

**Subject card**

<b>Subject name and code</b>	Chemical bonding via quantum chemistry tools, PG_00129572						
<b>Field of study</b>	Chemistry						
<b>Date of commencement of studies</b>	October 2024	<b>Academic year of realisation of subject</b>			2025/2026		
<b>Education level</b>	Master's studies	<b>Subject group</b>			Optional subject group		
<b>Mode of study</b>	full-time studies	<b>Mode of delivery</b>			at the university		
<b>Year of study</b>	2	<b>Language of instruction</b>			English		
<b>Semester of study</b>	4	<b>ECTS credits</b>			2.0		
<b>Learning profile</b>	academic	<b>Assessment form</b>					
<b>Conducting unit</b>							
<b>Name and surname of lecturer (lecturers)</b>	<b>Subject supervisor</b>		prof. dr hab. Iwona Anusiewicz				
	<b>Teachers</b>						
<b>Lesson types</b>	<b>Lesson type</b>	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	<b>Number of study hours</b>	0.0	30.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						
<b>Learning activity and number of study hours</b>	<b>Learning activity</b>	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	<b>Number of study hours</b>	30		5.0		15.0	50
<b>Subject objectives</b>	Explaining how to identify via quantum chemical calculations types of various chemical bonding. Teaching students about the applications of computational methods to chemical bonding analysis.						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently. Develops the ability to work in a team.	[SK2] presentation/project/paper/report
	[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	Student knows how to choose the proper theoretical methods and how to perform the study of a given molecule.	[SW2] presentation/project/paper/report
	[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Student has the ability of visualizing and interpreting the results of the performed theoretical calculations.	[SU2] presentation/project/paper/report
	[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student explains the stability of molecular systems by characterizing the most important interactions responsible for binding.	[SW2] presentation/project/paper/report
	[CHEMMU2_W01] Uses knowledge of spectroscopic methods of chemical compound analysis.	Student defines and describes basic types of chemical bonding.	[SW2] presentation/project/paper/report
	[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	Student has the ability of estimating the stability of various molecular systems, develops the ability of choosing a proper quantum chemistry method to investigate the type of chemical bonding.	[SU2] presentation/project/paper/report
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Student knows what theoretical method to choose for the determination of physical properties of a given molecule.	[SW2] presentation/project/paper/report	
Subject contents	<p>Various types of chemical bonding: covalent bonding, ionic bonding, intermolecular forces; theoretical methods used for identification of chemical bonding in molecular structure; determination of physical properties (bond lengths, bond energy, charge distribution, polarizability, dipole moments) related to different types of chemical bonding/molecular interactions; molecular orbitals- visualization and interpretations; natural bond orbital calculation and analysis; visualization of NBO plots. The calculation and interpretation of Wiberg bond orders.</p>		
Prerequisites and co-requisites	basic knowledge in chemistry		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Assessment criteria in accordance with the University of Gdańsk Study Regulations. The main criteria for evaluation of reports are the correct answers to the questions in the exercise instructions.	51.0%	100.0%
Recommended reading	Basic literature	Atkins Molecules, P. Atkins, Cambridge University Press, 2003	
	Supplementary literature	Handbook of Computational Chemistry, ed. J. Leszczyński, Springer, Science+Business Media B.V. 2012	
	eResources addresses	Adresy na platformie eNauczanie:	
Example issues/example questions/tasks being completed	Describe the electronic structure of the NaCl and its corresponding anion at the MP2/aug-cc-pVDZ level of theory.		
Work placement	Not applicable		

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