University of Gdańsk

Subject card

Subject name and code	Chemical bonding via quantum chemistry tools, PG_00129572						
Field of study	Chemistry						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2027/2028			
Education level	Master's studies		Subject group	Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	2		Language of instruction	English			
Semester of study	4		ECTS credits	2.0			
Learning profile	academic		Assessment form	credit			
Conducting unit							
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Iwona Anusiewicz				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	30.0	0.0	0.0	0.0	30
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours	Self-study	SUM	
	Number of study hours	30		5.0	15.0	50	
Subject objectives	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

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.

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	

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

Document generated electronically. Does not require a seal or signature.