AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Module name: Foundations of Quantum Chemistry

Academic year: 2019/2020 Code: ZSDA-3-0039-s ECTS credits: 3

Faculty of: Szkoła Doktorska AGH

Field of study: Szkoła Doktorska AGH Specialty: —

Study level: Third-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 quantum mechanics as an additional tool in solving common problems met in chemistry, physics or materials science	SDA3A_K01	Activity during classes
Skills: he can			
M_U001	Student can analyze practical problem he/she is facing from the quantum mechanical viewpoint, select the appropriate approach to solve it and analyze the results of ab initio calculations carried out for a particular system.	SDA3A_U01	Examination
Knowledge: he knows and understands			
M_W001	Student has basic knowledge of fundamentals of quantum mechanics and its most important approximations.	SDA3A_W01	Examination
M_W002	Student knows modern methods and tools of quantum mechanics.	SDA3A_W02	Examination

Number of hours for each form of classes

	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	30	0	0	0	0	0	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	Form of classes										
		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 quantum mechanics as an additional tool in solving common problems met in chemistry, physics or materials science	+	-	-	-	-	-	-	-	-	-	-
Skills: he can												
M_U001	Student can analyze practical problem he/she is facing from the quantum mechanical 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 mechanics.	+	-	-	-	-	-	-	-	-	-	-

Student workload (ECTS credits balance)

Student activity form	Student workload
Udział w zajęciach dydaktycznych/praktyka	30 h
Realization of independently performed tasks	50 h
Examination or Final test	2 h
Contact hours	5 h
Summary student workload	87 h
Module ECTS credits	3 ECTS

Additional information

Module content

Lectures

Topics covered in this course:
1)Wave mechanics, wave-particle duality, Heisenberg’s uncertainty principle.
2)Hilbert space, operators, Dirac’s notation, Fourier transform.
3)Hermitian Operators, eigenfunctions, eigenvalues, eigenvalue problem.
4)Quantum non-locality, quantum contextuality, quantum entanglement,
5)Bell pairs, rotational invariance of Bell pairs, Bell inequalities.
6)Average values, Ehrenfest’s theorem.
7)Particle in a box, particles in “square” potentials.
8)Time evolution of wave functions and wave packets, the harmonic oscillator.
9)Postulates of quantum mechanics.
10)Schrodinger representation of QM.
11)The Hydrogen atom, hydrogen-like ions, multi-electron atoms, the Pauli principle, electron spin, electronic configuration
12)Born-Oppenheimer approximation, Hartree Fock/SCF method, basis sets (Gaussian, Slater, APW, etc.)
13)Post Hartree-Fock methods: Møller-Plesset perturbation theory, Configuration Interaction, Coupled Clusters, Quantum Monte Carlo
14)Density Functional Theory – Hohenberg-Kohn theorems, Kohn-Sham equations, exchange-correlation potential approximations
15)Practical applications of quantum mechanics to molecules, clusters, and solids (periodic and amorphous)

Teaching methods and techniques:

Lectures: Lectures in a form of multimedia presentation and animations

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

At least 80% attendance rate is required in order to be allowed to take the final exam.

Zasady udziału w poszczególnych zajęciach, ze wskazaniem, czy obecność

studenta na zajęciach jest obowiązkowa:

Lectures:
– Attendance is mandatory: Yes
– Participation rules in classes: Lecture attendance is obligatory.

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:

This will be discussed at the beginning of the first class.

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. C. Kittel, Introduction to Solid State Physics, 8th Edition (2004)
2. S. Altmann, Band Theory of Solids: An Introduction from the Point of View of Symmetry, Oxford University Press (1994).
3. S.R. Elliot, The physics and chemistry of solids, Wiley (1998).
4. M. Springborg, Methods of Electronic-Structure Calculations: From Molecules to Solids, Wiley (2000).
5. P. A, Cox, The Electronic Structure and Chemistry of Solids, Oxford University Press (1987).
6. V. V. Nemoshkalenko, V. N. Antonov, Computational methods in solid state physics, CRC Press (1999).
7. D. S. Sholl, J. Steckel, Density Functional Theory: a practical introduction, John Wiley & Sons, Inc. (2009).
8. R. Dronskowski, Computational Chemistry of Solid State Materials, Wiley-VCH (2005).

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.