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"MEASURING THE MECHANICAL PROPERTIES OF BIOMOLECULES IN LIQUIDS WITH LARGE-SCALE ATOMISTIC MOLECULAR DYNAMICS SIMULATIONS"

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INM, Leibniz-Saal, Campus D2 5
Gastgeber: Prof. Dr. Roland Bennewitz

Multiple biological processes involve the mechanical response of proteins and nucleic acids. Stretching and compressive forces induce local changes in their structure that can inhibit or enhanced the binding to other biomolecules, thus affecting their functionality. Experimental tools like optical and magnetic tweezers [1], and atomic force microscopy (AFM) [2] have paved the way for measuring the force-structure relation under physiological conditions in systems ranging from single molecules to viruses and cells.
In this talk, I'll discuss the challenges involved in simulating the adsorption of large biomolecules and their mechanical response. We have developed tools, based on robust and well-tested molecular dynamics (MD) biochemistry codes [3,4], to calculate the mechanical properties of complex systems composed by millions of atoms, while retaining an atomistic detailed description of the system. In particular, we'll show how these methods allow us to describe the mechanical properties of systems with an increasing range of complexity: (i) The dynamical ordering of water molecules over hydrophobic surfaces (e.g. graphene) and how it can be detected using AFM [5]; (ii) How MD simulations allow us to understand and guide the controlled adsorption of the most abundant plasma proteins (albumin and antibodies) to hydrophobic surfaces, thus enabling the development of better biosensors [6-8]; (iii) the atomistic origin of the striking differences in the mechanical properties of DNA and RNA is spite of their common double helix structure [9]; (iv) the electronic transport across redox metalloproteins [10], and (v) the atomistic deformation mechanisms behind the local effective elastic modulus extracted with continuum models from AFM measurements on antibodies.

[1] C. Bustamante, Z. Bryant, and S. B. Smith, Nature 421, 423 (2003) .
[2] Y. F. Dufrêne, et al., Nat. Nanotechnol. 12, 295 (2017) .
[3] M. Karplus and J.A. McCammon, Nature Struct. Biology 9, 646 (2002)
[4] D.A. Case et al., Amber17, University of California, San Francisco, CA. (2017)
[5] J. G. Vilhena et al, ACS Nano 10, 4288 (2016).
[6] J. G. Vilhena et al, Langmuir 32, 1742 (2016).
[7] J. G. Vilhena et al, Nanoscale 8, 13436 (2016).
[8] P. Rubio-Pereda et al, J. Chem. Phys, 146, 214704 (2017).
[9] Alberto Marin-Gonzalez, et al., PNAS 114, 7049 (2017).
[10] Marta P. Ruiz et al, J. Am. Chem. Soc., 139, 15337 (2017).

Wir laden 15 Minuten vor Beginn zu einem Get-together mit dem Referenten ein.

KONTAKT

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