Theoretische und Computergestützte Biophysik (WS 2016/17)

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 16:00-17:30 (16:15-17:45) in Lecture Hall HS3 (A0.105) and PC-Pool C.00.110, Physics Faculty

Date	Topic	Type/Room
2016-10-17	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L1 = Lecture in lecture hall 3
2016-10-24	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (BdG)	P1= Practical training in PC-Pool C.00.110
2016-10-31	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (JH)	Lecture 2
2016-11-07	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (JH)	Practical Training 2
2016-11-14	Protein data bank, structure determination by NMR / x-ray, refinement (JH)	Lecture 3
2016-11-21	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	Practical Training 3
2016-11-28	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (JH)	Lecture 4
2016-12-05	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	Practical Training 4
2016-12-12	Monte Carlo, normal mode analysis, principal components (HG)	Lecture 5
2016-12-19	Monte Carlo, normal mode analysis, principal components (BdG)	Practical Training 5
2017-01-09	Charge transfer & photosynthesis, electrostatics methods (HG)	Lecture 6
2017-01-16	Aquaporin / ATPase: two examples from current research (HG)	Lecture 7
2017-01-23	Charge transfer & photosynthesis, electrostatics methods (BdG)	Practical Training 6
2017-01-30	Aquaporin / ATPase: two examples from current research (BdG)	Practical Training 7

Potential exam Dates: Feb/March 2017

27.2.-3.3.2017 (week 9)

6.-10.3.2017 (week 10)

Lecture period 17.10.2016-3.2.2017

Semester break 24.12.2016-6.1.2017