SYLLABUS

1. Information regarding the program

| 1.1 Higher education institution | Babeş-Bolyai University |
|-----------------------------------|----------------------------------|
| 1.2 Faculty | Faculty of Physics |
| 1.3 Department | Doctoral School of Physics |
| 1.4 Field of study | Physics |
| 1.5 Study cycle | Doctorate |
| 1.6 Study program / Qualification | Doctoral training/PhD in Physics |

2. Course data

| 2.1 Name of disc | ipli | ne | Applications of bio(nano)medical spectroscopy and imaging | | | | g |
|-----------------------------|------|-----------|---|---|---|------------|----|
| 2.2 Teacher responsible for | | | Pr | Prof.dr. Zoltan Balint, Prof.dr. Vasile Chiș, Conf.dr. Monica | | | |
| lectures | | | Focșan, Prof.dr. Nicolae Leopold | | | | |
| 2.3 Teacher resp | ons | sible for | Prof.dr. Zoltan Balint, Prof.dr. Vasile Chiş, Conf.dr. Monica | | | | |
| seminars | | | Focșan, Prof.dr. Nicolae Leopold | | | | |
| 2.4 Year of | I | 2.5 | I | 2.6 Type of | Е | 2.7 Course | DS |
| study | | Semester | | evaluation | | framework | |

3. Estimated total time of teaching activities (hours per semester)

| 3.1 Hours per week | 3 | Out of which: | 2 | 3.3 Seminars / | 1 |
|---|-----|---------------|----|--------------------|----|
| | | 3.2 Lectures | | Laboratory classes | |
| 3.4 Total hours in the curriculum | 36 | Out of which: | 24 | 3.6 Seminars / | 12 |
| | | 3.5 Lectures | | Laboratory classes | |
| Allocation of study time: | | | | | 89 |
| Study supported by textbooks, other course materials, recommended bibliography and | | | | 34 | |
| personal student notes | | | | | |
| Additional learning activities in the library, on specialized online platforms and in the field | | | | | 24 |
| Preparation of seminars/laboratory classes, topics, papers, portfolios and essays | | | | 15 | |
| Tutoring | | | | 12 | |
| Examinations | | | | 4 | |
| Other activities: - | | | | _ | |
| | 2.0 | | | | - |

| 3.9 Total individual study hours | 89 |
|----------------------------------|-----|
| 3.10 Total hours per semester | 125 |
| 3.11 Number of ECTS credits | 10 |

4. Prerequisites (if necessary)

| 4.1 Curriculum | Quantum mechanics, Statistical physics, Physics of atoms and molecules, |
|-----------------|---|
| | Numerical methods, Calculus, Algebra, Probability theory |
| 4.2 Competences | - computational skills for molecular modeling |
| | - skills in using programming environments and graphical applications |
| | - skills in using the research equipments |

5. Conditions (where applicable)

| 5.1 Conducting lectures | Course hall, appropriate board, projector, dedicated software, |
|--|--|
| | computer |
| 5.2 Conducting Course hall, appropriate board, projector, dedicated softw | |
| seminars/laboratory classes | computer network |

6. Specific competences acquired

- Acquiring advanced concepts and models of molecular modeling.
- Abilities to build molecular models and prepare input data for advanced numerical codes.
- Ability to select appropriate models and options for complex simulations.
- Correct use of quantum chemistry methods and appropriate models for calculating molecular properties
- Correlation of theoretical and computational data with experimental ones
- Communicating complex scientific ideas, the conclusions of experiments or the results of a scientific project.
- Ability to obtain and support scientifically argued results; ability to develop scientific papers.
- Use of scientific methods and models in narrow or interdisciplinary fields.
- Advanced ability to plan and organize.
- Operation with the principles of digital image data processing. Ability to analyze and synthesize data; the ability to model the effect of external factors on images.
- Use and adaptation of software packages for data analysis and processing. Use of automated computer systems for processing and extracting data from 2D and 3D digital images, respectively.
- Carrying out data processing experiments and evaluating their results based on existing theoretical models. Multi- and interdisciplinary way of thinking through biomedical applications.
- Modeling and analysis skills in an interdisciplinary context.
- Competences in using high performance computing technology.
- Carrying out professional tasks efficiently and responsibly, in compliance with the legislation and field-specific deontology.
- The application, in the context of compliance with the legislation, of intellectual property rights (including technology transfer), of the product certification methodology, of the principles, norms and values of the code of professional ethics within its own rigorous, efficient and responsible work strategy.
- Application of efficient work techniques in multidisciplinary team on various levels hierarchical. Identify roles and responsibilities in a team, apply techniques effective relationships, and work within the team.
- Efficient use of information sources and communication and training resources professional, both in Romanian and English.
- Demonstrate involvement in scientific activities, such as the development of specialized articles and studies.
- To participate in scientific projects, compatible with the requirements of integration in European education and research.

