# Bad Honnef Physics School „Molecular Dynamics Simulations in Biophysics“

## April 26 – May 1, 2020, Physikzentrum Bad Honnef, Germany

| *Time* | *Sunday Apr 26* | *Monday Apr 27* | *Tuesday Apr 28* | *Wednesday Apr 29* | *Thursday Apr 30* | *Friday May 1* |
|---|---|---|---|---|---|---|
| 08:00 | | Breakfast | | | | |
| 09:00 – 10:00 | | **Martin Zacharias** Molecular Dynamics /Advanced Sampling | **Martin Zacharias** Protein/peptide Simulations | **Petra Imhof** Simulation studies on systems containing RNA and DNA | **Pavel Jungwirth** Charge scaling methods and applications | **Gerhard Stock** Collective motions and Markov Modeling of simulation data |
| 10:00 – 10:30 | | Discussion | Discussion | Discussion | Discussion | Discussion |
| 10:30 | | Coffee Break | | | | |
| 11:00 – 12:00 | | **Lars Schäfer** Membrane and membrane protein systems | **Dominik Horinek** Free energy simulations | **Helmut Grubmüller** Simulations studies on molecular machines | **Roland Netz** Non-Markovian simulation of equilibrium and non-equilibrium systems | **Bettina Keller** Extracting kinetics form enhanced sampling and Markov models |
| 12:00 – 12:30 | | Discussion | Discussion | Discussion | Discussion | Discussion |
| 12:30 | | Lunch | | | | |
| 14:00 – 15:00 | Arrival | **Nico van der Vegt** Macromolecular solvation | **Chris Oostenbrink** Alchemical Transformations | Excursion | **Frauke Gräter** Multi-Scale Simulations and force distribution analysis | End of the School |
| 15:00 – 15:30 | | Discussion | Discussion | | Discussion | |
| 15:30 | | Coffee Break | | | Coffee Break | |
| 16:00 – 18:80 | | Poster/Talks by students | Poster/Talks by students | | Poster/Talks by students | |
| 18:30 | Dinner | | | | | |
| 20:00 – … | Intro-Talk | | | Special talk | | |