SYLLABUS

1. Information regarding the program

1.1 Higher education institution	Babeş-Bolyai University
1.2 Faculty	Faculty of Physics
1.3 Department	Doctoral School of Physics
1.4 Field of study	Physics
1.5 Study cycle	Doctorate
1.6 Study program / Qualification	Doctoral training/PhD in Physics

2. Course data

2.1 Name of discipline			Theoretical models and simulation methods in physics				
2.2 Teacher responsible for lectures			Prof. dr. Titus Beu, Prof. dr. Vasile Chiş, Prof. dr. Ladislau Nagy, Prof. dr. Zoltan Neda, Conf. dr. Zoltan Balint				
2.3 Teacher responsible for seminars			Prof. dr. Titus Beu, Prof. dr. Vasile Chiş, Prof. dr. Ladislau Nagy, Prof. dr. Zoltan Neda, Conf. dr. Zoltan Balint				
2.4 Year of study	I	**2.5 Semester**	I	**2.6 Type of evaluation**	E	**2.7 Course framework**	DS

3. Estimated total time of teaching activities (hours per semester)

3.1 Hours per week	3	Out of which: 3.2 Lectures	2	3.3 Seminars / Laboratory classes	1
3.4 Total hours in the curriculum	36	Out of which: 3.5 Lectures	24	3.6 Seminars / Laboratory classes	12
Allocation of study time:					
Study supported by textbooks, other course materials, recommended bibliography and personal student notes					36
Additional learning activities in the library, on specialized online platforms and in the field					36
Preparation of seminars/laboratory classes, topics, papers, portfolios and essays					50
Tutoring					12
Examinations					10
Other activities: -					–

3.9 Total individual study hours	144
3.10 Total hours per semester	180
3.11 Number of ECTS credits	10

4. Prerequisites (if necessary)

4.1 Curriculum	Quantum mechanics, Statistical physics, Physics of atoms and molecules, Numerical methods, Calculus, Algebra, Probability theory
4.2 Competences	- analytical calculation skills - programming skills (Python, C / C ++, Mathematica) - skills in using programming environments and graphical applications

5. Conditions (where applicable)

5.1 Conducting lectures	Course hall, appropriate board, projector, computer, dedicated software
5.2 Conducting seminars/laboratory classes	Course hall, appropriate board, projector, computer, dedicated software, computer network

6. Specific competences acquired

Professional competences	- Acquiring advanced concepts and models of molecular dynamics. - Abilities to build molecular models and prepare input data for advanced numerical codes. - Ability to select appropriate models and options for complex simulations. - Correct use of quantum chemistry methods and appropriate models for calculating molecular properties - Ability to solve the Schrodinger equation for the external atom-field interaction by applying various numerical methods - Correlation of theoretical and computational data with experimental ones - Communicating complex scientific ideas, the conclusions of experiments or the results of a scientific project. - Ability to obtain and support scientifically argued results; ability to develop scientific papers. - Use of scientific methods and models in narrow or interdisciplinary fields. - Advanced ability to plan and organize. - Operation with the principles of digital image data processing. Ability to analyze and synthesize data; the ability to model the effect of external factors on images. - Use and adaptation of software packages for data analysis and processing. Use of automated computer systems for processing and extracting data from 2D and 3D digital images, respectively. - Carrying out data processing experiments and evaluating their results based on existing theoretical models. Multi- and interdisciplinary way of thinking through biomedical applications.
Transversal competencies	- Modeling and analysis skills in an interdisciplinary context. - Competences in using high performance computing technology. - Carrying out professional tasks efficiently and responsibly, in compliance with the legislation and field-specific deontology. - The application, in the context of compliance with the legislation, of intellectual property rights (including technology transfer), of the product certification methodology, of the principles, norms and values of the code of professional ethics within its own rigorous, efficient and responsible work strategy. - Application of efficient work techniques in multidisciplinary team on various levels hierarchical. Identify roles and responsibilities in a team and apply techniques effective relationships and work within the team. - Efficient use of information sources and communication and training resources professional, both in Romanian and English. - Demonstrate involvement in scientific activities, such as the development of specialized articles and studies. - To participate in scientific projects, compatible with the requirements of integration in European education and research.

7. Course objectives (based on the acquired competencies grid)

7.1 The general objective of the discipline	- Learning physical models and advanced numerical methods used to simulate the structural and dynamic properties of atomic and molecular systems.
7.2 Specific objectives	- Developing of an algorithmic way of thinking, specific to numerical simulations. - Acquiring the ability to use advanced numerical methods and algorithms in complex simulation projects in the fields of computational physics, physical chemistry, materials science and biophysics. - Familiarization of doctoral students with the most used models of statistical and computational physics in interdisciplinary applications. - Encourage interdisciplinary research. - Learning the principles, methods and computational techniques for calculating different molecular properties. - Efficient use of computational resources for molecular modeling. - Training in the skills of calculation and analysis of atomic and molecular properties and digital information.

