



Subject card

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| Subject name and code | , PG_00059468 | | | | | | |
| Field of study | Nanotechnology | | | | | | |
| Date of commencement of studies | February 2023 | | Academic year of realisation of subject | | 2023/2024 | | |
| Education level | second-cycle studies | | Subject group | | Optional subject group Subject group related to scientific research in the field of study | | |
| Mode of study | Full-time studies | | Mode of delivery | | at the university | | |
| Year of study | 1 | | Language of instruction | | Polish | | |
| Semester of study | 2 | | ECTS credits | | 2.0 | | |
| Learning profile | general academic profile | | Assessment form | | exam | | |
| Conducting unit | Instytut Nanotechnologii i Inżynierii Materiałowej -> Faculty of Applied Physics and Mathematics | | | | | | |
| Name and surname of lecturer (lecturers) | Subject supervisor | | dr inż. Michał Winiarski | | | | |
| | Teachers | | dr inż. Michał Winiarski | | | | |
| Lesson types and methods of instruction | Lesson type | Lecture | Tutorial | Laboratory | Project | Seminar | SUM |
| | Number of study hours | 15.0 | 0.0 | 0.0 | 0.0 | 0.0 | 15 |
| | E-learning hours included: 0.0 | | | | | | |
| Learning activity and number of study hours | Learning activity | Participation in didactic classes included in study plan | | Participation in consultation hours | | Self-study | SUM |
| | Number of study hours | 15 | | 0.0 | | 0.0 | 15 |
| Subject objectives | The aim of the course is to introduce selected methods for analyzing the electronic structures of solids, including the tight binding method, Wannier representation and techniques for analyzing the electron density | | | | | | |
| Learning outcomes | Course outcome | | Subject outcome | | Method of verification | | |
| | K7_W04 | | The student is able to compare the results of model calculations with experimental data (eg. ARPES) | | [SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects | | |
| | K7_W02 | | The student can apply the introduced methods to analyze the electronic structure of nanostructures | | [SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects | | |
| | K7_W01 | | The student knows the tight binding method and Wannier representation and can use them to create simple models of the electronic structures of solids. | | [SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects | | |
| Subject contents | 1 Tight binding method applied to electronic structure analysis - introduction and mathematical background - calculations and analysis of simple 2D and 3D models using the Python 3.x programming language2 Description of electronic structure using Wannier representation - Bloch and Wannier functions - calculations employing Quantum Espresso and Wannier90 packages3 Methods electron density visualization and analysis - electron density and ELF - Quantum theory of atoms in molecules | | | | | | |
| Prerequisites and co-requisites | | | | | | | |

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| Assessment methods and criteria | Subject passing criteria | Passing threshold | Percentage of the final grade |
| | Homeworks | 50.0% | 50.0% |
| | Colloquia | 50.0% | 50.0% |
| Recommended reading | Basic literature | 1. W. A. Harrison, Electronic structure and the properties of solids : the physics of the chemical bond, New York : Dover Publications, Inc., 1989 2. R.F.W. Bader, Atoms in molecules : a quantum theory, Oxford : Clarendon Press, 2003 | |
| | Supplementary literature | C M Goringe <i>et al</i> 1997 <i>Rep. Prog. Phys.</i> 60 1447 | |
| | eResources addresses | Podstawowe https://www.youtube.com/watch?v=T8r_3vzWCUM&list=PLYc-eBolpXTJIIUVgoqhJMa2CunCTURr - Lecture on Wannier functions Uzupełniające Adresy na platformie eNauczanie: Metody Analizy Struktury Elektronowej - Moodle ID: 34408 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=34408 | |
| Example issues/ example questions/ tasks being completed | Draw a band structure of an infinite chain of s orbitals. Explain the instability of the model towards structural distortion, | | |
| Work placement | Not applicable | | |