SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babes-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 semester of all master programmes**

2. Information regarding the discipline

2.1 Name of the discipline	**Advanced atomic and molecular physics**						
2.2 Course coordinator	**Ladislau Nagy/ Leontin David**						
2.3 Seminar coordinator	**Ladislau Nagy/ Leontin David**						
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		Of which: 3.5 course		3.6 seminar/laboratory	

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

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

4. Prerequisites (if necessary)

4.1. curriculum	•
4.2. competencies	•

5. Conditions (if necessary)

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

6. Specific competencies acquired

Professional competencies	
Transversal competencies	

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 quantummechanical 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, and the application of these in the hybridization of atomic orbitals, the splitting of degenerated atomic levels in crystal fields of different symmetry, electron states in diatomic molecules, and calculation of molecular wavefunctions

8. Content

8.1 Course	Teaching methods	Remarks
The hydrogen atom. Nonrelativistic and relativistic treatment.		
Perturbational treatment of spin-orbit interaction. Fine structure. The Lamb shift. Hyperfine structure		
The helium atom. Ortho and parahelium		
Calculating the energy levels and wavefunctions of the helium using the variational and perturbational methods. The Hartree method.		
Multielectron atoms. The Hartree-Fock method.		
The atoms in magnetic field. The normal and anomal Zeeman effect. The Paschen-Back effect. Electron Spin Resonance		
The atoms in electric field. The Stark effect for the		

hydrogen (linear) and for multielectron atoms (square)		
Elements of group theory. Symmetry operations and elements in molecules. Symmetry groups. Equivalent atoms		
The representation of groups. Character tables. Irreducible representations.		
Atomic and molecular wavefunctions as basis of irreducible representations. Electron configurations for diatomic molecules N_2, O_2, NO, CO.		
Electronic states and spectral terms for diatomic molecules. Selection rules.		
The hybridization of atomic orbitals. σ hybridization schemes. The calculation of the coefficients		
The LCAO-MO method for polyatomic molecules. π approximation. The Hückel method, self-consistent field method (SCF-MO) and Pariser-Parr-Pople (PPP)		
The use of molecular symmetry properties in the calculation of molecular orbitals. Projection operators. Symmetrized wavefunctions.		

Bibliography

1. H. Haken, H.C. Wolf, The Physics of atoms and Quanta, Ed. Springer-Verbag, Berlin, New York, 1996
2. B. M. Bransden, C. J. Joachain, Fizica atomului şi moleculei. Ed. Tehnică, Bucureşti, 1998
3. T. Crețu, St. Tudorache, Fizica atomului, Ed.Ştiintifică şi Enciclopedică, Bucureşti, 1985
4. V. Malinovschi, I.Ştefănescu, Fizică atomică, Ed.Conphys, Rm. Vâlcea, 2001
5. C. Cosma, C.Simuț, Elemente de fizică atomică. Aplicații, Ed. Univ., Oradea, 2001
6. C. J. Ballhausen, H.B. Gray, Molecular Orbital Theory, Ed. W. A. Benjamin Inc., New York, 1965
7. O. Cozar, Teoria grupurilor în fizica atomului şi moleculei, Ed. U.B.B., Cluj-Napoca, 1986
8. A. Hernanz, Metodos teoricos de la quimica fisica, vol. 2, Ed. R. G. Blanca, Madrid, 1991
9. F. L. Pilar, Elementary Quantum Chemistry, Ed. McGraw-Hill B.C., New York, 1968
10. O. Cozar, V. Grecu, V. Znamirovschi, Rezonanța electronica de spin pe complecşi metalici, Ed. Acad., Bucureşti, 2001
11. L. David, O. Cozar, C. Crăciun, V. Chiş, Rezonanța electronica de spin, Ed. Presa Universitară Clujeană 2001

8.2 Seminar / laboratory	Teaching methods	Remarks
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Bibliography		

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

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10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Knowlidge, 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			
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Date	Signature of course coordinator	Signature of seminar coordinator
..30.09.2013………..	....	....

Date of approval	Signature of the head of department
....	...........….............................