

## Theoretische und Computergestützte Biophysik (WS 2015/16)

Theoretical and Computational Biophysics

Helmut Grubmüller (HG), Bert de Groot (BdG) and Jochen Hub (JH)

Modul B.Phy.5648 (Lehramt: M.Phy.710.Mp)

Mondays 16:15-17:45 in HS3 (A0.105) and PC-Pool A.02.115 or SR1 (A1.101), Physics Faculty

Date	Topic	Type/Room
2015-10-26	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L1 = Lecture in lecture hall 3
2015-11-02	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (JH)	P1= Practical training in room A.02.115
2015-11-09	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (JH)	L2
2015-11-16	Protein data bank, structure determination by NMR / x-ray, refinement (JH)	L3
2015-11-23	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	P2 in room A.02.115
2015-11-30	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	P3 in room A.02.115
2015-12-07	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (JH)	L4
2015-12-14	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	P4 in room SR1 (A1.101)
2015-12-21	Monte Carlo, normal mode analysis, principal components (HG)	L5
2016-01-11	Monte Carlo, normal mode analysis, principal components (BdG)	P5 in room SR1 (A1.101)
2016-01-18	Charge transfer & photosynthesis, electrostatics methods (HG)	L6
2016-01-25	Charge transfer & photosynthesis, electrostatics methods (BdG)	P6 in room SR1 (A1.101)
2016-02-01	Aquaporin / ATPase: two examples from current research (HG)	L7
2016-02-08	Aquaporin / ATPase: two examples from current research (BdG)	P7 in room SR1 (A1.101)

### Potential exam Dates: Feb/March 2016

24.-25.2.2016

14.-16.03.2016

Lecture period 26.10.2015-12.02.2016

Semester break 23.12.2015-05.01.2016