AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Code:	UBPJO-158	Module name:	Introductory quantum chemistry		
Academic year:	2017/2018	Semester:	Fall, Spring	ECTS credits:	4
Programme:	AGH UST International Courses				
Course homepage:	https://intcourses.agh.edu.pl/	Lecture language:	English		
Responsible teacher:	prof. dr hab. inż. Koleżyński Andrzej (kolezyn@agh.edu.pl)				
Academic teachers:	prof. dr hab. inż. Koleżyński Andrzej (kolezyn@agh.edu.pl)				

Module summary

The course is intended for undergraduate students and majors interested in gaining basic knowledge about foundations of modern quantum chemistry and its practical applications.

Description of learning outcomes for module

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Method of learning outcomes verification (form of completion)
Social competence		
M_K001	Student is prepared to effectively select appropriate methods of computational chemistry as an additional tool in solving common problems met in chemistry and materials science	
Skills		
M_U001	Student can analyze practical problem he/she is facing from quantum chemical viewpoint, select the appropriate approach to solve it and analyze the results of ab initio calculations carried out for particular system.	Examination
Knowledge		
M_W001	Student has basic knowledge of fundamentals of quantum mechanics and its most important approximations.	Examination
M_W002	Student knows modern methods and tools of quantum chemistry.	Examination

FLO matrix in relation to forms of classes

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Form of classes										
		Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Others	E-learning
Social competence												
M_K001	Student is prepared to effectively select appropriate methods of computational chemistry as an additional tool in solving common problems met in chemistry and materials science	+	-	-	-	-	-	-	-	-	-	-
Skills												
M_U001	Student can analyze practical problem he/she is facing from quantum chemical viewpoint, select the appropriate approach to solve it and analyze the results of ab initio calculations carried out for particular system.	+	-	-	-	-	-	-	-	-	-	-
Knowledge												
M_W001	Student has basic knowledge of fundamentals of quantum mechanics and its most important approximations.	+	-	-	-	-	-	-	-	-	-	-
M_W002	Student knows modern methods and tools of quantum chemistry.	+	-	-	-	-	-	-	-	-	-	-

Module content

Lectures

Topics covered in this course

1)Wave mechanics, wave-particle duality, Heisenberg’s uncertainty principle.
2)Operators, eigenfunctions, eigenvalues, the Dirac function, Fourier transforms.
3)Wave function space, Dirac notation, Hermitian Operators, eigenvalue problem.
4)Average values, Ehrenfest’s theorem.
5)Particle in a box, particles in “square” potentials.
6)Time evolution of wave functions and wave packets, the harmonic oscillator.
7)Postulates of quantum mechanics.
8)Schrodinger representation of QM.
9)The Hydrogen atom, hydrogen-like ions, multi-electron atoms, the Pauli principle, electron spin, electronic configuration
10)Hartree Fock/SCF method, Gaussian basis sets
11)Post Hartree-Fock methods: Møller-Plesset perturbation theory, Configuration Interaction, Coupled Clusters, Quantum Monte Carlo

12)Application of quantum mechanics to molecules: Born-Oppenheimer approximation
13)Molecular Orbital vs Valence Bond theory
14)Molecular vibrations and rotations
15)Density Functional Theory – Hohenberg-Kohn theorems, Kohn-Sham equations, exchange – correlation potential approximations

Method of calculating the final grade

The final grade is calculated as an weighted average of partial grades: activity during lectures (20%), attendance (10%) and exam results (70%).

Prerequisites and additional requirements

The course is intended for undergraduate students and majors interested in gaining basic knowledge about foundations of modern quantum chemistry and its practical applications for molecular and (to some extent) periodic systems.

