NAME OF THE COURSE	Computer Methods and Applications in Nano and Biophysics						
Code	PMP409	Year of study	DS-2				
Course teacher	prof.dr. dr. h.c. Vlasta Bonačić Koutecky	Credits (ECTS)	5,0				
Associate teachers		Type of instruction (number of hours)	L	S	E	F	
			30	15			
Status of the course	elective	Percentage of application of e-learning					

COURSE DESCRIPTION						
Course objectives	Ability to model nanostructures and their properties for interpretation of experimental results and stimulation of new experiments.					
Course enrolment requirements and entry competences required for the course	Knowledge of classical physics and basics of quantum physics					
Learning outcomes expected at the level of the course (4 to 10 learning outcomes)	1. Selection of suitable methods for simulating system properties within nanophysics and biophysics 2. Independent evaluation and interpretation of results obtained by simulations 3. Comparison with experimental results 4. The skills to compare achievements in the relevant literature					
Course content broken down in detail by weekly class schedule (syllabus)	1. Basic theoretical methods for determining the structures and optical properties of molecules and nanoparticles 2. Their application for determining the optical properties of nano biomolecular hybrid systems 3. Fundamentals of molecular dynamics methods: ground and excited states for research of dynamic properties of molecules, nanoparticles and their hybrid systems 4. Application of molecular dynamics to determine the fluorescence of nano bio systems for biosensors 5. Simulation of catalytic properties of metal particles and applications for fuel cell improvement 6. Computational methods for structural and optical properties of two-dimensional periodic system and their use for improving the properties of materials for solar cells					
Format of instruction	☒ lectures ☐ seminars and workshops ☒ exercises ☐ *on line* in entirety ☐ partial e-learning ☐ field work		☒ independent assignments ☐ multimedia ☐ laboratory ☐ work with mentor ☐ (other)			
Student responsibilities	Attending lectures and exercises. Two tests (colloquia) from the material covered in the lectures. Written exam (a student who collects more than 50% of points from both colloquia is exempted from taking the written part of the exam). Oral exam. Preparation of the presentation of the selected scientific article.					
Screening student work *(name the proportion of ECTS credits for each activity so that the total number of ECTS credits is equal to the ECTS value of the course)*	Class attendance	2	Research		Practical training	
	Experimental work		Report		(Other)	
	Essay		Seminar essay		(Other)	
	Tests	2	Oral exam	1	(Other)	
	Written exam		Project		(Other)	

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<tr><td>Grading and evaluating student work in class and at the final exam</td><td colspan="3">Two tests (colloquia) from the material covered in the lectures
Oral exam</td></tr>
<tr><td rowspan="9">Required literature (available in the library and via other media)</td><td>Title</td><td>Number of copies in the library</td><td>Availability via other media</td></tr>
<tr><td>[1] F. Jensen: “Introduction to computational chemistry”, John Wiley and Sons, 2007.</td><td></td><td></td></tr>
<tr><td>[2] M.P.Allen, D.J.Tildesley: “Computer Simulationin Chemical Physics”, Kluwer Academic Publishers, 1993.</td><td></td><td></td></tr>
<tr><td>[3] Carsten A. Ullrich: „Time-Dependent Density-Functional Theory; Concepts and Applications“, Oxford Graduate Texts, 2011.</td><td></td><td></td></tr>
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<tr><td>Optional literature (at the time of submission of study programme proposal)</td><td colspan="3">[1] R. Antoine, V. Bonačić-Koutecký: Liganded Silver and Gold Quantum Clusters. Towards a New Class of Nonlinear Optical Nanomaterials, Springer, SpringerBriefs in Materials, 2018.
[2] R. Mitrić, J. Petersen, V. Bonačić-Koutecký: Nonadiabatic Dynamics “on the fly” in Complex Systems and its Control by Laser Fields", in Conical Intersections II, Ed. by H. Köppel, W. Domckeand D. Yarkony, World Scientific 2011.
[3] W. Domcke, D. R. Yarkony, H. Köppel Conical Intersections, World scientific Publishing, 2011.
[4] P. E. Hoggan, E. J. Brändas, J. Maruani, P. Piecuch, G. Delgado-Barrio Advances in the Theory of Quantum Systems in Chemistry and Physics, Springer, 2012.</td></tr>
<tr><td>Quality assurance methods that ensure the acquisition of exit competences</td><td colspan="3">An anonymous post-course survey will be used to identify weaknesses in course structure and performance.
Exam results statistics and student evaluation through an anonymous survey at the end of the course. The survey is conducted according to the regulations of the University of Split</td></tr>
<tr><td>Other (as the proposer wishes to add)</td><td colspan="3"></td></tr>
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