

## Molecular Dynamics Simulations in Biophysics

April 26 - May 1, 2020, Physikzentrum Bad Honnef, Germany

Organised by

**Dominik Horinek (University of Regensburg) and Martin Zacharias (TU Munich)**

Molecular Dynamics (MD) simulations have become a powerful tool in modern biomolecular science and allow one to follow the motion of molecules at high spatial and time resolution. The full potential of MD lies in the link between this information and experimental properties: with the help of statistical mechanics it is possible to extract a variety of thermodynamic and kinetic properties of a molecular system. A major focus will be on efficient methods to extract thermodynamic quantities such as solvation properties and free energies from simulations. Advanced techniques such as multi-scale methods and combinations of classical molecular mechanics combined with quantum mechanical approaches will also be covered. The methods will be illustrated on several examples and further evaluated in Discussion sessions. Participants are invited to present posters or to give short talks in extra sessions.

### Confirmed Speakers:

Frauke Graeter (HITS Heidelberg, Germany)

Helmut Grubmüller (MPI Göttingen, Germany)

Dominik Horinek (University of Regensburg, Germany)

Petra Imhof (University of Stavanger, Norway)

Pavel Jungwirth (Charles University, Prague, Czech Rep.)

Bettina Keller (FU-Berlin, Germany)

Roland Netz (FU-Berlin, Germany)

Chris Oostenbrink (BOKU, Vienna, Austria)

Lars Schäfer (University of Bochum, Germany)

Gerhard Stock (University of Freiburg, Germany)

Nico van der Vegt (TU Darmstadt, Germany)

Martin Zacharias (TU Munich, Germany)

### Fees:

Covering full board and lodging at the Physikzentrum Bad Honnef  
200 € (for DPG members 100 €).

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