Carl von Ossietzky
Universität
Oldenburg

Institut für PHYSIK

PHYSICAL COLLOQUIUM

INVITATION

Monday, 12.12.2022, 4.15 p.m., Room W02 1-148 and per
video conference: https://meeting.uol.de/b/anj-2vc-j6s-fwe

speaks

Dr. Till Rudack

Project Group Leader (PG Biomolecular Simulations),
Ruhr-Universität Bochum, Bochum (RUB), Germany

about

"Calculating the Secrets of Life -
Quantum Mechanics and Molecular Mechanics Simulations of Vital Molecular Machines“

Life is motion driven through cellular processes carried out by molecular machines. In order to understand and manipulate such cellular processes, scale-spanning knowledge of structure, dynamics, and function of molecular machines is needed. This knowledge cannot be obtained by one method alone. Therefore, I developed a strategy that combines quantum mechanical calculations, molecular mechanics simulations and artificial intelligence-based structure prediction with data from structure resolving experiments to investigate the assembly and functional cycle of molecular machines from the electron up to the molecular level. The strategy provides insights into the interplay between local processes like chemical reactions and global conformational changes driving cellular function. Derived structural dynamic models are validated based on comparison of calculated infrared and UV/VIS spectroscopic data with experimental measurements. Methods and application of the strategy will be presented for a small molecular switch, an ion channel, and a large molecular motor.

spectroscopy of a photonic mode.

All interested persons are cordially invited.

Prof. Dr. Ilia Solov’yov