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| 1. | Nazwa kierunku | biofizyka |
| 2. | Wydział | Wydział Nauk Ścisłych i Technicznych |
| 3. | Cykl rozpoczęcia | 2021/2022 (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 | <p>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.</p> <p>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</p> |

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| | 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 |