SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babeș-Bolyai University**
1.2 Faculty	**Physics**
1.3 Department	**Physics**
1.4 Field of study	**Physics**
1.5 Study cycle	**Master**
1.6 Study programme / Qualification	**Common course for all master programmes / Physicist**

2. Information regarding the discipline

2.1 Name of the discipline	**Advanced atomic and molecular physics**						
2.2 Course coordinator	**Ladislau Nagy / Vasile Chiș**						
2.3 Seminar coordinator	**Ladislau Nagy / Vasile Chiș**						
2.4. Year of study	**1**	2.5 Semester	**1**	2.6. Type of evaluation	**E**	2.7 Type of discipline	**Fundamental**

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	3	Of which: 3.2 course	2	3.3 seminar/laboratory	1
3.4 Total hours in the curriculum	52	Of which: 3.5 course	28	3.6 seminar/laboratory	14

Time allotment:	hours
Learning using manual, course support, bibliography, course notes	16
Additional documentation (in libraries, on electronic platforms, field documentation)	16
Preparation for seminars/labs, homework, papers, portfolios and essays	32
Tutorship	4
Evaluations	
Other activities:	

3.7 Total individual study hours	68
3.8 Total hours per semester	120
3.9 Number of ECTS credits	6

4. Prerequisites (if necessary)

4.1. curriculum	• quantum mechanics, basic atomic and molecular physics
4.2. competencies	• quantum mechanics, basic atomic and molecular physics

5. Conditions (if necessary)

5.1. for the course	•
5.2. for the seminar /lab activities	•

6. Specific competencies acquired

Professional competencies	• *Using in-depth knowledge of physics, mathematics, and programming in various multi- and inter-disciplinary fields.* • *Applying atomic and molecular physics to understand of complex scientific phenomena.* • *Making effective use of in-depth knowledge of physics and mathematics in solving real problems in atomic and molecular physics* • *Using advanced information technology and electronic communication in order to analyse, model, simulate, and aggregate data from various branches of physics or other related fields.* • *Solving advanced problems of atomic and molecular physics by means of field-related mathematical and computer instruments (analytical, numerical, or statistical tools).* • *Communicating complex scientific ideas, experiments or outcomes of a scientific project.*
Transversal competencies	• *Implementing the values and ethics of the scientific research profession, carrying out professional tasks in a responsible manner in autonomous conditions, as well as making decisions based on assessment and self assessment.* • *Carrying out teamwork activities and assuming specific roles at various hierarchical levels, demonstrating initiative and entrepreneurial spirit, as well as leadership in promoting dialogue, cooperation, positive attitudes, mutual respect, diversity, and multiculturalism and a constant preoccupation for continuous self improvement.* • *Objective self evaluation of professional and continuous training needs to enable labour market insertion and adaptability to changing market demands, as well as for personal and professional development to ensure effective use of multilingual abilities and IT & communication knowledge.*

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• The students should acquire basic knowledge about the quantum-mechanical treatment of the atoms and molecules.
7.2 Specific objective of the discipline	• They should be able to use the variational and perturbational methods in order to discuss the structure, energy and wavefunctions of the multielectron atoms, the relativistic effects (spin-orbit interaction), and the Zeeman and Stark effects. Students should have the basic knowledge also on group theory, molecular symmetry, group representation, projection operators, direct products and the application of these concepts for analysing the hybridization of atomic orbitals, identifying the symmetry species of normal modes of vibration, electronic states of molecules, and calculation of molecular wavefunctions.

