum chemistry program package. *The Journal of Chemical Physics, 152*(22), 224108. https://doi.org/10.1063/5.0004608
3. **Leach, A. R., & Gillet, V. J.** (2023). *An introduction to chemoinformatics* (3rd ed.). Springer.
4. **Hafner, J., Wolverton, C., & Ceder, G.** (2023). Toward computational materials design: Density functional theory and beyond. *Nature Reviews Materials, 8*(9), 641–658. https://doi.org/10.1038/s41578-023-00568-2
5. Lab work presentations, 2025.

8. Corrrelation of the discipline content with the expectations of representatives of the epistemic community, professional associations, and representative employers in the field related to the program

The discipline content is aligned with the standards and expectations of the international epistemic community in theoretical and computational chemistry, as well as with the recommendations of relevant professional associations (IUPAC, European Chemical Society – EuChemS), through ensuring a strong theoretical grounding, methodological transparency, and reproducibility of scientific results. It provides advanced theoretical and methodological competences in abstract reasoning, model construction, and theoretical analysis required by research institutions, R&D centers, and doctoral programmes in the field of Advanced Chemistry.

9. Evaluation

Activity	9.1. Evaluation criteria	9.2. Evaluation method	9.3. Contribution to final score
9.4. Course	1. Correct understanding of theoretical concepts 2. Ability to follow and reproduce formal derivations 3. Critical analysis of approximations and theoretical limits 4. Coherent use of scientific terminology	Written examination: theory-based problems and conceptual questions	50%
		Oral examination: structured theoretical discussion	20%
9.5. Lab	1. Correct application of computational methods 2. Quality and rigor of computational analysis 3. Interpretation of results in relation to theory 4. Clarity and structure of laboratory reports	- Evaluation of laboratory reports - Assessment of computational assignments - Oral presentation and discussion of results	30%

9.6. Minimum performance standard
To successfully complete the discipline, students must demonstrate the minimum level of competences required for advanced study in theoretical and computational chemistry: • At the theoretical level, this includes the ability to understand and explain core concepts, to follow formal mathematical derivations, and to critically assess the validity and limitations of computational models and approximations. • At the practical level, students must demonstrate the competence to apply fundamental computational chemistry methods in a controlled laboratory setting, to perform standard calculations, and to interpret computational outputs in a manner consistent with the underlying theoretical framework. Students must also show the ability to document computational procedures and results clearly, ensuring logical coherence and reproducibility.

Date
22.09.2025

Course coordinator,
Lect.dr. Aurelian Dobrițescu

Date of approval
25.09.2025

Head of Department,
Conf.dr. Nicoleta Cioateră