

<b>Course title in English</b>	<b>Molecular simulations in chemistry</b>
Course title in Polish	Symulacje molekularne w chemii
Course code	
Type of course	Lecture
Level of course	PhD
Year of study	1-4
Semester/trimester	1/3/5/7
Number of hours/credits allocated	30/2
Name of lecturer	Józef Adam Liwo
Objective of the course (expected learning outcomes and competences to be acquired)	<p><u>Knowledge:</u></p> <p>Acquisition of the knowledge specified in the "Course contents" section.</p> <p><u>Skills:</u></p> <p>Ability to select appropriate simulation method(s) to solve a given chemical or biochemical problem, ability to use the simulation methods and interpret their results.</p> <p><u>Social competence:</u></p> <p>Work in a team, ability to take active part in constructive discussions.</p>
Prerequisites	Theoretical chemistry including quantum chemistry and statistical mechanics, physical chemistry, mathematics, information technology
Course contents	<ol style="list-style-type: none"> <li>1. Purpose, time-, and size-scales of molecular simulations.</li> <li>2. Energy surfaces of molecules.</li> <li>3. All-atom force fields: purpose, derivation, and parameterization</li> <li>4. Treatment of solvent in force fields. Models of water.</li> <li>5. Metropolis Monte Carlo.</li> <li>6. Molecular dynamics.</li> <li>7. Calculating ensemble-averages and error estimation in simulations.</li> <li>8. Umbrella-sampling simulations and the weighted-histogram analysis method.</li> </ol>

	<p>9. Generalized-ensemble simulations.</p> <p>10. Enlarging the time- and size-scale of simulations: coarse-grained models. The CABS and UNRES force fields.</p> <p>11. Thermodynamics and kinetics of protein folding from simulations. QM/MM simulations.</p>
Recommended reading	<p>A.1. Leach: <i>Molecular Modeling: Principles and Applications</i>, Pearson Education EMA, 2001.</p> <p>A.2. D. Frenkel, B.A. Smit, <i>Understanding Molecular Simulation: From Algorithms to Applications</i>. Academic Press, 2000.</p>
Teaching methods	Lecture with multimedia presentation.
Assessment methods	Doing assignments throughout the course, final exam
Language of instruction	Polish