"Babeş-Bolyai" University, Cluj-Napoca
Faculty of Physics, Department of Biomedical Physics
Academic Year 2012/2013
1st Semester

SYLLABUS

I. General information about the course

Discipline: Complements of atomic and molecular physics
Year of study: I (1st sem.)
Code: FMS0002
No of credits: 5
No hours /week: 2 course + 1 laboratory
Place: Aula „Victor Marian"
Schedule: Thursday 16-18

II. Information about the instructor

Name: Ladislau Nagy, Leontin David
Position: professor
Degree: PhD
E-mail: lnagy@phys.ubbcluj.ro
Phone: 405300 ext 5107 (Nagy)
Personal contact: Friday 10-12

III. Objectives and competences

Objectives:
The students should acquire basic knowledge about the quantummechanical treatment of the atoms and molecules. 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
Competences:
The students should have the skills to use the basic approximation methods (variational and perturbational) to calculate the wavefunctions and energy levels in multielectron atoms and molecules. They should understand and be able to use a series of experimental techniques (IR, Raman, ESR, NMR) used in the study of crystalline and nanostructured materials, magnetic and superconducting materials, complex molecules of biomedical interest etc.

IV. 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. Creţu, 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.Simuţ, Elemente de fizică atomică. Aplicaţii, 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, Rezonanţa electronica de spin pe complecşi metalici, Ed. Acad., Bucureşti, 2001
11. L. David, O. Cozar, C. Crăciun, V. Chiş, Rezonanţa electronica de spin, Ed. Presa Universitară Clujeană 2001

V. Used equipment:

a) at course: multimedia projector
b) at laboratory: the equipment of the atomic and molecular physics laboratory

VI. The detailed schedule of the courses, laboratory works and examination

V. a. COURSE

No	Topic	Hours	Bibliography
1.	The hydrogen atom. Nonrelativistic and relativistic treatment.	2	[1]: 243-249; 271-278 [3]: 164-183
2.	Perturbational treatment of spin-orbit interaction. Fine structure. The Lamb shift. Hyperfine structure	2	[1]: 347-360 [4]: 162-168 [5]: 214-221
3.	The helium atom. Ortho and parahelium	2	[1]: 297-307 [5]: 221-232
4.	Calculating the energy levels and wavefunctions of the helium using the variational and perturbational methods. The Hartree method.	2	[2] 292-336
5.	Multielectron atoms. The Hartree-Fock method.	2	[1]: 335-343 [2]: 338-394 [9]: 341-384
6.	The atoms in magnetic field. The normal and anomal Zeeman effect. The Paschen-Back effect. Electron Spin Resonance	2	[1]: 205-220 [2]: 233-246 [3]: 324-358
7.	The atoms in electric field. The Stark effect for the hydrogen (linear) and for multielectron atoms (quadratic)	2	[1]: 251-260 [2]: 259-270 [7]: 152-176
8.	Elements of group theory. Symmetry operations and elements in molecules. Symmetry groups. Equivalent atoms	2	[7]: 1-48 [8]: 19-94
9.	The representation of groups. Character tables. Irreducible representations.	2	[7]: 49-106 [8]: 121-204

10.	Atomic and molecular wavefunctions as basis of irreducible representations. Electron configurations for diatomic molecules N_2, O_2, NO, CO.	2	[7]: 112-144 [8]: 235-292
11.	Electronic states and spectral terms for diatomic molecules. Selection rules.	2	[6]: 73-115
12.	The hybridization of atomic orbitals. σ hybridization schemes. The calculation of the coefficients	2	[7]: 184-208 [8]: 293-330
13.	The LCAO-MO method for polyatomic molecules. π approximation. The Hückel method, self-consistent field method (SCF-MO) and Pariser-Parr-Pople (PPP)	2	[9]: 523-607 668-690
14.	The use of molecular symmetry properties in the calculation of molecular orbitals. Projection operators. Symmetrized wavefunctions.	2	[7]: 212-258

VI. c. Laboratory work

No	Topic	Hours	Bibliography
1.	Determination of ionization potentials of atoms by mass spectrometry. Comparison with calculation results.	2	[9]: 341-384
2.	Observation and interpretation of the helium spectrum. Identification of ortho and para lines.	2	[1]: 297-307
3.	The study of the Zeeman effect. Determination of effective spin from fine structure ESR spectra.	2	[1]: 271-278 [10]: 146-164
4.	The analyze of hyperfine structures in ESR spectra. Hyperfine tensors for complex ions and molecules.	2	[10]: 64-96 [11]: 114-145
5.	Mass spectrometry study of the fragmentation of organic molecules and their interpretation on the basis of LCAO-MO calculations.	2	[9]: 523-607; 668-690
6.	Determination of d-d transitions in UV-VIS spectra of molecular complexes of different symmetries (Oh, D_4h, C_4v) and their comparison with LCAO-MO calculation results.	2	[10]: 81-102; 155-169
7.	Determination of MO coefficients from ESR and optical data for metallic complexes with axial and rhombic symmetry.	2	[10]: 121-145

VII. Evaluation method

- 25% problem solving (atomic physics);
- 25% oral exam (atomic physics);
- 50% written exam (molecular physics);

Date,
30.09.2013

Signature,