#### **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 discipline			Ap	Applications of bio(nano)medical spectroscopy and imaging				
2.2 Teacher responsible for			Prof.dr. Zoltan Balint, Prof.dr. Vasile Chiş, Conf.dr. Monica					
lectures			Fo	Focșan, Prof.dr. Nicolae Leopold				
2.3 Teacher responsible for			Prof.dr. Zoltan Balint, Prof.dr. Vasile Chiş, Conf.dr. Monica					
seminars			Fo	Focșan, Prof.dr. Nicolae Leopold				
2.4 Year of	I         2.5         I         2.6 Type of         E         2.7 Course				2.7 Course	DS		
study Semester			evaluation		framework			

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

6		· ·	-		
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: -					_
3.9 Total individual study hours 8	9				-

-	
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 software,
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
ces	- Correlation of theoretical and computational data with experimental ones
enc	- Communicating complex scientific ideas, the conclusions of experiments or the results of a
Jet	scientific project.
lui	- Ability to obtain and support scientifically argued results; ability to develop scientific papers.
l co	- Use of scientific methods and models in narrow or interdisciplinary fields.
nal	- Advanced ability to plan and organize.
sio	- Operation with the principles of digital image data processing. Ability to analyze and
fes	synthesize data; the ability to model the effect of external factors on images.
Pro	- 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.
es	- The application, in the context of compliance with the legislation, of intellectual property
nci	rights (including technology transfer), of the product certification methodology, of the
ete	principles, norms and values of the code of professional ethics within its own rigorous,
du	efficient and responsible work strategy.
C01	- Application of efficient work techniques in multidisciplinary team on various levels
sal	hierarchical. Identify roles and responsibilities in a team, apply techniques effective
/er:	relationships, and work within the team.
NSU	- Efficient use of information sources and communication and training resources
ſra	professional, both in Romanian and English.
<b>-</b>	- 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.
	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

7.1 The general objective of the	I coming physical models and advanced computational		
dissipling	- Learning physical models and advanced computational		
discipline	methods used to calculate spectroscopic properties of		
	The second 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 higherdical image analysis		
	-gating familiar with modern fluorescent techniques and		
	aquipmont in biomodical research		
	Impuladas in single melecule fluoressense techniques and		
	- knowledge in single molecule nuorescence techniques and		
	super resolution hubrescence 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	l 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	toaching	
	obtained by MRI and CT.	teaching	

2. Techniq results a automa process as 3D in 3D imag	ues for simulating the effect of noise on the of digital image data analysis. Automatic and semi- tic operations and processes for 3D image data ing. Biomedical applications: data processing such hages obtained with the microscope, respectively ges obtained by CT and MRI.		2 hours
<ol> <li>Decision supervis image se input.</li> </ol>	n support tools in medicine: Development of sed and unsupervised algorithms for biomedical egmentation using microscopy, CT and MRI as		2 hours
4. Modelin dispersi of host- molecul	g weak intermolecular interactions: the role of on in weakly bound molecular systems; Modeling guest systems; Modeling the adsorption of es on surfaces.		2 hours
5. Calculat systems fluoresc fluoresc	ion of photophysical parameters of molecular : modeling of electronic absorption and ence emission spectra; calculation of radiative ence lifetime.		2 hours
6. Introdu Concept applicat	ction to fluorescence spectroscopy and imaging; ; Overview of fluorescence measurements and ions; Fluorescence Sensing		2 hours
7. Fluores Principl Principl Tissue Fluores Fluores	cence Lifetime Spectroscopy and Imaging es; Applications in biomedical diagnostics. es of Fluorescence Lifetime Instrumentation. Fluorescence Lifetime Spectroscopy. Tissue cence Lifetime Imaging - Endogenous. cence Lifetime Imaging - Exogenous Probes.		2 hours
8. Plasmon Imaging	n-enhanced Fluorescence Spectroscopy and ; Enhanced Fluorescence Sensing		2 hours
9. Fluores Single M	cence super-resolution microscopy; Principles; Iolecule Fluorescence Detection		2 hours
10. Electric	al and optical properties of materials		2 hours
11. Surface applicat	enhanced Raman scattering: Theory and ions		2 hours
12. Clinical	Raman Spectroscopy		2 hours
0.0.0		The solution of the later	Com i
8.2 Semina	Irs / laboratory classes	I eaching methods	Lomments
1. Auvanced	a methous of 2D image data processing.	Learning Droject	1 110UI
2. Automate	ea 2D image segmentation techniques:	hased learning	1 hour
microscopy	images with application in histology.	Inquiry guided	
3. Medical o	lecision support tools: methods for extraction and	learning, Experiential	1 hour
characterization of various organs and features from MRI		learning	
acquisition 3D model p	s – from image segmentation to texture analysis. reparation.		
4. Modeling surface. Mo energy calc	the adsorption of molecules on a graphene model deling the host-guest complexes. Interaction ulation and BSSE correction.		1 hour

5. Calculation of the electronic transitions (absorption and fluorescence emission) spectrum for solvated molecules using the "state specific" approach. Calculation of the radiative lifetimes of solvated molecule	1 hour
6. Instrumentation for fluorescence spectroscopy; Spectrofluorometers used.	1 hour
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 examples	1 hour
11. Experimental setups in surface-enhanced Raman scattering	1 hour
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.
- Digital Image Processing W. Burger, M.J. Burge Springer 2008 ISBN 978-1-84628-379-6 -<u>https://imagingbook.files.wordpress.com/2013/06/</u>burgerburgeen20071104\_ijreference\_le tter.pdf
- 3. Platform ImageJ: <u>http://imagej.net/Introduction</u>
- 4. Platform ZEN: https://www.zeiss.com/microscopy/int/products/microscope-software/zenlite.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/
- 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	0.4 Lectures Assessment of knowledge		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	
	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	
	0:	

Date	Signature
	Head of department
21.09.2024	Prof. dr. Vasile Chiș