Warsaw University of Technology

# COURSE OFFERED IN THE DOCTORAL SCHOOL

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| Code of the course | 4606-ES-DEGIKLP-0282 | Name of the course | Polish | **Zastosowanie krystalograficznych baz danych w analizie i projektowaniu różnych materiałów funkcjonalnych, katalizatorów i produktów farmaceutycznych** |
| | | | English | **Application of crystallographic database in the analysis and design of various functional materials, catalysts and pharmaceutical products** |

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| Type of the course | Special courses | | |
| Course coordinator | dr hab. inż. Izabela Madura, prof. WUT | Course teacher | dr hab. inż. Izabela Madura, prof. WUT |
| Implementing unit | Faculty of Chemistry | Scientific discipline / disciplines* | Chemical sciences, Physical sciences, Chemical engineering , Materials engineering, Biomedical engineering, Biotechnology, Environmental engineering, mining and energy, biotechnology |

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| Level of education | Doctoral studies | Semester | Summer | | |
| Language of the course | English | | | | |
| Type of assessment | Pass for assessment - final project with presentation | Number of hours in a semester | 45 | ECTS credits | 3 |
| Minimum number of participants | 10 | Maximum number of participants | 24 | Available for students (BSc, MSc) | Yes/~~No~~ |

| Type of classes | | Lecture | Auditory classes | Project classes | Laboratory | Seminar |
|---|---|---|---|---|---|---|
| Number of hours | in a week | 1 | | 1 | 1 | |
| | in a semester | 15 | | 15 | 15 | |

* does not apply to the Researcher's Workshop

## 1. Prerequisites

General knowledge of the structure of matter or chemistry

## 2. Course objectives

The aim of the course is to familiarize students with the Cambridge Structural Database (CSD) and its integrated data analysis tools.

The CSD is a database of fully curated and enhanced organic and metal-organic structures with software enabling drug discovery and design, protein-ligand docking algorithms, design and new materials development, evaluation of solid materials stability, prediction of crystallites' shape, void and pore analysis, catalysts and MOF analysis

## 3. Course content (separate for each type of classes)

### Lecture

The lecture will cover the following topics:

- Basics of X-ray crystallography (symmetry, group theory, X-ray diffraction theory, X-ray diffraction techniques and their main applications)
- Basics of chemical bonds and intermolecular interactions (basic concepts with quantum chemistry elements)
- Importance of knowledge of crystal structures in selected industrial applications
- Overview of crystallographic databases and crystallographic information file formats
- Presentation of the CSD-Core and specialized functionalities of CSD-Materials, CSD-Discovery and CSD-Particles

### Laboratory

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| During the laboratory classes, students will solve on their own (or in pairs) problems prepared so that they can master the basic functionalities of the CSD database. The tasks will be optimized to the students' preliminary knowledge and area of interests |
| Project |
| Depending on the student's interest, the project will require the use one of the CSD-Core, CSD-Materials, CSD-Discovery or CSD-Particles modules at the intermediate or advanced level. The tasks will be discussed with students, aiming for their engagement in the real scientific problems solving. If the group is numerous, the pair or group projects will be regarded. |

4. Learning outcomes

| Type of learning outcomes | Learning outcomes description | Reference to the learning outcomes of the WUT DS | Learning outcomes verification methods* |
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| Knowledge | | | |
| K01 | Student has knowledge of discovering problems in her/his area of interest regarding the use of the solid forms of matter | SD_W1 | Project evaluation |
| K02 | Student has theoretical knowledge of X-ray crystallography and bond theory | SD_W2 | Project evaluation |
| K03 | Student has knowledge about the use of crystallographic databases in the scientific discipline being pursued and the related research methodologies | SD_W3 | Project evaluation |
| Skills | | | |
| S01 | Student has ability of use crystallographic databases in the field of her/his interest | SD_U1 | Project evaluation |
| S02 | Student has ability to select a research methodology depending on the analyzed materials | SD_U2 | Project evaluation |
| S03 | Student is capable of planning and implementing a knowledge discovery process as well as of interpreting its results | SD_U4 | Project evaluation |
| S04 | Student is improving teamwork skills | SD_U7 | Project evaluation |
| Social competences | | | |
| SC01 | Student is thinking and acting in a creative and entrepreneurial way | SD_K4 | Project evaluation |
| SC02 | Presentation of own concepts, analyses and guidelines and the ability to conduct an informed discussion in this area | SD_K2 | Project evaluation |

5. Assessment criteria

Preparing the tasks on the auditory classes and elaboration of the final topic related to selected area of interests which will be checked by lecturer and discussed the results with students (a presentation). Final mark will be given after discussion and correction of work by student.

6. Literature

Primary references:

[1] Introduction to crystallography or Basics of X-ray crystallography – any book avaiable

[2] https://www.ccdc.cam.ac.uk/

Secondary references:

[1] https://www.youtube.com/c/CCDCCambridge

[2] https://www.iucr.org/education/pamphlets

| 7. PhD student's workload necessary to achieve the learning outcomes** | | |
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| No. | Description | Number of hours |
| 1 | Hours of scheduled instruction given by the academic teacher in the classroom | 30 |
| 2 | Hours of consultations with the academic teacher, exams, tests, etc. | 15 |
| 3 | Amount of time devoted to the preparation for classes, preparation of presentations, reports, projects, homework | 30 |
| | | |
| | **Total number of hours** | **75** |
| | **ECTS credits** | **3** |

** 1 ECTS = 25-30 hours of the PhD students work (2 ECTS = 60 hours; 4 ECTS = 110 hours, etc.)

| 8. Additional information | |
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| Number of ECTS credits for classes requiring direct participation of academic teachers | 2 |
| Number of ECTS credits earned by a student in a practical course | 1 |