8. Content

8.1 Lectures	**Teaching methods**	**Comments**
1. Advanced molecular dynamics. Atomic and coarse-graining force fields. Propagators and reservoirs. Simulations in different statistical sets. Modern implementations of the Ewald sum method for electrostatic interactions.	Lecture, demonstration, debate, the experiment demonstration, presentations on the computer, case studies	2.5 hours
2. Models and fundamentals in the use of NAMD and Gromacs codes. Trajectory analysis. Applications of molecular dynamics in the biomolecular field and materials science.		2 hours
3. Analysis of the conformational space of molecules and modeling of ligand-receptor interactions. Simulation of experimental spectra based on relative Boltzmann populations.		1.5 hours
4. Modeling of weak intermolecular interactions: the role of dispersion in weakly bound molecular systems; Modeling of host-guest systems; Modeling the adsorption of molecules on surfaces.		1.5 hours
5. Calculation of photophysical parameters of molecular systems: modeling of electronic absorption and fluorescence emission spectra; calculation of radiative fluorescence lifetime.		1.5 hours
6. Theoretical models in the physics of atomic collisions: classification, areas of use.		1.5 hours
7. Ionization of atoms and molecules by charged particles; interference effects.		2 hours
8. Ionization of atoms by intense laser fields. Photoelectron holography.		2 hours

9. Basic analytical models of statistical physics with interdisciplinary applications: Ising model, Kuramoto model, percolation model, simple randomness model, masters equations.		2.5 hours
10. Basic computational models with interdisciplinary applications: Vicsek's "flocking" model, sandpile model, restricted randomness, percolations with geometric objects.		2 hours
11. Digital image data processing. Theoretical methods for improving and analyzing digital image data. Filters and automatic and semi-automatic 2D data processing modes. Biomedical applications: data processing such as 2D images obtained with a fluorescence microscope, respectively 2D images obtained by cardiac MRI.		2.5 hours
12. Techniques for simulating the effect of noise on the results of digital image data analysis. Automatic and semi-automatic operations and processes for 3D data processing. Biomedical applications: data processing such as 3D images obtained with a fluorescence microscope, respectively 3D images obtained by pulmonary CT.		2.5 hours
1.		
8.2 Seminars / laboratory classes	Teaching methods	Comments
1. Tutorial on using the NAMD code to simulate ubiquitin. Preparation of the molecular model and input files.	Projection, demonstration, modeling, debate	1.5 hours
2. Tutorial on using the NAMD code to simulate ubiquitin. Trajectory analysis.		1 hour
3. Optimization of fluorodeoxyglucose molecule conformations and calculation of the IR spectrum of the molecule, mediated by relative Boltzmann populations.		0.5 hours
4. Modeling the adsorption of the adenine molecule on a graphene model surface. Interaction energy calculation and BSSE correction.		0.5 hours
5. Calculation of the electronic transitions (absorption and fluorescence emission) spectrum for the solvated aldehyde molecule using the "state specific" approach.		0.5 hours
6. Current applications of models in the physics of atomic collisions.		1 hour
7. Analytical calculations for the discussed models. Mean-field methods. Langevin and Fokker-Planck equations.		1 hour
8. Computational simulation codes for the discussed models. Discussion of simple programs written in C.		0.5 hours
9. Advanced methods of 2D data processing.		1 hours
10. Automated image segmentation techniques: methods for extracting and characterizing the heart from 2D cardiac MRI acquisitions, respectively from the contours of cells and objects of interest from 2D fluorescence microscopy images.		0.5 hours
Case studies prepared with the doctoral students, based on		4

