Module title			Abbreviation
Computational Materials Science (DFT)			11-CMS-Int-201-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

Theoretical treatment of the above topics complemented by hands-on tutorials to be held in the CIP-Pool. Familiarity with DFT software packages such as VASP or Wien2k and construction of maximally localized Wannier functions by projecting DFT results onto atomic orbitals using wannier90. Knowledge how to obtain many-body solutions of the AIM and explore some of its limiting cases such as the Kondo regime. Ability to use impurity solvers based on exact diagonalization or continuous-time quantum Monte Carlo for the solution of the DMFT self-consistency equations.

Courses (type, number of weekly contact hours, language — if other than German)

V (4) + R (2)
Module taught in: 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)

a) written examination (approx. 90 to 120 minutes) or
b) oral examination of one candidate each (approx. 30 minutes) or
c) oral examination in groups (groups of 2, approx. 30 minutes per candidate) or
d) project report (approx. 8 to 10 pages) or
e) 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.
Language of assessment: English
Assessment offered: In the semester in which the course is offered and in the subsequent semester

Allocation of places

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Additional information

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Workload

240 h

Teaching cycle
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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) Physics International (2020) exchange program Physics (2023) Master's degree (1 major) Physics International (2024)