

。 GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	MATHEMATICAL METHODS IN CHEMISTRY, PG_00038882							
Field of study	Chemistry							
Date of commencement of studies	February 2025		Academic year of realisation of subject		2024/2025			
Education level	second-cycle studies		Subject group			Obligatory subject group in the field of study		
Mode of study	Full-time studies		Mode of delivery			at the university		
Year of study	1		Language of instruction		Polish			
Semester of study	1		ECTS credits		2.0			
Learning profile	general academic profile		Assessmer	ssessment form		exam		
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry							
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. inż. Jacek Czub					
	Teachers							
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Projec	t	Seminar	SUM
	Number of study hours	15.0	15.0	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	The aim of the course is to provide students with general knowledge and skills in advanced mathematical methods used in chemistry and related fields, with a special emphasis on linear algebra, vector analysis, Fourier series and transform, probability theory and numerical methods.							

Learning outcomes	Course outcome	Subject outcome	Method of verification		
	K7_W01	The student acquires in-depth knowledge of mathematical methods and tools for the study of quantum and theoretical chemistry, spectroscopy, crystallography, statistical thermodynamics, molecular biophysics and related fields on a quantitative level. The student learns the terminology and mathematical formalism used in linear algebra, vector analysis, Fourier analysis, theory of stochastic processes and numerical methods. The student learns to use the theoretical knowledge gained during the lecture to solve mathematically advanced problems of chemical importance by writing computer programs.	[SW1] Assessment of factual knowledge		
Subject contents	К7_К01	The student understands the need for lifelong learning, and is able to inspire and organize the learning process of other people.	[SK5] Assessment of ability to solve problems that arise in practice		
	K7_U01	The student learns to confront the results of theoretical predictions with regard to the properties of chemical molecules with the literature and experimental data.	[SU1] Assessment of task fulfilment		
	K7_W02	The student learns the mathematical formalism of theoretical chemistry methods used to predict the properties of molecules, including the relationship between structure and reactivity.	[SW1] Assessment of factual knowledge		
	 Linear algebra (operations on vectors and matrices, inner product axioms, systems of linear equations, multiple linear regression, four fundamental subspaces, orthogonal bases, orthogonal (unitary) matrices, eigenvalue problem, diagonalization, properties of symmetric (hermitian) matrices, similarity transformation, spectral decomposition of a matrix, positive-definite matrices, singular value decomposition, introduction to LCAO-MO method, Hueckel method, normal mode analysis, principal component analysis) Vector analysis (parametric curves and surfaces, vectors tangent and normal to curves and surfaces, arc length, total differential and total derivative, chain rule, gradient and gradient operator, Lagrange multipliers, directional derivative, scalar and vector field, curl of a vector field, flux of a vector field, Stokes theorem, Green theorems, divergence of a vector field, curl of a vector field, flux of a vector field, Stokes theorem, Green theorems, divergence of a vector field, continuity equation, Gauss theorem, laplacian, diffusion equation, Poisson equation, Laplace equation, Poisson-Boltzmann equation, vector identities) Fourier analysis (brief introduction to Sturm-Liouville theory, representing functions in orthogonal function bases, orthogonal polynomials, Fourier series, Fourier transform, inverse Fourier transform, Dirac delta-function of Fourier transform, convolution theorem and its applications, Nyquist-Shannon sampling theorem) Stochastic processes theory (probability density, cumulative distribution function, stochastic processes and their properties, stationary stochastic processes, autocorrelation, white noise, Monte Carlo methods, Langevin equation and Brownian dynamics, introduction to Markov processes, Markov matrices and their properties, stationary stochastic processes, autocorrelation, white noise, Monte Carlo methods, Langevin equation and Brownian dynamics, introduction to Markov processes, Markov matrices and their properties, s				
	 Eigenvalue problem: normal mode analysis in the context of IR spectroscopy, numerical prediction of IR spectra Basics of vector analysis: numerical approach to optimization, minimization of multivariable function, optimization of the structure of atomic clusters Selected topics in Fourier analysis: application of the fast Fourier transform to analysis of time series, in particular, discrete Fourier transform of free induction decay data from an NMR spectrometer; Fourier transform of images 				

Prerequisites and co-requisites	Basic background in calculus and linear algebra.					
Assessment methods	Subject passing criteria	Passing threshold	Percentage of the final grade			
and criteria	Practicals	50.0%	70.0%			
	Lecture	50.0%	30.0%			
Recommended reading	Basic literature	 Donald A. McQuarrie "Mathematical Methods for Scientists and Engineers" Erich Steiner "The Chemistry Maths Book" Henry Margenau "The Mathematics of Physics and Chemistry" Zbigniew Skoczylas, "Elementy analizy wektorowej: teoria, przykłady, zadania" (in polish only) 				
	Supplementary literature	 Gilbert Strang "LInear Algebra and Its Applications", 4th ed. George B. Arfken, Hans J. Weber "Mathematics for Physicists", 7th ed. 				
	eResources addresses	Adresy na platformie eNauczanie:				
Example issues/ example questions/ tasks being completed	 Examples of problems to be solved in the MATLAB/Octave environment: 1. Create a routine z(v) that will take a vector of arguments, v = [x y], and return the value of an arbitra function z = f(x,y), e.g. z = x² + 4y². Based on this routine, create another routine grad(v) that will tak the vector of coordinates v = [x y] and return the normalized gradient, grad(v) = [gx gy]. Then, write program which will do the followng: (1) read the starting point P, (2) calculate the gradient at point P move point P by a given step along the direction of negative gradient, (4) compute the resulting cha in value of z = f(x,y), (5) repeat steps 2-4 until the value of the function ceases to decrease. 2. Use the toeplitz() function to create a tridiagonal matrix describing a hexatriene molecule according the Hückel theory. Calculate the electronic energy of the conjugated π-system. Repeat the procedu with the matrix modified to represent benzene instead of hexatriene. Compare and comment on the results. 					
Work placement	Not applicable					

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