

Module title		Abbreviation
Computational Materials Science (DFT)		11-CMS-161-m01
Module coordinator		Module offered by
Managing Director of the Institute of Theoretical Physics and Astrophysics		Faculty of Physics and Astronomy
ECTS	Method of grading	Only after succ. compl. of module(s)
8	numerical grade	--
Duration	Module level	Other prerequisites
1 semester	graduate	--
Contents		
<ol style="list-style-type: none"> 1. Density functional theory (DFT) 2. Wannier functions and localized basis functions 3. Numerical evaluation of topological invariants 4. Hartree-Fock and static mean-field theory 5. Many-body methods for solid state physics 6. Anderson impurity model (AIM) and Kondo physics 7. Dynamical mean-field theory (DMFT) 8. DFT + DMFT methods for realistic modeling of solids 9. Strongly correlated electrons 		
Intended learning outcomes		
<p>Aside from the theoretical discussion of these topics, the students carry out hands-on exercises from the CIP pool. The participants are introduced to the use of DFT software packages such as VASP or Wien2k and to the construction of maximally localised Wannier functions through the projection of DFT results on atom orbitals with the software wanniergo. Furthermore, the students learn how to construct many-particle solutions of AIM and observe border cases such as the Kondo regime. Impurity solvers such as exact diagonalisation or continuous-time quantum Monte Carlo are utilised to solve the self consistency equations of dynamic molecular field theory (DMFT). These steps are necessary to reach the peak of the lecture: a DFT-DMFT calculation of a strongly correlated transition metal oxide such as SrVO₃.</p>		
Courses (type, number of weekly contact hours, language – if other than German)		
V (4) + R (2) Module taught in: German or English		
Method of assessment (type, scope, language – if other than German, examination offered – if not every semester, information on whether module is creditable for bonus)		
<p>written examination (approx. 90 to 120 minutes) or oral examination of one candidate each (approx. 30 minutes) or oral examination in groups (groups of 2, approx. 30 minutes per candidate) or project report (approx. 8 to 10 pages) or presentation/talk (approx. 30 minutes).</p> <p>If a written examination was chosen as method of assessment, this may be changed and assessment may instead take the form of an oral examination of one candidate each or an oral examination in groups. If the method of assessment is changed, the lecturer must inform students about this by four weeks prior to the original examination date at the latest.</p> <p>Assessment offered: In the semester in which the course is offered and in the subsequent semester Language of assessment: German and/or English</p>		
Allocation of places		
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Additional information		
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Referred to in LPO I (examination regulations for teaching-degree programmes)		
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Module appears in		

Master's degree (1 major) Mathematics (2016)
Master's degree (1 major) Physics (2016)
Master's degree (1 major) Mathematical Physics (2016)
Master's degree (1 major) Computational Mathematics (2016)
Master's degree (1 major) Functional Materials (2016)
Master's teaching degree Gymnasium MINT Teacher Education PLUS, Elite Network Bavaria (ENB) (2016)
Supplementary course MINT Teacher Education PLUS, Elite Network Bavaria (ENB) (2016)
Master's degree (1 major) Computational Mathematics (2019)
Master's degree (1 major) Mathematics (2019)
Master's degree (1 major) Physics (2020)
Master's teaching degree Gymnasium MINT Teacher Education PLUS, Elite Network Bavaria (ENB) (2020)
Supplementary course MINT Teacher Education PLUS, Elite Network Bavaria (ENB) (2020)
Master's degree (1 major) Mathematical Physics (2020)