
Academic year: 2019/2020  Code: ZSDA-3-0037-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. nadzw. dr hab. inż. Koleżyński Andrzej (kolezyn@agh.edu.pl)

Module summary
The course is intended for Ph.D. students interested in exploring practical aspects of using theoretical methods of modern physics and chemistry for solving common problems for periodic systems.

Description of learning outcomes for module

<table>
<thead>
<tr>
<th>MLO code</th>
<th>Social competence: is able to</th>
<th>Skills: he can</th>
<th>Knowledge: he knows and understands</th>
</tr>
</thead>
<tbody>
<tr>
<td>M_K001</td>
<td>Student is prepared to effectively use chosen methods of computational solid state chemistry and physics as the complementary tool in solving common problems met in physics, chemistry and materials science</td>
<td>Student can choose appropriate theoretical methods in the calculations of electronic structure for 3D periodic systems and surfaces as well as the topological properties of total electron density. He/She can use the obtained results in the detailed analysis of structural, electronic and bonding properties of a given system.</td>
<td>Student has basic knowledge of quantum mechanics and the most important approaches to electronic structure calculations in periodic systems.</td>
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</table>
Student knows modern methods and tools used in the analysis of bonding properties in solids.

<table>
<thead>
<tr>
<th>Number of hours for each form of classes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Form of classes</strong></td>
</tr>
<tr>
<td>Lectures</td>
</tr>
<tr>
<td>Suma 30</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>FLO matrix in relation to forms of classes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>MLO code</strong></td>
</tr>
<tr>
<td>-------------------------------------------</td>
</tr>
<tr>
<td>Lectures</td>
</tr>
</tbody>
</table>
| Social competence: is able to

**M_K001**
Student is prepared to effectively use chosen methods of computational solid state chemistry and physics as the complementary tool in solving common problems met in physics, chemistry and materials science

**Skills: he can**

**M_U001**
Student can choose appropriate theoretical methods in the calculations of electronic structure for 3D periodic systems and surfaces as well as the topological properties of total electron density. He/She can use the obtained results in the detailed analysis of structural, electronic and bonding properties of a given system.

**Knowledge: he knows and understands**

**M_W001**
Student has basic knowledge of quantum mechanics and the most important approaches to electronic structure calculations in periodic systems.
M_W002 | Student knows modern methods and tools used in the analysis of bonding properties in solids.

| + | - | - | - | - | - | - | - | - |

**Student workload (ECTS credits balance)**

<table>
<thead>
<tr>
<th>Student activity form</th>
<th>Student workload</th>
</tr>
</thead>
<tbody>
<tr>
<td>Udział w zajęciach dydaktycznych/praktyka</td>
<td>30 h</td>
</tr>
<tr>
<td>Realization of independently performed tasks</td>
<td>30 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>67 h</td>
</tr>
<tr>
<td>Module ECTS credits</td>
<td>3 ECTS</td>
</tr>
</tbody>
</table>

**Additional information**

**Module content**

**Lectures**

Topics covered in this course:

1. Introduction: wave mechanics, wave-particle duality, Heisenberg’s uncertainty principle, Hilbert space, Dirac’s notation, linear Hermitian operators, eigenvalue problem.

2. Quantum Mechanics basics.: postulates of quantum mechanics, Schrodinger representation of QM, the Hydrogen atom, hydrogen-like ions.


5. Periodic systems: translational symmetry, planewaves, wave vectors, direct and momentum space, Brillouin zones.


8. Bandstructure, DOS vs bonding properties: chemist’s interpretation (band characters, occupation, DOS projected onto particular atoms and orbitals, COOP, COHP).

9. Electronic structure of 1D, 2D periodic systems (layers, slabs, wires).

10. Electron density topology – QTAIM, Bond critical points, $\nabla^2 \rho [r]$, ELF.


12. Practical calculations 1: nuts and bolts of DFT calculations.
13. Practical calculations 2: DFT calculations for periodic solids and surfaces, doped semiconducting systems, non-stoichiometric solids, calculations of vibrational frequencies, equilibrium phase diagrams from ab initio thermodynamics, electronic structure and transport properties.

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: The 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
Basic knowledge of calculus, vector analysis, crystallography (point symmetry, space symmetry, translational symmetry, reciprocal lattice).

Recommended literature and teaching resources
Suggested readings:

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

Additional information
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