

Course code																																	
Type and description	Elective Course in Physics																																
ECTS credit	1																																
Course name	Density Functional Theory 2																																
Course name in Polish	Teoria funkcjonału gęstości 2																																
Language of instruction	English																																
Course level	8 PRK																																
Course coordinator	prof. dr hab. Katarzyna Pernal																																
Course instructors	prof. dr hab. Katarzyna Pernal																																
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 at advanced level.																																
Learning outcomes	Student knows Kohn-Sham formulation of density functional theory. Student understands differences between semilocal and orbital-dependent functionals. (W4, U4, K1)																																
Assessment methods	Take-home exam and presentation.																																
Prerequisites	Knowledge of quantum mechanics (advanced level), many-electron physics (basic level) and density functional theory (basic level)																																
Course content with delivery methods	<ol style="list-style-type: none"> (1) Levy constrained search construction of density functionals (2) Matrix formulation of the Kohn-Sham equations (3) Orbital-dependent functionals.. 																																
Basic reference	Density-Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang (Oxford																																

materials	Science Publications). A primer in density functional theory, C.Fiolhais, F. Nogueira, M. Marques (Eds.) Springer
Other materials	reference Scientific papers.
Average workload classroom	student outside 10 h
Comments	
Last update	