AGH University of Science and Technology

Module name:	Introductory Quantum Chemistry
Academic year:	2019/2020
Code:	CIMT-1-002-s
ECTS credits:	3
Faculty of:	Materials Science and Ceramics
Field of study:	Materials Science
Specialty:	—
Study level:	First-cycle studies
Form and type of study:	Full-time studies
Lecture language:	English
Profile of education:	Academic (A)
Semester:	0
Course homepage:	—
Responsible teacher:	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	Connections with FLO	Method of learning outcomes verification (form of completion)
Social competence: is able to			
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	IMT1A_K01	Activity during classes
Skills: he can			
M_U001	Student can analyze practical problem he/she is facing from the quantum chemical viewpoint, select the appropriate approach to solve it and analyze the results of ab initio calculations carried out for a particular system.	IMT1A_U01, IMT1A_U05	Examination
Knowledge: he knows and understands			
M_W001	Student has basic knowledge of fundamentals of quantum mechanics and its most important approximations.	IMT1A_W01	Examination
M_W002	Student knows modern methods and tools of quantum chemistry.	IMT1A_W01	Examination

Number of hours for each form of classes

Suma	Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
30	0	0	0	0	0	30	0	0	0	0	0

FLO matrix in relation to forms of classes

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
Social competence: is able to												
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: he can												
M_U001	Student can analyze practical problem he/she is facing from the quantum chemical viewpoint, select the appropriate approach to solve it and analyze the results of ab initio calculations carried out for a particular system.	-	-	-	-	-	+	-	-	-	-	-
Knowledge: he knows and understands												
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.	-	-	-	-	-	+	-	-	-	-	-

Student workload (ECTS credits balance)

Student activity form	Student workload
Udział w zajęciach dydaktycznych/praktyka	30 h
Realization of independently performed tasks	40 h
Examination or Final test	2 h
Contact hours	5 h
Summary student workload	77 h
Module ECTS credits	3 ECTS

Additional information

Module content

Seminar classes

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

Teaching methods and techniques:

Seminar classes: Na zajęciach seminaryjnych podstawą jest prezentacja multimedialna oraz ustna prowadzona przez studentów. Kolejnym ważnym elementem kształcenia są odpowiedzi na powstałe pytania, a także dyskusja studentów nad prezentowanymi treściami.

Warunki i sposób zaliczenia poszczególnych form zajęć, w tym zasady zaliczeń poprawkowych, a także warunki dopuszczenia do egzaminu:

Nie określono

Zasady udziału w poszczególnych zajęciach, ze wskazaniem, czy obecność

studenta na zajęciach jest obowiązkowa:

Seminar classes:
– Attendance is mandatory: Yes
– Participation rules in classes: Studenci prezentują na forum grupy temat wskazany przez prowadzącego oraz uczestniczą w dyskusji nad tym tematem. Ocenie podlega zarówno wartość merytoryczna prezentacji, jak i tzw. kompetencje miękkie.

Method of calculating the final grade

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

Sposób i tryb wyrównywania zaległości powstałych wskutek nieobecności studenta na zajęciach:

Nie określono

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.