

## Vorlesung: Biomolekulare Physik und Simulationen (SS 2021)

Lecture: Biomolecular Physics and Simulations

Undergraduate Students: Modul B.Phy.5649, 4 Credits (compulsory examination)

PhD Candidates: 2 Credits (optional examination)

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

Tutor for practicals: Sara Gabrielli [sara.gabrielli@mpibpc.mpg.de](mailto:sara.gabrielli@mpibpc.mpg.de)

Time: Mondays, 16:00-17:30

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

<https://zoom.us/j/96771881823?pwd=QTVUdVdaK1A4ZGwvZTh1MjZENE0rQT09>

Meeting ID: 967 7188 1823

Passcode: 591549

Date	Topic	Type
2021-04-12	Short introduction to MD simulation, molecular machines, Markov theory (HG)	Lecture 1
2021-04-19	Short introduction to MD simulation, molecular machines, Markov theory (BdG)	Practical 1
2019-04-26	Quantum mechanical methods: Enzyme catalysis (HG)	Lecture 2
2021-05-03	Hartree-Fock, density functional theory (HG)	Lecture 3
2021-05-10	Quantum mechanical methods: Enzyme catalysis (BdG)	Practical 2
2021-05-17	Hartree-Fock, density functional theory (BdG)	Practical 3
2021-05-31	Free energy calculations: Molecular recognition (HG)	Lecture 4
2021-06-07	Non-equilibrium thermodynamics: Molecular driving forces (HG)	Lecture 5
2021-06-14	Rate theory: Biomolecular efficiency (HG)	Lecture 6
2021-06-21	Free energy calculations: Molecular recognition (BdG)	Practical 4
2021-06-28	Non-equilibrium thermodynamics: Molecular driving forces (BdG)	Practical 5
2021-07-05	Rate theory: Biomolecular efficiency (BdG)	Practical 6

Lecture period April 12 to July 11, 2021

Whit Monday/Pentecost: May 24, 2021

Examination block: July 26 to August 13, 2021