The Molecular Simulation Group (Schäfer Group)

Prof. Dr. Lars Schäfer
Lehrstuhl für Theoretische Chemie
Ruhr-Universität Bochum
D-44780 Bochum
Germany
Phone: +49 (0)234 32 21582
E-mail: lars.schaefer@ruhr-uni-bochum.de

Who we are and what we do

We investigate the link between structure, dynamics, and function of biological macromolecules by means of computer simulations. To that end, we develop and apply efficient computational methods to study biomolecular systems at the atomistic and coarse-grained level, mostly using classical molecular dynamics (MD) type simulations. Our group is also part of the RESOLV cluster of excellence, Solvation Science@RUB. Have a look at Research for more details.

Research

Group Members

List of Publications