Vorlesung: Biomolekulare Physik und Simulationen (SS 2018)

Lecture: Biomolecular Physics and Simulations

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

Modul B.Phy.5649

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
2018-04-09	Short introduction to MD simulation, molecular machines, Markov theory (HG)	Lecture 1
2018-04-16	Short introduction to MD simulation, molecular machines, Markov theory (BdG)	Practical 1
2018-04-23	Quantum mechanical methods: Enzyme catalysis + Hartree-Fock, density functional theory (HG)	Lecture 2 + 3
2018-04-30	--	--
2018-05-07	Quantum mechanical methods: Enzyme catalysis (BdG)	Practical 2
2018-05-14	Free energy calculations: Molecular recognition (HG)	Lecture 4
2018-05-28	Hartree-Fock, density functional theory (BdG)	Practical 3
2018-06-04	Free energy calculations: Molecular recognition (BdG)	Practical 4
2018-06-11	Non-equilibrium thermodynamics: Molecular driving forces (HG)	Lecture 5
2018-06-18	Protein Design (Leonard Heinz)	Extra Practical
2018-06-25	Non-equilibrium thermodynamics: Molecular driving forces (BdG)	Practical 5
2018-07-02	Rate theory: Biomolecular efficiency (HG)	Lecture 6
2018-07-09	Rate theory: Biomolecular efficiency (BdG)	Practical 6

Lecture period 9 April-13 July 2018
Whit Monday: 21 May 2018

Examination block: 30.7. - 10.8.2018