1.	**Nazwa kierunku**	**biofizyka**
2.	Wydział	Wydział Nauk Ścisłych i Technicznych
3.	Cykl rozpoczęcia	2022/2023 (semestr zimowy), 2023/2024 (semestr zimowy), 2024/2025 (semestr zimowy)
4.	Poziom kształcenia	studia drugiego stopnia
5.	Profil kształcenia	ogólnoakademicki
6.	Forma prowadzenia studiów	stacjonarna

Moduł kształcenia: Computational Materials Science

Kod modułu: W4-2BF-MB-21-34

1. Liczba punktów ECTS: 6

2. Zakładane efekty uczenia się modułu

kod	opis	efekty uczenia się kierunku	stopień realizacji (skala 1-5)
MB_34_1	the student can comprehend molecular modeling techniques currently used in the field of life and material sciences	KBF_W02	4
MB_34_2	The student develops competencies on some of the most common computational methodologies used in molecular sciences	KBF_W03 KBF_W08	4 4
MB_34_3	the student develop computational skills through tutorials and exercises	KBF_K04	4

3. Opis modułu

Opis	Intermolecular Forces: Hydrogen bonding, Electrostatic interactions, London forces. Molecular clusters, Supramolecular assemblies. Thermodynamics: Variational formulation. Free energy of a reaction, Equilibrium constants. Statistical Mechanics: Gibbs ensemble, Mechanical system, Generalized coordinates, Lagrangian formalism. Hamiltonian formalism, Hamilton's equation, Phase space. Properties of Hamiltonian systems, Conservation laws, Canonical transformation, Poisson brackets, Liouville's operator, Equation of motion of dynamical variables. Liouville's equation and theorem, Probability density, Microcanonical ensemble, Canonical ensemble. Molecular dynamics: Definition, Foundations of molecular simulations, Limits and approximations. Overview of the basic ingredients (Energy potential, Force fields, Numerical integrators). Energy potential, Force fields, Numerical integrators. Force field terms (bonding, bending, torsion, non-covalent interactions). Molecular Dynamics: Coordinate and Velocity initialization, Integrators. Numerical integrators (velocity Verlet, Leapfrog), Statistical mechanical ensemble, Thermal and pressure coupling. Enhanced Sampling Methods. Simulation of the Kv ion channel. Simulation of a lipid bilayer. Fundamentals of enhanced sampling techniques. Implicit solvent and continuum electrostatic modeling. From collisional theory to stochastic dynamical systems. Stochastic differential equations and Statistical Mechanics. Structural properties: distribution function, radial distribution functions. Monte Carlo methods: Numerical Integration, Importance sampling. Free Energy methods. Free Energy Methods: Thermodynamic Integration, Free energy perturbation, Umbrella Sampling Free Energy Methods: Metadynamics, Jarzinski method, Adiabatic free energy. The course aims to provide an overview of the theories and methodologies currently used in various fields of computational molecular sciences, ranging from biomedical sciences to material sciences. A special focus will be devoted to those models and algorithms related to molecular simulation

	techniques, including enhanced sampling and free energy methods. Such models will be illustrated along with relevant examples taken from recent literature and concerning different molecular modeling applications.
Wymagania wstępne	

4. Sposoby weryfikacji efektów uczenia się modułu

kod	nazwa (typ)	opis	efekty uczenia się modułu
MB_34_w_1	egzamin	Oral Exam. In addition to questions related to the basic knowledge of the course, students will be asked to present a scientific problem of their interest suitable to be treated with molecular modeling methodologies.	MB_34_1, MB_34_2, MB_34_3

5. Rodzaje prowadzonych zajęć

kod	rodzaj prowadzonych zajęć			praca własna studenta		sposoby weryfikacji efektów uczenia się
	nazwa	opis (z uwzględnieniem metod dydaktycznych)	liczba godzin	opis	liczba godzin	
MB_34_fs_1	wykład	detailed discussion by the lecturer of the issues listed in the table "module description" using the table and/or multimedia presentations	48	supplementary reading, working with the textbook	102	MB_34_w_1