

## Subject content

### 1. Program information

|                     |  |
|---------------------|--|
| 1.1 University      | West University of Timisoara                 |
| 1.2 Faculty         | Physics                                      |
| 1.3 Department      | Physics                                      |
| 1.4 Study direction | Physics                                      |
| 1.5 Study cycle     | Master                                       |
| 1.6 Study program   | Physics and technology of advanced materials |

### 2. Subject matter information

|                                  |   |                                     |   |                     |    |                  |              |
|----------------------------------|---|-------------------------------------|---|---------------------|----|------------------|--------------|
| 2.1 Subject matter               |   | Condensed Matter Spectroscopy       |   |                     |    |                  |              |
| 2.2 Subject teacher              |   | Associate Professor dr. Calin Avram |   |                     |    |                  |              |
| 2.3 Subject applications teacher |   | Associate Professor dr. Calin Avram |   |                     |    |                  |              |
| 2.4 Study year                   | 2 | 2.5 Semester                        | 3 | 2.6 Assessment type | Ex | 2.7 Subject type | Ob. PTAM2302 |

### 3. Study time distribution

|  |            |                      |    |             |              |
|--|------------|----------------------|----|-------------|--------------|
| 3.1 Nr. of hours/week  | 3          | In which: 3.2 course | 2  | 3.3 seminar | 1            |
| 3.4 Total hours in educational plan  | 42         | In which: 3.5 course | 28 | 3.6 seminar | 14           |
| <b>Time distribution:</b>  |            |                      |    |             | <b>hours</b> |
| Study after lecture notes, bibliography or notes                               |            |                      |    |             | 31           |
| Additional documentation in the library, electronic specialty platforms/ field |            |                      |    |             | 10           |
| Seminar / laboratory preparations, homework, portfolio and essays              |            |                      |    |             | 10           |
| Tutoring   |            |                      |    |             | 4            |
| Exams  |            |                      |    |             | 3            |
| Other activities.....  |            |                      |    |             |              |
| <b>3.7 Total number of personal study hour</b>                                 | <b>42</b>  |                      |    |             |              |
| <b>3.8 Total number of hours in semester</b>                                   | <b>100</b> |                      |    |             |              |
| <b>3.9 Number of credits</b>   | <b>6</b>   |                      |    |             |              |

#### 4. Preconditions (where appropriate)

|                |   |
|----------------|---|
| 4.1 curriculum | • |
| 4.2 skills     | • |

#### 5. Conditions (where appropriate)

|                     |   |
|---------------------|---|
| 5.1 for course      | • Physics of Atoms and Molecules; Quantum Mechanics; Solid State Physics; |
| 5.2 for seminar/lab | • Physics of Atoms and Molecules; Quantum Mechanics; Solid State Physics; |

#### 6. Specific skills gained

|                     |  |
|---------------------|--|
| Professional skills | <ul style="list-style-type: none"> <li>- Thorough knowledge and understanding of physical phenomena underlying the spectral methods to investigate condensed matter ;</li> <li>-Getting new deepening of professional skills closely related areas of undergraduate studies, and development capacity for scientific research in a world of knowledge.</li> <li>-Capacity of understanding, analyzing and description of the structure and basic interactions in condensed matter ;</li> <li>-Capacity of using models for transitional and rare-earth ions in crystals, ceramics and glasses;</li> <li>-Skills of standalone analysis and synthesis of complex systems and interactions between them;</li> <li>- Interpretation and correlations of the personal results with that of related professionals;</li> <li>- Skills on interpretation condensed state spectroscopy methods.</li> </ul> |
| Transversal skills  | <ul style="list-style-type: none"> <li>• Skills in research ethics</li> <li>• Skills in research project management</li> <li>• Team work in a research activity.</li> <li>• Efficient use of informational and communication resources in English language.</li> <li>• Improving investigation references;</li> </ul>  |

## 7. Course Objectives

|                         |  |
|-------------------------|--|
| 7.1 Main Objective      | <ul style="list-style-type: none"> <li>The main objective of this course is obtaining of new knowledge in the field of spectroscopy and use them to investigate condensed matter (undoped and doped crystals, nanocrystals, glasses, ceramics, etc.).</li> </ul>   |
| 7.2 Specific objectives | <ul style="list-style-type: none"> <li>Study interactions of the electromagnetic radiation with condensed matter in order to obtain information about structure and basic interactions in such systems;</li> <li>Modeling and simulation of spectral properties of systems with complex structure, forecasting this way of properties designated for the studied systems, especially for laser crystals doped with various impurity ions</li> <li>Use knowledge and skills acquired by graduates of this university master's program in order to access and continue their studies in the next cycle of initial training at the doctoral program;</li> </ul> |

## 8. Table of content

| 8.1 Course  | Teaching methods                                  | Observations  |
|---|---|---|
| 1. Spectroscopy of condensed matter. Introduction.                          | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 2. Spectra of many electron atoms   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 3. Symmetry in condensed matter physics. Symmetry operations.               | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 4. Symmetry groups.   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 5. Ions in anisotropic environment.   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 6. Single d-electron in a cubic field. 3d transition ions in crystal field. | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 7. General structure of a Hamiltonian of an ion in a crystal field.         | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 8. Many d-electrons in a crystal field and Tanabe-Sugano diagram.           | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |

|   |   |   |
|---|---|---|
| 9. Estimations of the crystal field strength $Dq$ and Racah parameters B, C from the experimental absorption spectra. Nephelauxetic effect. | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 10. Exchange charge model and superposition model of crystal field.   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 11. Adiabatic approximation and configurational coordinate model.   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 12. General picture of the Jahn-Teller effect.  | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 13. Spectroscopy of rare-earth ions doped in crystals.  | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |
| 14. Ab initio and DFT methods in condensed matter spectroscopy.   | Exposition, demonstration, heuristic conversation | Google Meet online conference, course support on e-mail |

