

Theoretische und Computergestützte Biophysik (WS 2019/20)

Theoretical and Computational Biophysics

Helmut Grubmüller (HG), Bert de Groot (BdG)

Tutor for Practical Trainings Tom Lam

Modul B.Phys.5648 (Lehramt: M.Phys.710.Mp), 4 C

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

Date	Topic	Type/Room
2019-10-21	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (HG)	Lecture 1
2019-10-28	Introduction, protein structure and function, molecular dynamics, approximations, numerical integration (BdG)	Practical Training 1
2019-11-04	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (HG)	Lecture 2
2019-11-11	Protein data bank, structure determination by NMR / x-ray, refinement (HG)	Lecture 3
2019-11-18	Tertiary structure, force field contributions, efficient algorithms, protonation, periodic boundaries, solvent, ions, NVT/NPT ensembles (BdG)	Practical Training 2
2019-11-25	Protein data bank, structure determination by NMR / x-ray, refinement (BdG)	Practical Training 3
2019-12-02	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (HG)	Lecture 4
2019-12-09	Bioinformatics: Sequence alignment & evolution, structure prediction, homology modelling (BdG)	Practical Training 4
2019-12-16	Monte Carlo, normal mode analysis, principal components (HG)	Lecture 5
2020-01-06	Monte Carlo, normal mode analysis, principal components (BdG)	Practical Training 5
2020-01-13	Charge transfer & photosynthesis, electrostatics methods (HG)	Lecture 6
2020-01-20	Charge transfer & photosynthesis, electrostatics methods (BdG)	Practical Training 6
2020-01-27	Aquaporin / ATPase: two examples from current research (HG)	Lecture 7
2020-02-03	Aquaporin / ATPase: two examples from current research (BdG)	Practical Training 7

Potential exam Dates: March 2020

02.-13. March 2019

Lecture period 21.10.2019-07.02.2020

Semester break 21.12.2019-05.01.2020