Module name: Introductory Quantum Chemistry


Faculty of: Materials Science and Ceramics
Field of study: Materials Science  Specialty: Mikro i nanotechnologie materiałowe
Study level: Second-cycle studies  Form and type of study: Full-time studies

Lecture language: English  Profile of education: Academic (A)  Semester: 3

Course homepage: —

Responsible teacher: prof. nadzw. dr hab. inż. Koleżyński Andrzej (kolezyn@agh.edu.pl)

Academic teachers: prof. nadzw. 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

<table>
<thead>
<tr>
<th>MLO code</th>
<th>Student after module completion has the knowledge/ knows how to/is able to</th>
<th>Connections with FLO</th>
<th>Method of learning outcomes verification (form of completion)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M_K001</td>
<td>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</td>
<td>IM2A_K08</td>
<td>Activity during classes</td>
</tr>
<tr>
<td>M_U001</td>
<td>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.</td>
<td>IM2A_U02, IM2A_U05</td>
<td>Examination</td>
</tr>
<tr>
<td>M_W001</td>
<td>Student has basic knowledge of fundamentals of quantum mechanics and its most important approximations.</td>
<td>IM2A_W03</td>
<td>Examination</td>
</tr>
<tr>
<td>M_W002</td>
<td>Student knows modern methods and tools of quantum chemistry.</td>
<td>IM2A_W03</td>
<td>Examination</td>
</tr>
</tbody>
</table>
Module card - Introductory Quantum Chemistry

FLO matrix in relation to forms of classes

<table>
<thead>
<tr>
<th>MLO code</th>
<th>Student after module completion has the knowledge/ knows how to/is able to</th>
<th>Form of classes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Lectures</td>
</tr>
<tr>
<td>M_K001</td>
<td>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</td>
<td>-</td>
</tr>
<tr>
<td>M_U001</td>
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<td>-</td>
</tr>
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<td>-</td>
</tr>
<tr>
<td>M_W002</td>
<td>Student knows modern methods and tools of quantum chemistry.</td>
<td>-</td>
</tr>
</tbody>
</table>

Social competence

Skills

Knowledge

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 \( \delta \) 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 a 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)

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

<table>
<thead>
<tr>
<th>Student activity form</th>
<th>Student workload</th>
</tr>
</thead>
<tbody>
<tr>
<td>Participation in lectures</td>
<td>30 h</td>
</tr>
<tr>
<td>Realization of independently performed tasks</td>
<td>40 h</td>
</tr>
<tr>
<td>Examination or Final test</td>
<td>2 h</td>
</tr>
<tr>
<td>Contact hours</td>
<td>5 h</td>
</tr>
<tr>
<td>Summary student workload</td>
<td>77 h</td>
</tr>
<tr>
<td>Module ECTS credits</td>
<td>3 ECTS</td>
</tr>
</tbody>
</table>