their individual doctoral research topics		

Bibliography

1. D. C. Rapaport, "The Art of Molecular Dynamics Simulation" (Cambridge, 2010).
2. T. A. Beu, "Molecular dynamics simulations", http://phys.ubbcluj.ro/~tbeu/courses.htm
3. NAMD – Scalable Molecular Dynamics, http://www.ks.uiuc.edu/Research/namd/
4. Martini Coarse Grain Force Field for Biomolecules, http://cgmartini.nl/
5. Aron J. Cohen, Paula Mori-Sanchez, and Weitao Yang, Challenges for Density Functional Theory, Chem. Rev., 112 (2012) 289-320.
6. P. Lazar, F. Karlický, P. Jurečka, M. Kocman, E. Otyepková, K. Šafářová, M. Otyepka, Adsorption of Small Organic Molecules on Graphene, J. Am. Chem. Soc. 2013, 135, 6372−6377, DOI: dx.doi.org/10.1021/ja403162r
7. E. Vinteler, N.-F. Stan, R. Luchian, C. Cainap, J.P. Prates-Ramalho, V. Chis, Conformational landscape and low lying excited states of imatinib, Journal of Molecular Modeling, 21 (2015) 84, DOI: 10.1007/s00894-015-2639-8
8. M. Oltean, G.S. Mile, M. Vidrighin, N. Leopold, V. Chis , Weakly bound PTCDI and PTCDA dimers studied by using MP2 and DFT methods with dispersion correction, Physical Chemistry Chemical Physics, 15 (2013) 13978-13990, DOI: 10.1039/C3CP44644A
9. R.-A. Domokos, M. Potara, S. Aştilean, V. Chiş, Adsorption of Trans- and cis-Resveratrol on Graphene, Physica Status Solidi B, 256 (2018) 1800335, DOI: 10.1002/pssb.201800335
10. M. Savarese, A. Aliberti, D. De Santo, E. Battista, F. Causa, P.A. Netti, N. Rega, Fluorescence Lifetimes and Quantum Yields of Rhodamine Derivatives: New Insights from Theory and Experiment, J. Phys. Chem. A, 2012, 116, 7491-7497, DOI: dx.doi.org/101021/jp30214851
11. L. Nagy, Multi-electron processes in atomic collisions – Theory, Nucl. Instr. Meth B154 (1999) 23-130.
12. L. Nagy, L. Kocbach, K Póra and J.P. Hansen, Interference effects in the ionization of H2 by fast charged projectiles, J Phys. B 35 (2002) L453-L459.
13. S. Borbely, A Toth, K, Tokesi and L. Nagy, Spatial and temporal interference during the ionization of H by few-cycle XUV laser pulses, Phys. Rev. A 87 (2013) 013405.
14. Photoelectron holography of atomic targets, S. Borbély, A. Tóth, D. G. Arbó, K. Tőkési and **L.** Nagy, Phys. Rev. A 99 (2019) 013413.
15. R. Baxer, Exactly Solved Models in Statistical Mechanics (Dover Books, 2008)
16. H. Gould, J. Tobochnik and W. Christian, Computer Simulation Methods (Addison-Wesley, 2006)
17. Advanced image Processing Techniques and Applications - N. Suresh Kumar, A. Kumar Sangaiah, M. Arun, S. Anand, ISBN-13: 978-1522520535. IGI Global 2017.
18. Digital Image Processing – W. Burger, M.J. Burge - Springer 2008 - ISBN 978-1-84628-379-6 - https://imagingbook.files.wordpress.com/2013/06/ burgerburgeen20071104_ijreference_letter.pdf
19. NAMD – Scalable Molecular Dynamics, http://www.ks.uiuc.edu/Research/namd/
20. P. Geerlings, F. De Proft, W. Langenaeker, Conceptual Density Functional Theory, , Chem. Rev., 103, 1793-1873, (2003)
21. J.B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd edition, 2015, http://expchem3.com/
22. L. Czipa and L. Nagy, Two-center interference in the ionization of H2 by ion impact: Comparison of different models, Phys. Rev. A 95 (2017) 062709
23. L. Nagy, F. Járai-Szabó and S. Borbély, The effect of projectile wave packet width on the fully differential ionization cross-sections, J. Phys. B: At. Mol. Opt. Phys. 51 (2018) 144005.
24. C. Gross, Complex and Adaptive Dynamical Systems (Springer, 2008)
25. Z. Neda, Introduction to Stochastic Simulation Methods,

http://www.phys.ubbcluj.ro/~zneda/edu/mc.htm
26. Platform ImageJ: http://imagej.net/Introduction
27. Platform ZEN: https://www.zeiss.com/microscopy/int/products/microscope-software/zen-lite.html

9. Alining the contents of the discipline with the expectations of the epistemic community, representatives, professional associations and standard employers operating in the program field

The content of the discipline is in line with what is studied in other university centers in the country and abroad. In order to adapt to the requirements imposed by the labor market, the content of the discipline was harmonized with the requirements imposed by the specifics of postgraduate education, research institutes and the business environment.

10. Examination

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight in the final grade
10.4 Lectures	Assessment of knowledge	Written exam	25%
	Assessment of knowledge	Ongoing tests	25%
10.5 Seminars / laboratory classes	Activity during seminars	Discussions, answers to questions	25%
	Assessment of knowledge	Written exam	25%
10.6 Minimum performance standard			
Correct assessment of methods and models to be used to solve a particular problem. Proper use of computational techniques and available hardware and software resources.			

Signature of course coordinator	Signature of seminar coordinator
Prof. dr. Titus Beu	Prof. dr. Titus Beu
Prof. dr. Vasile Chiş	Prof. dr. Vasile Chiş
Prof. dr. Ladislau Nagy	Prof. dr. Ladislau Nagy
Prof. dr. Zoltan Neda	Prof. dr. Zoltan Neda
Conf. dr. Zoltan Balint	Conf. dr. Zoltan Balint

Date	Signature Head of department
21.09.2021	Prof. dr. Simion Aştilean

Date of approval by the doctoral school council
08.10.2021