Georg-August-Universität Göttingen **Module B.Phy.5723: Hands-on course on Density-Functional calculations 1**	3 C 3 WLH

Learning outcome, core skills:	**Workload:**
Students will be able to perform first-principles electronic-structure and ab-initio molecular dynamics simulations, understand the results and judge their accuracy. They will have a basic knowledge of the underlying methods. They will know simple methods of anticipating and describing electronic and atomic structure and chemical bonds.	Attendance time: 40 h Self-study time: 50 h

Course: B.Phy.5723.C **Hands-on course on Density-Functional calculations 1 (Block course)** *Contents*: 1. Theoretical foundation of first-principles calculations (lecture 10 h) 2. Simple concepts of electronic structure and chemical binding (lecture 10 h) 3. Hands on Course with the CP-PAW code (Exercise 20 h)	
Examination: oral (approx 30 min), presentation (30 min) or report B.Phy.5723.Mp: Hands-on course on Density-Functional calculations 1 **Examination prerequisites:** regular participation **Examination requirements:** The student is able to describe topics from the course and to respond to questions. A presentation or a report will describe a specified home project.	3 C

Admission requirements: none	**Recommended previous knowledge:** none
Language: English, German	**Person responsible for module:** Prof. Bloechl
Course frequency: each summer semester	**Duration:** 1 semester[s]
Number of repeat examinations permitted: three times	**Recommended semester:** Bachelor: 6; Master: 1 - 4
Maximum number of students: 20	