Module title	Abbreviation
Computational Materials Science	11-CMS-131-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 semesters.

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

The students have advanced knowledge of mathematical methods of material sciences. They are able to develop algorithms for the application of these methods and to implement them into programmes.

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 (approx. 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, 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)