SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babes-Bolyai University
1.2 Faculty	Physics
1.3 Department	Department of solid state physics and advanced technologies
1.4 Field of study	Physics
1.5 Study cycle	Master of Science
1.6 Study programme / Qualification	MSc./Solid State Physics

2. Information regarding the discipline

2.1 Name of the discipline	Ab initio computational methods in solids						
2.2							
2.3 Laboratory coordinator	Diana Benea, Scientific researcher Dr.						
2.4. Year of study	**MSc. 2**	2.5 Semester	**II**	2.6. Type of evaluation	**C**	2.7 Type of discipline	**DC**

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

3.1 Hours per week	3	Of which: 3.2 course	0	3.3 seminar/laboratory	3
3.4 Total hours in the curriculum	42	Of which: 3.5 course	0	3.6 seminar/laboratory	42
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					32
Additional documentation (in libraries, on electronic platforms, field documentation)					64
Preparation for seminars/labs, homework, papers, portfolios and essays					30
Tutorship					7
Evaluations					3
Other activities:					

3.7 Total individual study hours	126
3.8 Total hours per semester	126
3.9 Number of ECTS credits	3

4. Prerequisites (if necessary)

4.1. curriculum	• Solid State and semiconductor Physics • Quantum Physics • Statistical Physics
4.2. competencies	• Knowledge related to computer operation, use of programs for editing and for graphical representation

5. Conditions (if necessary)

5.1. for the labs	•

5.2. for the seminar /lab activities	• Computer + beamer for practical demonstrations • Seminar hall with computers + programs installed

6. Specific competencies acquired

Professional competencies	• The use of theoretical concept of the solid-state physics. • The use of computer codes to determine the properties of solids • Critical/constructive analysis of the results by using advanced models/theories.
Transversal competencies	• Search and identification of the advanced formation opportunities and effective exploitation of learning techniques for the own development.

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

7.1 General objective of the discipline	This discipline uses the knowledge aquired in the (Advanced) Solid State Physics and (based on the theoretical ab initio methods) allows to determine main electronic and magnetic properties of solids. It will develop the basic knowledge underlining the relationship between the crystal structure and the electronic properties of solids. The laboratory work will provide the basis for the theoretical description of solids, allowing the comparison with the main experimental methods used in our laboratory.
7.2 Specific objective of the discipline	• the students will be able to initiate modern research work, by combining the theoretical and experimental methods of investigation in the solid state physics. • the students will be able to characterize the solids from electronic and magnetic points of view. • the students will also be able to find the correlations between the chemical/crystal structure and the electronic properties of solids.

8. Content

8.2 Seminar/Laboratory	Teaching methods	Remarks
Each student will learn to use the SPRKKR program and the XBAND interface to perform band structure calculations for the themes described in the lectures. The laboratory consist in band structure calculations for the proposed subjects.		
Linux tutorial (commands, editing programs, programs for graphical representation)	Demonstration, didactic modelling, e-	3 hours
Introduction.Density functional theory. Principles. Kohn-		6 hours

Sham equations. Local density approximation.	learning	
Electronic structure of solids. One electron model. Multiple scattering theory (Korringa-Kohn-Rostocker). Green functions. Calculation of observables. Self-consistent calculations for metals and alloys (for ex. Fe, FeCo and $Fe_{0.5}Co_{0.5}$)		6 hours
Self-consistent calculations for compounds with many atoms in the unit cell (for ex. Mn_2VAl and CrAs)		3 hours
Density of states. Density of states calculations for selected systems.		3 hours
Dispersion relation. Bloch spectral functions Dispersion relation calculations for selected systems, along different paths. Bloch spectral function calculations for the alloys		3 hours
Photoemission. Calculation of the valence-band photoemission spectra for several metals and alloys.		6 hours
Heisenberg model for exchange coupling. Calculation of the exchange-coupling parameters for several magnetic materials. Stability of spin structures.		3 hours
X-ray absorption (XAS). X-ray circular dichroism in absorption spectra. Calculation of the XAS spectra for several metals and alloys.		3 hours
Equilibrium lattice constants. Magnetic moments vs. lattice constants dependence. Atomic substitutions and prefferential site occupation.		6 hours

Bibliography

1. C. Kittel, Introduction to Solid State Physics (7ed., Wiley, 1996)
2. N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, Saunders, 1976.
3. SPRKKR manual – H. Ebert , LMU Munich 2017 (http://ebert.cup.uni-muenchen.de)
4. Structura electronica de benzi cu aplicatii in solide, D. Benea 2014 (lucrari de laborator).
5. P. Strange, *Relativistic Quantum Mechanics* (Cambridge University Press, 1998).
6. H. Ebert, J. Minar, and D. Kodderitzsch, Rep. Prog. Phys. **74**, 096501 (2011).
7. A. I. Liechtenstein,M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, J.Magn.Magn. Materials **67**, 65 (1987).
8. Introduction to photoemission spectroscopy, M. Singh, Univ. Wuerzburg, https://www.cond-mat.de/events/correl14/manuscripts/sing.pdf
9. James E Penner- Hahn, , X-Ray Absorption Spectroscopy, Willey 2005 https://doi.org/10.1038/npg.els.0002984
10. C.S. Schnohr and M.C. Ridgway, X-Ray Absorption Spectroscopy of Semiconductors, Springer Series in Optical Sciences 190, DOI 10.1007/978-3-662-44362-0_1

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

- The content of the course is congruent to the similar matter studied in representative European and national universities. In order to better adapt to the work market requirements, the content of the course was related with the main trends from this field in the regional scientific research, industry and business environment.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Courses	-	-	-
10.5 Seminar/lab activities	-ability to use the computer programs to generate the requested solids properties -correct interpretation of the results	Colloquium consists of computational projects (selected tasks). Time for solving the tasks: 3 h	50 %
	criteria related to the dutifulness, the interest for individual study.	Active presence at labs. Projects.	50 %
10.6 Minimum performance standards			
➢ basic elements of theory/computational skills are requested. A candidate shall be declared to have passed the examination in a subject of study only if he/she secures not less than 50% of the total marks.			

Date | Signature of discipline coordinator | Signature of seminar coordinator

15.09.2021

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Date of approval | Signature of the head of department

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