

## Vorlesung: Biomolekulare Physik und Simulationen (SS 2020)

Lecture: Biomolecular Physics and Simulations

Modul B.Phy.5649, 4 Credits

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

Tutor for practicals: Tom Lam

Time: Mondays, 16:00-17:30

Location: Lectures and practicals will be conducted as virtual classes this summer term

Date	Topic	Type
2020-04-20	Short introduction to MD simulation, molecular machines, Markov theory (HG)	Lecture 1
2019-04-27	Quantum mechanical methods: Enzyme catalysis (HG)	Lecture 2
2020-05-04	Short introduction to MD simulation, molecular machines, Markov theory (BdG)	Practical 1
2020-05-11	Quantum mechanical methods: Enzyme catalysis (BdG)	Practical 2
2020-05-18	Hartree-Fock, density functional theory (HG)	Lecture 3
2020-05-25	Hartree-Fock, density functional theory (BdG)	Practical 3
2020-06-08	Free energy calculations: Molecular recognition (HG)	Lecture 4
2020-06-15	Free energy calculations: Molecular recognition (BdG)	Practical 4
2020-06-22	Non-equilibrium thermodynamics: Molecular driving forces (HG)	Lecture 5
2020-06-29	Non-equilibrium thermodynamics: Molecular driving forces (BdG)	Practical 5
2020-07-06	Rate theory: Biomolecular efficiency (HG)	Lecture 6
2020-07-13	Rate theory: Biomolecular efficiency (BdG)	Practical 6

Lecture period 14 April-17 July 2020

Whit Monday: 1 June 2020

Examination block: 3 to 14 August 2020