Recommended literature and teaching resources

1. Ira N. Levine, Quantum Chemistry, (obligatory)
2. Lucjan Piela, “Ideas of Quantum Chemistry”, Second Edition (optional)
3. Martin C.R. Cockett, Graham Doggett, “Maths for Chemists Vol. 1 : Numbers, Functions and Calculus (Tutorial Chemistry Texts)”, (optional)
4. Martin C.R. Cockett, Graham Doggett, “Maths for Chemists Vol 2: Power Series, Complex Numbers and Linear Algebra (Tutorial Chemistry Texts)”, (optional)

Scientific publications of module course instructors related to the topic of the module

1. A. Koleżyński, “FP-LAPW study of anhydrous cadmium and silver oxalates: electronic structure and electron density topology”, **Phys. B**, **405** 3650–3657 (2010); DOI: 10.1016/j.physb.2010.05.059.
2. J. Leszczyński, A. Koleżyński, K.T. Wojciechowski, “Electronic and transport properties of polycrystalline Ba8Ga15Ge31 type I clathrate prepared by SPS method”, **J. Sol. State Chem.**, **193** 114-121 (2012); DOI: 10.1016/j.jssc.2012.03.067.
3. W. Szczypka, P. Jeleń, A. Koleżyński, “Theoretical studies of bonding properties and vibrational spectra of chosen ladder-like silsesquioxane clusters”, **J. Mol. Struct.**, **1075** 599–604 (2014), DOI: 10.1016/j.molstruc.2014.05.037.
4. A. Koleżyński, P. Nieroda, K. T. Wojciechowski, “Li doped Mg2Si p-type thermoelectric material: theoretical and experimental study”, **Comp. Mat. Sci.**, **100** 84–88 (2015), DOI: 10.1016/j.commatsci.2014.11.015.
5. A. Mikuła, M. Król, A. Koleżyński, “The influence of the long-range order on the vibrational spectra of structures based on sodalite cage”, **Spectrochim. Acta. A**, **144** 273–280 (2015), DOI: 10.1016/j.saa.2015.02.073.
6. P. Nieroda, A. Kolezynski, M. Oszajca, J. Milczarek, K. T. Wojciechowski, “Structural and Thermoelectric Properties of Polycrystalline p-Type Mg2-xLixSi”, **J. Electronic Mat.**, **45** 3418-3426 (2016), DOI: 10.1007/s11664-016-4486-5.
7. A. Koleżyński, W. Szczypka, “First-Principles Study of the Electronic Structure and Bonding Properties of X8C46 and X8B6C40 (X: Li, Na, Mg, Ca) Carbon Clathrates”, **J. Electronic Mat.**, **45** 1336–1345 (2016), DOI: 10.1007/s11664-015-4028-6.
8. A. Koleżyński, W. Szczypka, “Towards band gap engineering in skutterudites: The role of X4 rings geometry in CoSb3-RhSb3 system”, **J. Alloys Compd.**, **691** 299-307 (2017), DOI: 10.1016/j.jallcom.2016.08.235
9. E. Drożdż, A. Koleżyński, “The structure, electrical properties and chemical stability of porous Nb-doped SrTiO3 – experimental and theoretical studies”, **RSC Advances**, **7** 28898-28908 (2017), DOI: 10.1039/C7RA04205A.
10. J. Leszczyński, W. Szczypka, Ch. Candolfi, A. Dauscher, B. Lenoir, A. Koleżyński, “HPHT synthesis of highly doped InxCo4Sb12 – experimental and theoretical study”, **J. Alloys Compd.**, DOI: 10.1016/j.jallcom.2017.08.194.

Additional information

During lectures the foundations of quantum mechanics and particular techniques, approximations and applications to question of chemical interest will be covered. In this course, you will learn the basics of how to describe the electronic structure of atoms and molecules and calculate their properties using quantum chemistry methods.

Student workload (ECTS credits balance)

Student activity form	Student workload
Participation in lectures	30 h
Realization of independently performed tasks	40 h
Examination or Final test	2 h
Contact hours	30 h
Summary student workload	102 h
Module ECTS credits	4 ECTS