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

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

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 wannier90. 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 $SrVO_3$.

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)

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).
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.
Assessment offered: In the semester in which the course is offered and in the subsequent semester
Language of assessment: German and/or English

Allocation of places

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Additional information

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Workload

240 h

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) Master's degree (1 major) Computational Mathematics (2022) Master's degree (1 major) Functional Materials (2022) Master's degree (1 major) Mathematics (2022) Master's degree (1 major) Mathematical Physics (2022)