

Course code																																	
Type and description	Elective Course in Physics																																
ECTS credit	1																																
Course name	Density Functional Theory 1																																
Course name in Polish	Teoria funkcjonału gęstości 1																																
Language of instruction	English																																
Course level	8 PRK																																
Course coordinator	prof. dr hab. Katarzyna Pernal																																
Course instructors	prof. dr hab. Katarzyna Pernal, dr inż. Ewa Pastorczak																																
Delivery methods and course duration	<table border="1"> <thead> <tr> <th></th> <th>Lecture</th> <th>Tutorials</th> <th>Laboratory</th> <th>Project</th> <th>Seminar</th> <th>Other</th> <th>Total of teaching hours during semester</th> </tr> </thead> <tbody> <tr> <td>Contact hours</td> <td></td> <td></td> <td></td> <td>15</td> <td></td> <td></td> <td>15</td> </tr> <tr> <td>E-learning</td> <td>No</td> <td>No</td> <td>No</td> <td>No</td> <td>No</td> <td>No</td> <td></td> </tr> <tr> <td>Assessment criteria (weightage)</td> <td></td> <td></td> <td></td> <td>100%</td> <td></td> <td></td> <td></td> </tr> </tbody> </table>		Lecture	Tutorials	Laboratory	Project	Seminar	Other	Total of teaching hours during semester	Contact hours				15			15	E-learning	No	No	No	No	No	No		Assessment criteria (weightage)				100%			
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Course objective	Theoretical foundations of density functional theory, its approximate formulations, and present-days applications of DFT.																																
Learning outcomes	Student knows theoretical foundations of density functional theory. Student recognizes differences between local and semilocal exchange-correlation density functionals. (W4, U4, K1)																																
Assessment methods	Take-home exam and presentation.																																
Prerequisites	Knowledge of quantum mechanics (advanced level), many-electron physics (basic level)																																
Course content with delivery methods	<ol style="list-style-type: none"> (1) Hohenberg-Kohn theorems. (2) Kohn-Sham equations. (3) Approximate density functionals. 																																

		(4) Examples of applications of DFT methods.
Basic materials	reference	Density-Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang (Oxford Science Publications).
Other materials	reference	Scientific papers.
Average workload classroom	student outside	10 h
Comments		
Last update		