Theoretische und Computergestützte Biophysik (WS 2017/18)

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 Lecture Hall HS3 (A0.105) and PC-Pool C.00.110, Physics Faculty

Date	Topic	Type/Room
2017-10-16	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	L1 = Lecture in lecture hall 3
2017-10-23	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (BdG)	P1= Practical training in PC-Pool C.00.110
2017-10-30	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (HG)	Lecture 2
2017-11-06	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	Practical Training 2
2017-11-13	Protein data bank, structure determination by NMR / x-ray, refinement (HG)	Lecture 3
2017-11-20	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	Practical Training 3
2017-11-27	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (JH)	Lecture 4
2017-12-04	Monte Carlo, normal mode analysis, principal components (HG)	Lecture 5
2017-12-11	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	Practical Training 4
2017-12-18	Monte Carlo, normal mode analysis, principal components (BdG)	Practical Training 5
2018-01-08	Charge transfer & photosynthesis, electrostatics methods (HG)	Lecture 6
2018-01-15	Charge transfer & photosynthesis, electrostatics methods (BdG)	Practical Training 6
2018-01-22	Aquaporin / ATPase: two examples from current research (HG)	Lecture 7
2018-01-29	Aquaporin / ATPase: two examples from current research (BdG)	Practical Training 7

Potential exam Dates: Feb/March 2018

26.02.-09.03.2018, weeks 9 and 10

Lecture period	16.10.2017-02.02.2018
Semester break	23.12.2017-07.01.2018