8. Content

8.1 Course	Teaching methods	Remarks
1. The hydrogen atom. Nonrelativistic treatment.	Presentation, interactive methods	
2. Relativistic treatment. Perturbational approximation of spin-orbit interaction. Fine structure. The Lamb shift. Hyperfine structure		
3. The helium atom. Ortho and parahelium		
4. Calculating the energy levels and wavefunctions of the helium using the variational and perturbational methods. The Hartree method.		
5. Multielectron atoms. The Hartree-Fock method.		
6. The atoms in magnetic field. The normal and anomal Zeeman effect. The Paschen-Back effect.		
7. The atoms in electric field. The Stark effect for the hydrogen (linear) and for multielectron atoms (quadratic)		
8. Molecular symmetry. Groups – fundamental properties. Classes. Properties of conjugate elements		
9. Symmetry point groups. Symmetry and physical-chemical properties. Group representation		
10. Bases of representations. Types of representations. Equivalent representations		
11. Characters of representations and their properties. Reducible and irreducible representations. Reduction of reducible representations		
12. Character tables. Correlation tables. Descent symmetry. Representations of continuous groups		
13. Projection operators. Symmetry-adapted combinations of atomic orbitals		
14. Direct products of representations. Vanishing integrals.		
Bibliography 1. H. Haken, H.C. Wolf, The Physics of atoms and Quanta, Ed. Springer-Verbag, Berlin, New York, 1996 2. W. Demtroder, Atoms, Molecules and Photons, Springer, 2006 3. B. M. Bransden, C. J. Joachain, Fizica atomului şi moleculei. Ed. Tehnică, Bucureşti, 1998		

4. C. J. Ballhausen, H.B. Gray, Molecular Orbital Theory, Ed. W. A. Benjamin Inc., New York, 1965 5. V. Chiş, O. Cozar, L. David, Simetrie moleculară, Ed. Napoca Star, Cluj-Napoca, 2007 6. A. Hernanz, Metodos teoricos de la quimica fisica, vol. 2, Ed. R. G. Blanca, Madrid, 1991 7. D.A. McQuarrie, J.D. Simon, Physical Chemistry, A Molecular Approach, University Science Books, Sausalito, 1997 8. Atkins's Physical Chemistry, 11-th edition, Peter Atkins, Julio de Paula, James Keeler, Oxford University Press, 2017. 9. P.W. Atkins, Molecular Quantum Mechanics 5-th edition, Oxford University Press, 2011		
8.2 Seminar / Laboratory	Teaching methods	Remarks
1. The hydrogen atom	Problem solving	
2. Multielectron atoms	Problem solving	
3. The atom in magnetic field	Problem solving	
4. Symmetry point groups; classes; equivalent atoms; chemical properties of molecules	Problem solving	
5. Symmetry species for normal modes; Hybridization schemes of atomic orbitals	Problem solving	
6. Projection operators; symmetry-adapted linear combinations of atomic orbitals	Problem solving	
7. Direct products; Determining new bases for representations; Vanishing integrals; Selection rules	Problem solving	
Bibliography 1. H. Haken, H.C. Wolf, The Physics of atoms and Quanta, Ed. Springer-Verbag, Berlin, New York, 1996 2. W. Demtroder, Atoms, Molecules and Photons, Springer, 2006 3. B. M. Bransden, C. J. Joachain, Fizica atomului şi moleculei. Ed. Tehnică, Bucureşti, 1998 4. V. Chiş, O. Cozar, L. David, Simetrie moleculară, Ed. Napoca Star, Cluj-Napoca, 2007 5. A. Hernanz, Metodos teoricos de la quimica fisica, vol. 2, Ed. R. G. Blanca, Madrid, 1991 6. D.A. McQuarrie, J.D. Simon, Physical Chemistry, A Molecular Approach, University Science Books, Sausalito, 1997 7. Atkins's Physical Chemistry, 11-th edition, Peter Atkins, Julio de Paula, James Keeler, Oxford University Press, 2017. 8. P.W. Atkins, Molecular Quantum Mechanics 5-th edition, Oxford University Press, 2011 9. P.W. Atkins, Solutions Manual for Molecular Quantum Mechanics, Oxford University Press, 1983.		

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

Course content is consistent with master classes in atomic and molecular in other universities at home and abroad. To adapt to the requirements of the labor market, the content was adjusted to the specific requirements of master level education, research institutes and businesses media.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Knowledge, understanding and capacity of application of atomic structure (atomic physics).	Oral exam	25
	Molecular physics	Written exam	50
10.5 Seminar/lab activities	Homework, activity (atomic physics)	Problem solving	25
10.6 Minimum performance standards			
➢ At least grade 5 (from a scale of 1 to 10) for all evaluations ➢			

Date

30.06.2023

Signature of course coordinator

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Signature of seminar coordinator

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Date of approval

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Signature of the head of department

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