Transversal competencies

Professional competences

7.1 The general objective of the - Learning physical models and advanced computational discipline methods used to calculate spectroscopic properties of molecular systems. - Foster interdisciplinary collaboration between fields such as spectroscopy, and clinical biophysics, enhancing research that spans across physics, chemistry, and biomedical engineering. - Learning basic concepts and principles of fluorescence spectroscopy and imaging with particular emphasis on applications in nanotechnology, sensing and clinical diagnostic. - Learning interdisciplinary applications of biomedical image analysis for the development of integrated clinical decision support systems. 7.2 Specific objectives - Acquiring the ability to use advanced computational methods and algorithms in complex simulation projects in the fields of computational spectroscopy, physical chemistry. materials science, imaging and biophysics. - Familiarization of doctoral students with the most used models molecular models and methods in interdisciplinary applications. - Encourage interdisciplinary research. - Learning the principles, methods and computational techniques for calculating different molecular properties. - Efficient use of computational resources for molecular modeling. - knowledge of designing and utilizing nanostructured materials (such as metal nanoparticles) to amplify Raman scattering. -skills in interpreting Raman spectra from biological samples (such-acquiring knowledge in biomedical image analysis. -geting familiar with modern fluorescent techniques and equipment in biomedical research. - knowledge in single molecule fluorescence techniques and super resolution fluorescence imaging. - acquiring knowledge in biomedical image analysis. - insight into novel techniques for decision support tool development. - knowledge upon integrating various modalities in a decision pipeline. - getting familiar with novel, AI-algorithm based approaches for image segmentation, feature extraction, texture analysis

8. Content

| 8.1 Lectures | Teaching methods | Comments |
|---|------------------------|----------|
| 1. Digital image data processing. Theoretical methods for | Interactive lecture, | 2 hours |
| improving and analyzing digital image data. Filters for | Directed discussion, | |
| automatic and semi-automatic 2D data processing. | debate, Case-based | |
| Biomedical applications: data processing of 2D images | learning, Just-in-time | |
| obtained by a microscope, respectively 2D images | teaching | |
| obtained by MRI and CT. | | |

