Georg-August-Universität Göttingen **Module B.Phy.5648: Theoretical and Computational Biophysics**	4 C 2 WLH

Learning outcome, core skills: This combined lecture and hands-on computer tutorial focuses on the basics of computational biophysics and deals with questions like "How can the particle dynamics of thousands of atoms be described precisely?" or "How does a sequence alignment algorithm function?" The aim of the lecture with exercises is to develop a physical understanding of those "nano maschines" by using modern concepts of non-equilibrium thermodynamics and computer simulations of the dynamics on an atomistic scale. Moreover, the lecture shows (by means of examples) how computers can be used in modern biophysics, e.g. to simulate the dynamics of biomolecular systems or to calculate or refine a protein structure. No cell could live without the highly specialized macromolecules. Proteins enable virtually all tasks in our bodies, e.g. photosynthesis, motion, signal transmission and information processing, transport, sensor system, and detection. The perfection of proteins had already been highly developed two billion years ago. 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.	**Workload:** Attendance time: 28 h Self-study time: 92 h

Course: B.Phy.5648.Lec **Theoretical and Computational Biophysics** (Lecture, Exercise)	
Examination: Oral examination (approx. 30 minutes) B.Phy.5648.Mp: Theoretical and Computational Biophysics **Examination requirements:** Protein structure and function, physics of protein dynamics, relevant intermolecular interactions, principles of molecular dynamics simulations, numeric integration, influence of approximations, efficient algorithms, parallel programing, methods of electrostatics, protonation balances, influence of solvents, protein structure determination (NMR, X-ray), principal component analysis, normal mode analysis, functional mechanisms in proteins, bioinformatics: sequence comparison, protein structure prediction, homology modeling, and hands-on computer simulation.	4 C

Admission requirements: none	**Recommended previous knowledge:** • Introduction to Biophysics • Introduction to Physics of Complex Systems
Language: English, German	**Person responsible for module:** Hon.-Prof. Dr. Karl Helmut Grubmüller
Course frequency: each winter 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	