Georg-August-Universität Göttingen **Module B.Phy.5649: Biomolecular Physics and Simulations**	4 C 2 WLH

	Workload:
Learning outcome, core skills: **Learning objectives:** This combined lecture and hands-on computer tutorial offers the possibility to deepen the knowledge about theory and computer simulations of biomolecular systems, particularly proteins, and can be understood as continuation of the lecture with exercises "Theoretical and Computational Biophysics" (usually taking place in the previous winter semester). During the exercises, the knowledge presented in the lecture will be applied to practical examples to further deepen and strengthen the understanding. By completing homework sets, which will be distributed after each lecture, additional aspects of the addressed topics during the lecture shall be worked out. The homework sets will be collected during the corresponding exercises. **Competencies:** Whereas the winter term lecture with exercises "Theoretical and Computational Biophysics" emphasized the principles of running and analysing simple atomistic force field-based simulations, this advanced course will broaden our view and introduce basic principles, concepts and methods in computational biophysics, particularly required to understand biomolecular function, namely thermodynamic quantities such as free energies and affinities. Further, inclusion of quantum mechanical simulation techniques will allow to also simulate chemical reactions, e.g., in enzymes.	Attendance time: 28 h Self-study time: 92 h

Course: Lecture with Exercises Biomolecular Physics and Simulations	

Examination: Oral examination (approx. 30 minutes) **Examination requirements:** Basic knowledge and understanding of the material covered in the course such as: Free energy calculations, Rate Theory, Non-equilibrium thermodynamics, Quantum mechanical methods (Hartree-Fock and Density Functional Theory), enzymatic catalysis; "handson" computational calculations and simulations	4 C

Admission requirements: none	**Recommended previous knowledge:** B.Phy.5648 Theoretical and Computational Biophysics
Language: English, German	**Person responsible for module:** Hon.-Prof. Dr. Karl Helmut Grubmüller
Course frequency: each summer semester	**Duration:** 1 semester[s]
Number of repeat examinations permitted: three times	**Recommended semester:** Bachelor: 5 - 6; Master: 1 - 4
Maximum number of students: 30	