| | ı | T = 1 |
|--|------------------------------------|----------|
| 2. Techniques for simulating the effect of noise on the results of digital image data analysis. Automatic and semi-automatic operations and processes for 3D image data processing. Biomedical applications: data processing such as 3D images obtained with the microscope, respectively | | 2 hours |
| 3D images obtained by CT and MRI. 3. Decision support tools in medicine: Development of supervised and unsupervised algorithms for biomedical image segmentation using microscopy, CT and MRI as input. | | 2 hours |
| 4. Modeling weak intermolecular interactions: the role of dispersion in weakly bound molecular systems; Modeling of host-guest systems; Modeling the adsorption of molecules on surfaces. | | 2 hours |
| 5. Calculation of photophysical parameters of molecular systems: modeling of electronic absorption and fluorescence emission spectra; calculation of radiative fluorescence lifetime. | | 2 hours |
| 6. Introduction to fluorescence spectroscopy and imaging; Concept; Overview of fluorescence measurements and applications; Fluorescence Sensing | | 2 hours |
| 7. Fluorescence Lifetime Spectroscopy and Imaging Principles; Applications in biomedical diagnostics. Principles of Fluorescence Lifetime Instrumentation. Tissue Fluorescence Lifetime Spectroscopy. Tissue Fluorescence Lifetime Imaging - Endogenous. Fluorescence Lifetime Imaging - Exogenous Probes. | | 2 hours |
| 8. Plasmon-enhanced Fluorescence Spectroscopy and Imaging; Enhanced Fluorescence Sensing | | 2 hours |
| 9. Fluorescence super-resolution microscopy; Principles; Single Molecule Fluorescence Detection | | 2 hours |
| 10. Electrical and optical properties of materials | | 2 hours |
| 11. Surface-enhanced Raman scattering: Theory and applications | | 2 hours |
| 12. Clinical Raman Spectroscopy | | 2 hours |
| 8.2 Seminars / laboratory classes | Teaching methods | Comments |
| 1. Advanced methods of 2D image data processing. | Problem based | 1 hour |
| 2. Automated 2D image segmentation techniques: | learning, Project | 1 hour |
| characterizing cells and objects of interest from 2D | based learning, | 1 Hour |
| microscopy images with application in histology. | Inquiry guided | |
| 3. Medical decision support tools: methods for extraction and characterization of various organs and features from MRI acquisitions – from image segmentation to texture analysis. | learning, Experiential learning | 1 hour |
| 3D model preparation. | | |
| 4. Modeling the adsorption of molecules on a graphene model surface. Modeling the host-guest complexes. Interaction energy calculation and BSSE correction. | | 1 hour |
| | 1 | |

| 5. Calculation of the electronic transitions (absorption and | 1 hour |
|--|--------|
| fluorescence emission) spectrum for solvated molecules | |
| using the "state specific" approach. Calculation of the | |
| radiative lifetimes of solvated molecule | |
| 6. Instrumentation for fluorescence spectroscopy; | 1 hour |
| Spectrofluorometers used. | |
| 7. Analysis of Fluorescence Lifetime Data. | 1 hour |
| 8. Nanoplatforms for Metal Enhanced Fluorescence detection. | 1 hour |
| 9. Single molecule fluorescence detection. | 1 hour |
| 10. Electrical and optical properties of materials. Selected | 1 hour |
| examples | |
| 11. Experimental setups in surface-enhanced Raman | 1 hour |
| scattering | |
| 12. Assignment of biofluids SERS spectra | 1 hour |

Bibliography

- 1. Advanced image Processing Techniques and Applications N. Suresh Kumar, A. Kumar Sangaiah, M. Arun, S. Anand, ISBN-13: 978-1522520535. IGI Global 2017.
- 2. Digital Image Processing W. Burger, M.J. Burge Springer 2008 ISBN 978-1-84628-379-6 https://imagingbook.files.wordpress.com/2013/06/ burgerburgeen 2007 1104_ijreference_le tter.pdf
- 3. Platform ImageJ: http://imagej.net/Introduction
- 4. Platform ZEN: https://www.zeiss.com/microscopy/int/products/microscope-software/zen-lite.html
- 5. Nketiah, G.A., Elschot, M., Scheenen, T.W. et al. Utility of T2-weighted MRI texture analysis in assessment of peripheral zone prostate cancer aggressiveness: a single-arm, multicenter study. *Sci Rep* 11, 2085 (2021). https://doi.org/10.1038/s41598-021-81272-x
- 6. Huang, S., Shi, K., Zhang, Y. *et al.* Texture analysis of T2-weighted cardiovascular magnetic resonance imaging to discriminate between cardiac amyloidosis and hypertrophic cardiomyopathy. *BMC Cardiovasc Disord* **22**, 235 (2022). https://doi.org/10.1186/s12872-022-02671-0
- 7. J.B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd edition, 2015, http://expchem3.com/
- 8. P. Lazar, F. Karlický, P. Jurečka, M. Kocman, E. Otyepková, K. Šafářová, M. Otyepka, Adsorption of Small Organic Molecules on Graphene, J. Am. Chem. Soc. 2013, 135, 6372–6377, DOI: dx.doi.org/10.1021/ja403162r
- 9. M. Oltean, G.S. Mile, M. Vidrighin, N. Leopold, V. Chiş, Weakly bound PTCDI and PTCDA dimers studied by using MP2 and DFT methods with dispersion correction, Physical Chemistry Chemical Physics, 15 (2013) 13978-13990, DOI: 10.1039/C3CP44644A
- 10. M. Savarese, A. Aliberti, D. De Santo, E. Battista, F. Causa, P.A. Netti, N. Rega, Fluorescence Lifetimes and Quantum Yields of Rhodamine Derivatives: New Insights from Theory and Experiment, J. Phys. Chem. A, 2012, 116, 7491-7497, DOI: dx.doi.org/101021/jp30214851
- 11. Kasap, S. O. Principles of Electronic Materials and Devices. 4th ed. New York: McGraw-Hill Education, 2018.
- 12. Maier, Stefan A. Plasmonics: Fundamentals and Applications. New York: Springer, 2007.
- 13. Le Ru, Eric C., and Pablo G. Etchegoin. Principles of Surface-Enhanced Raman Spectroscopy and Related Plasmonic Effects. Amsterdam: Elsevier, 2009.

