

A U S H A N G

FREIE UNIVERSITÄT BERLIN

Fachbereich Physik

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D I S P U T A T I O N

Freitag, 16. Juli 2021, 16:30 Uhr

[WebEx](#)

Disputation über die Doktorarbeit von

Herrn Richard Schwarzl

Das Thema der Arbeit lautet:

Elasticity of Proteins and Polymers from Molecular Dynamics Simulations

Die Arbeit wurde unter der Betreuung von **Prof. Dr. R. Netz** durchgeführt.

Abstract: The functions of biomolecules are often linked to conformational changes on a molecular level. Force is a key factor in driving these conformational changes. Atomic force spectroscopy is commonly used to quantify the force response of individual molecules along a single reaction coordinate. Computational studies can elucidate unfolding mechanisms on an atomistic scale. Using molecular dynamics simulations in explicit water, I investigated different homopeptides. From the simulations, parameters relevant for a full model description, which employs the inhomogeneous partially rotating chain, are derived. A full description of the force-extension by a single heuristic formula is given at the end, including the force-dependent stretching of the contour length. I also present simulation results on a coiled coil linker, which is a common motif in signal transduction. By means of linear response functions, I analyze three different relative motions and quantify their suitability for signal transduction by calculating their respective transfer functions.

Die Disputation besteht aus einem Vortrag und einer angrenzenden Aussprache.

Der Vortrag ist öffentlich.

Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission

Prof. Dr. R. Bittl