### Bibliography

1. B. Henderson, R.H. Bartram, “*Crystal-Field Engineering of Solid-State Laser Materials*”, Cambridge University Press, Cambridge, 2000;
2. M.G. Brik, I. Sildos, V. Kiisk, “*Introduction in Spectroscopy of Atomic, Molecular and Crystals*”, Tartu, 2008
3. H. Kuzmany, “*Solid-State Spectroscopy*”, Springer, Berlin, 1998
4. D.R. Vij, “*Handbook of Applied Solid State Spectroscopy*, Springer, Heidelberg, 2006.
5. Feng Duan, Jin Goujun, “*Introduction to Condensed Matter Physics*”, Vol.1, World Scientific Publishing Co., Singapore, 2005

| 8.2 Seminar / labs  | Teaching methods                         | Observations                  |
|---|--|-------------------------------|
| 1. Introduction. Spectra of condensed matter.               | Conversation, investigation, case study. | Google Meet online conference |
| 2. Terms of many electron free atoms. Classifications.      | Conversation, investigation, case study. | Google Meet online conference |
| 3. Symmetry elements of molecules. Point group of symmetry. | Conversation, investigation, case study. | Google Meet online conference |
| 4. Symmetry of the crystals(I): Space group .               | Conversation, investigation, case study. | Google Meet online conference |
| 5. Symmetry of the crystals(II): Site symmetry group.       | Conversation, investigation, case study. | Google Meet online conference |
| 6. Classification of the electronic state using symmetry.   | Conversation, investigation, case study. | Google Meet online conference |

|  |  |                               |
|--|--|-------------------------------|
| 7. Calculation of Racah Parameters from absorption spectra                                       | Conversation, investigation, case study. | Google Meet online conference |
| 8. Modeling the crystal field parameters for $\text{Cr}^{3+}:\text{LiCaAlF}_6$ .                 | Conversation, investigation, case study. | Google Meet online conference |
| 9. Simulation of energy levels for $\text{Ni}^{2+}:\text{MgGa}_2\text{O}_4$ .                    | Conversation, investigation, case study. | Google Meet online conference |
| 10. Jahn-Teller effect in ${}^4\text{T}_{2g}$ excited states of $\text{V}^{2+}:\text{CsCaF}_3$ . | Conversation, investigation, case study. | Google Meet online conference |
| 11. Calculations of energy levels with CASSCF and NEVPT2 .                                       | Conversation, investigation, case study. | Google Meet online conference |
| 12. Modeling spin-Hamiltonian parameters in crystal field parameters.                            | Conversation, investigation, case study. | Google Meet online conference |
| 13 Modeling spin-Hamiltonian parameters  | Conversation, investigation, case study. | Google Meet online conference |
| 14. Modeling spin-Hamiltonian parameters with DFT methods.                                       | Dialogue                                 | Google Meet online conference |

### Bibliography

1. N.M. Avram, C.N. Avram, *"Nivelele energetice ale ionilor în cristale"*, Editura Mirton, Timișoara, 2001
2. M.G. Brik, N.M. Avram and C.N. Avram, „*Exchange charge model of crystal field for 3d ions* ” in N.M. Avram and M.G. Brik (Eds), *"Optical Properties of 3d-Ions in Crystals. Spectroscopy and Crystal Field Analysis"*, Tsinghua University Press, Beijing and Springer-Verlag, Berlin, Heidelberg, 2013.
3. D.R. Vij, *"Handbook of Applied Solid State Spectroscopy"*, Springer, Heidelberg, 2006.
4. Published papers by C.N. Avram.

### 9. Relation between subject content and the expectations of employers

Condensed Matter Spectroscopy gives work skills in domain topics and related topics in which the future graduate could work. Mainly are related to physics, chemistry, material science, etc.

### 10. Assessment

| Activity type | 10.1 Assessment criteria | 10.2 Assessment method | 10.3 Percent in final mark |
|---------------|--------------------------|------------------------|----------------------------|
|---------------|--------------------------|------------------------|----------------------------|

|   |  |                  |     |
|---|--|------------------|-----|
| 10.4 Course   | The assimilation level of knowledge gained | Oral examination | 60% |
| 10.5 Seminar / labs   | Capacity of solving specific problem       | Written test     | 40% |
| 10.6 Minimum performance standards  |  |                  |     |
| -To know the basic terminology<br>-To correct address three topics, even if they cannot develop completely;<br>-Do not make major mistakes. |  |                  |     |

Data  
completării:  
21.09.2020

Semnătura titularului de curs:  
Conf. dr. Călin Avram

Semnătura titularului de seminar/laborator:  
Conf. dr. Călin Avram

Semnătura directorului de departament:  
Lect. dr. Nicoleta Ștefu

