1.	**Field of study**	**Materials Science and Engineering**
2.	Faculty	Faculty of Science and Technology
3.	Academic year of entry	2019/2020 (winter term), 2020/2021 (winter term), 2021/2022 (winter term), 2022/2023 (winter term), 2023/2024 (winter term), 2024/2025 (winter term)
4.	Level of qualifications/degree	second-cycle studies (in engineering)
5.	Degree profile	general academic
6.	Mode of study	full-time

Module: Computer modelling of materials structure and properties

Module code: IM2A_KMSM

1. Number of the ECTS credits: 4

2. Learning outcomes of the module

code	description	learning outcomes of the programme	level of competence (scale 1-5)
IM2A_KMSM_1	Students know and understand basic notions and postulates of quantum mechanics and have basic knowledge in the field of precise quantum modelling of small systems. They have basic knowledge in the field of electron structure models for periodic systems: nearly free electrons model, a tight bond approximation. They know and understand approximate quantum mechanic methods: perturbation theory, calculus of variations.	IM2A_W01 IM2A_W11	5 1
IM2A_KMSM_2	Students have basic knowledge about the quantum description of multi-electron systems - understand the essence of Born-Oppenheimer approximation, of quantum single-particle methods (Hartree, Hartree-Fock, Thomas-Fermi) and the method of Hohenberg-Kohn-Sham density functional. On a basic level they know at least one dedicated software package used for quantum computations of microscopic and macroscopic properties of engineering materials.	IM2A_W01 IM2A_W15	5 5
IM2A_KMSM_3	In an understandable way students can formulate quantum mechanics definitions and postulates. They use quantum calculus for simple quantum-mechanical systems. In an understandable way they can discuss assumptions and fundamental results of basic quantum models of periodic systems electron structure.	IM2A_U02 IM2A_U09	5 1
IM2A_KMSM_4	In an understandable way students can present limitations of quantum mechanics applied to the problem of multi-electron systems and discuss approximations necessary for a quantum resolution of the problem. They can carry out computations ab initio of the electron structure of atomically ordered systems and interpret computation results with the use of WIEN2k software	IM2A_U07 IM2A_U08	4 4
IM2A_KMSM_5	Students are aware of individual research method limitations and see the need of a thorough scientific analysis of problems in the field of materials engineering. They are aware of and know possibilities of further learning in the field of modern computer simulation methods applied to materials engineering.	IM2A_K01 IM2A_K04	3 3
IM2A_KMSM_6	Ma świadomość ograniczenia jednostkowej metody badawczej i widzi konieczność wszechstronnej, naukowej analizy problemów z zakresu inżynierii materiałowej. Ma świadomość i zna możliwości dalszego dokształcania się w zakresie nowoczesnych metod symulacji komputerowych w zastosowaniu w inżynierii materiałowej.	IM2A_K01 IM2A_K04	3 3

3. Module description

Description	The module Computer modelling of materials structure and properties shall enable students learning the quantum formalism applied to numerical computations of microscopic properties of small (finite) and bulk (periodical) physical systems. Owing to that students will be prepared to use the software, available in research laboratories, for electron structure computations and thermodynamic modelling of new materials as well as to use the results to determine physical and chemical properties of materials studied and designed.
Prerequisites	It is required to achieve effects of education of the modules: calculus, solid state physics, chemistry, crystallography, materials testing methods and thermodynamics.

4. Assessment of the learning outcomes of the module

code	type	description	learning outcomes of the module
IM2A_KMSM_w_1	Written examination	Verification of the knowledge based on the lectures content, recommended literature and attended classes	IM2A_KMSM_1, IM2A_KMSM_2, IM2A_KMSM_3, IM2A_KMSM_4, IM2A_KMSM_5, IM2A_KMSM_6
IM2A_KMSM_w_2	Written test	Checking the acquired skills in the field of quantum computations for model quantum systems	IM2A_KMSM_1, IM2A_KMSM_2, IM2A_KMSM_3, IM2A_KMSM_4
IM2A_KMSM_w_3	Practical test	Assessment of mastering the basic knowledge necessary for individual performance of quantum computations of engineering materials.	IM2A_KMSM_1, IM2A_KMSM_2
IM2A_KMSM_w_4	Report	Assessment of the skill to understand results of computations and to connect them with engineering materials properties by a correct formulation of conclusions.	IM2A_KMSM_3, IM2A_KMSM_4, IM2A_KMSM_5

5. Forms of teaching

code	form of teaching			required hours of student's own work		assessment of the learning outcomes of the module
	type	description (including teaching methods)	number of hours	description	number of hours	
IM2A_KMSM_fs_1	lecture	The lecture shall enable learning basics and procedures for quantum description of small quantum systems and periodic multi-electron structures and to teach students the principles and procedures for quantum modelling applied to materials engineering. The lecture is delivered with the use of multimedia, demonstrations and the WIEN2k software.	30	The work with the recommended literature comprising independent acquisition of knowledge related to basic issues	20	IM2A_KMSM_w_1
IM2A_KMSM_fs_3	laboratory classes	Application of the acquired theoretical knowledge to practical computations of the structure and microscopic and macroscopic properties of engineering materials. Exercises are performed by students individually with the use of teaching laboratories equipment.	60	Preparation of theoretical basics and issues related to the topic of performed exercise. Independent preparation of a theoretical introduction. Individual preparation of exercise results.	15	IM2A_KMSM_w_2, IM2A_KMSM_w_3, IM2A_KMSM_w_4