1.	Field of study	Materials Science and Engineering
2.	Academic year of entry	2018/2019 (summer term)
3.	Level of qualifications/degree	second-cycle studies
4.	Degree profile	general academic
5.	Mode of study	full-time

Module: Monographic lecture 1. Advanced numerical methods in materials modelling

Module code: IM2A_WM1_MMM

1. Number of the ECTS credits: 2

2. Learning outcomes of the module

code	description	learning outcomes of the programme	level of competence (scale 1-5)
IM2A_WM1_MMM_1	Knowledge of numerical methods used in materials modelling based on a classical molecular dynamics.	IM2A_W01	3
IM2A_WM1_MMM_2	Knowledge of selected numerical methods used to analyse simulation results.	IM2A_W02	2
IM2A_WM1_MMM_3	The skill to use computational capabilities of LAMMPS software and AtomEye software to visualise simulation results.	IM2A_U01	3

3. Module description

Description	The module Advanced numerical methods in materials modelling shall enable students learning issues of using a classical molecular dynamics method in simulations of physical phenomena and processes. Owing to learning specialised numerical methods used in LAMMPS and AtomEye software students shall understand benefits and limitations of a classical molecular dynamics method in testing properties and designing new materials. The accomplishment of the above objective will require learning a number of issues from the field of numerical methods used in computer simulations by the molecular mechanics method, such as: Verlet algorithms, Berendesen algorithm for temperature and pressure control of the simulated physical system, slip vector method or computation of internal stresses field used during the analysis of simulation results.
Prerequisites	The knowledge of issues from the field of mathematics, physics, programming languages and numerical methods is required.

4. Assessment of the learning outcomes of the module

code	type	description	learning outcomes of the module
IM2A_WM1	Written test	Verification of knowledge based on the lectures content and recommended literature.	

_MMM_w_1			IM2A_WM1_MMM_1, IM2A_WM1_MMM_2, IM2A_WM1_MMM_3

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_WM1_MMM_fs_1	lecture	The lecture shall enable understanding a classical molecular dynamics method. The lecture is delivered with the use of multimedia based on a recommended set of handbooks.	30	The work with the recommended literature comprising independent acquisition of knowledge related to issues presented during the lectures.	35	IM2A_WM1_MMM_w_