AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

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| Code: | UBPJO-157 | Module name: | Electronic structure and bonding in solids: practical approach | | |
| Academic year: | 2017/2018 | Semester: | Spring | ECTS credits: | 6 |
| Programme: | AGH UST International Courses | | | | |
| Course homepage: | http://upel.agh.edu.pl/wimic/course/view.php?id=12 | 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) | | | | |

## 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 use chosen methods of computational solid state chemistry as the complementary tool in solving common problems met in materials science | Execution of laboratory classes |
| Skills | | |
| M_U001 | Student can calculate the electronic structure for 3D periodic systems and surfaces as well as the topological properties of total electron density and use the obtained results in the detailed analysis of structural, electronic and bonding properties of a given system. | Execution of laboratory classes |
| Knowledge | | |
| M_W001 | Student has basic knowledge of quantum mechanics and the most important approaches to electronic structure calculations in periodic systems. | Execution of laboratory classes |
| M_W002 | Student knows modern methods and tools used in the analysis of bonding properties in solids. | 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 use chosen methods of computational solid state chemistry as the complementary tool in solving common problems met in materials science | + | - | - | - | - | - | - | - | - | - | - |
| Skills | | | | | | | | | | | | |
| M_U001 | Student can calculate the electronic structure for 3D periodic systems and surfaces as well as the topological properties of total electron density and use the obtained results in the detailed analysis of structural, electronic and bonding properties of a given system. | - | - | + | - | - | - | - | - | - | - | - |
| Knowledge | | | | | | | | | | | | |
| 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. | + | - | - | - | - | - | - | - | - | - | - |

## Module content

**Lectures**

List of lecture topics

1. Introduction, Quantum Mechanics basics – short overview, what is Density Functional Theory?
2. DFT: Hohenberg-Kohn theorem, Kohn-Sham equations, XC potential approximations – LDA, GGA, meta-GGA.
3. Periodic systems: translational symmetry, planewaves, wave vectors, direct and momentum space, Brillouin zones.
4. Bloch’s function, Brillouin zones and energy bands, bandstructure, Nearly Free Electrons approximation, Tight binding approximation.
5. Bandstructure: ionic, covalent and metallic crystals. Density of states (total and

projected ones), short description of some experimental methods (XPS, XAS, EXAFS, AES, XES).
6. Bandstructure, DOS vs bonding properties: chemist’s interpretation (band characters, occupation, DOS projected onto particular atoms and orbitals, COOP, COHP).
7. Electronic structure of 1D, 2D periodic systems (layers, slabs, wires).
8. Electron density topology – QTAiM, Bond critical points, ∇2r®, ELF.
9. Electronic structure calculations – standard methods (APW, OPW, KKR, pseudopotentials). Linearization – pros and cons; linearized methods (LMTO, LASW, LAPW, LKKR).
10. Practical calculations 1: DFT calculations for simple solids, nuts and bolts of DFT calculations.
11. Practical calculations 2: DFT calculations for surfaces of solids.
12. Practical calculations 3: DFT calculations of vibrational frequencies
13. Practical calculations 4: equilibrium phase diagrams from ab initio thermodynamics
14. Practical calculations 5: electronic structure and magnetic properties

**Laboratory classes**

Practical calculations
Every student is supposed to carry out full calculations for a series of model systems by means of WIEN2k package and to analyze in detail the obtained results.

## Method of calculating the final grade

The final grade is calculated as an average of all partial grades achieved in class.

## Prerequisites and additional requirements

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

## Recommended literature and teaching resources

Suggested readings
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).
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).
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)

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).
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)

### Additional information
None

## Student workload (ECTS credits balance)

| Student activity form | Student workload |
|---|---|
| Participation in lectures | 30 h |
| Realization of independently performed tasks | 30 h |
| Participation in laboratory classes | 30 h |
| Preparation for classes | 34 h |
| Examination or Final test | 30 h |
| Summary student workload | 154 h |
| Module ECTS credits | 6 ECTS |