GESELLSCHAFT DEUTSCHER CHEMIKER

Ortsverband Osnabrück

“Probing the Chemomechanics of Membrane-Bound Biomolecular Machines with Molecular Simulations”

Prof. Dr. Lars Schäfer

Ruhr-Universität Bochum, Theoretische Chemie, Molekulare Simulation

The central theme of the talk is how small-scale chemical reactions, which involve the making and breaking of chemical bonds, are coupled to large conformational changes that are linked to the biological functions of proteins.

As a prime example, we will discuss ATP-binding cassette (ABC) transporters, a class of membrane proteins that translocate substrate molecules across biological membranes by chemomechanically coupling ATP binding and hydrolysis in the nucleotide-binding domains to large-scale conformational changes of the transmembrane domains. Despite recent progress in the determination of high-resolution structures of substrate-bound ABC exporters, the inherently dynamic mechanism of substrate transport remained unclear at the atomic level.

We combined atomistic molecular dynamics (MD) simulations and hybrid quantum mechanics/molecular mechanics (QM/MM) simulations to reveal the atomic-level mechanisms of how the ATP-related “power stroke” ultimately leads to the conformational changes of the transporter that drive substrate translocation across the membrane. Analogies to the chemomechanics of other ATP-powered biomolecular machines will be discussed.

Der Vortrag findet am **Di., 13.05.2025, 16:15 Uhr** im CellNanOs statt:
Raum 38/201, Barbarastr. 11, 49076 Osnabrück

Besucher sind herzlich willkommen!

Der Ortsverbandsvorsitzende:
Prof. Dr. Andreas Hennig, Chemie Osnabrück, Universität Osnabrück
Tel.: 0541 969-2495; Email: andreas.hennig@uni-osnabrueck.de