Module title			Abbreviation
Computational Materials Science			11-CMS-122-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	Certain prerequisites must be met to qualify for admission to assessment. The lecturer will inform students about the respective details at the beginning of the course. Registration for the course will be considered a declaration of will to seek admission to assessment. If students have obtained the qualification for admission to assessment over the course of the semester, the lecturer will put their registration for assessment into effect. Students who meet all prerequisites will be admitted to assessment in the current or in the subsequent semester. For assessment at a later date, students will have to obtain the qualification for admission to assessment anew.	

Contents

Density functional theory (DFT)/local-density approximation (exercise with "Wien2k"; band structure programme, Green's functions, quantum dots, Anderson impurity model (exercise, implementation of the exact diagonalisation/Lanczos), introduction to continuous-time quantum Monte Carlo (exercise), crystal field symmetry, Coulomb interaction, dynamic mean field theory (DMFT exercise). Lecture + 4-5 exercises in the CIP pool. The exercises implement the basic ideas of different algorithms, either based on template programmes or on completely self-written programmes. Electronic submission of all exercises and approx. 20 minutes presentation about one of the 4-5 topics of the lecture/exercise (freely chosen by the student) with a little more elaboration on the topic than in the exercise.

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 and construction of maximally localized Wannier functions by projecting DFT results onto atomic orbitals using wannier90. Focus on applications to topological materials. 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 + R (no information on SWS (weekly contact hours) and course language available)

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 (90 minutes) or b) oral examination of one candidate each or oral examination in groups (approx. 30 minutes per candidate) or c) project report (approx. 8 to 10 pages, time to complete: 1 to 4 weeks) or d) presentation/seminar presentation (approx. 30 minutes)
Assessment offered: When and how often assessment will be offered depends on the method of assessment and will be announced in due form under observance of Section 32 Subsection 3 ASPO (general academic and examination regulations) 2009.
Language of assessment: German or English

Allocation of places

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Additional information

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Workload
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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 (2010) Master's degree (1 major) Physics (2011) Master's degree (1 major) Nanostructure Technology (2011) Master's degree (1 major) Nanostructure Technology (2010) Master's degree (1 major) FOKUS Physics (2010)