

Vorlesung: Biomolekulare Physik und Simulationen (SS 2019)

Lecture: Biomolecular Physics and Simulations

Lecturer: Helmut Grubmüller (HG) and Bert de Groot (BdG)

Tutor for practicals: Malte Schäffner

Modul B.Phys.5649, 4C

Mondays, 16:00-17:30 in Lecture in Lecture Hall 3 (HS3, A0.105) or Practical in Seminar Room 1 (SR1, A1.101), both in the Physics Faculty

Date	Topic	Type/Room
2019-04-15	Short introduction to MD simulation, molecular machines, Markov theory (HG)	Lecture 1 Lecture Hall 3
2019-04-29	Short introduction to MD simulation, molecular machines, Markov theory (BdG)	Practical 1 SR1, A1.101
2019-05-06	Quantum mechanical methods: Enzyme catalysis (HG)	Lecture 2
2019-05-13	Quantum mechanical methods: Enzyme catalysis (BdG)	Practical 2
2019-05-20	Hartree-Fock, density functional theory (HG)	Lecture 3
2019-05-27	Free energy calculations: Molecular recognition (HG)	Lecture 4
2019-06-03	Hartree-Fock, density functional theory (BdG)	Practical 3
2019-06-17	Free energy calculations: Molecular recognition (BdG)	Practical 4
2019-06-24	Non-equilibrium thermodynamics: Molecular driving forces (HG)	Lecture 5
2019-07-01	Rate theory: Biomolecular efficiency (HG)	Lecture 6
2019-07-08	Non-equilibrium thermodynamics: Molecular driving forces (BdG)	Practical 5
2019-07-15	Rate theory: Biomolecular efficiency (BdG)	Practical 6

Lecture period 15 April-19 July 2019

Whit Monday: 10 May 2019

Examination block: 29.7. to 09.8.2019