- 14. V. Moisoiu, S. D. Iancu, A. Stefancu, T. Moisoiu, B. Pardini, M. P. Dragomir, N. Crisan, L. Avram, D. Crisan, I. Andras, D. Fodor, L. F. Leopold, C. Socaciu, Z. Bálint, C. Tomuleasa, F. Elec and N. Leopold, SERS liquid biopsy: An emerging tool for medical diagnosis, Colloids and Surfaces B: Biointerfaces 2021, 208, 112064.
- 15. Lakowicz, J. R.: Principles of Fluorescence Spectroscopy, 3rd ed., Springer Science + Business Media, LLC (2006), ISBN: 978-0-387-46312-4
- 16. Ana-Maria Craciun, Simion Astilean, Monica Focsan, Marc Lamy de la Chapelle, Gold nanoparticles conjugated with fluorophore-labeled DNA: overview of sensing and imaging applications, TrAC Trends in Analytical Chemistry, 180, 2024, 117913

9. Aligning the contents of the discipline with the expectations of the epistemic community, representatives, professional associations and standard employers operating in the program field

The content of the discipline is in line with what is studied in other university centers in the country and abroad. In order to adapt to the requirements imposed by the labor market, the content of the discipline was harmonized with the requirements imposed by the specifics of postgraduate education, research institutes and the business environment.

10. Examination

| Activity type | 10.1 Evaluation criteria | 10.2 Evaluation | 10.3 Weight in | |
|---|--------------------------|----------------------|-----------------|--|
| | | methods | the final grade | |
| 10.4 Lectures | Assessment of knowledge | Written exam | 25% | |
| | Assessment of knowledge | Ongoing tests | 25% | |
| 10.5 Seminars / | Activity during seminars | Discussions, answers | 25% | |
| laboratory classes | | to questions | | |
| | Assessment of knowledge | Written exam | 25% | |
| 10.6 Minimum performance standard | | | | |
| Correct assessment of methods and models to be used to solve a particular problem. | | | | |
| Proper use of computational techniques and available hardware and software resources. | | | | |

| Signature of course coordinator | Signature of seminar | |
|---------------------------------|--------------------------|---|
| organization course coordinator | coordinator | |
| Prof.dr. Zoltan Balint | Prof.dr. Zoltan Balint | |
| Prof.dr. Vasile Chiş | Prof.dr. Vasile Chiş | |
| Conf.dr. Monica Focșan | Conf.dr. Monica Focșan | |
| Prof.dr. Nicolae Leopold | Prof.dr. Nicolae Leopold | |
| Date | | Signature |
| 21.09.2025 | | Head of department Prof. dr. Vasile Chiș |