Advances in Computational Mechanics

Einladung zum Vortrag

Models of Cellular Mechanobiology, from Focal Adhesions to Nuclear Pores

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It is now widely established that living cells sense mechanical signals, and respond actively by changing their phenotype accordingly. Cellular mechanotransduction is mediated by a combination of biochemical and biophysical mechanisms via mechanically induced changes in the structure and function of specific molecules. These mechanosensing molecules can function to initiate key biological processes, e.g. focal adhesion formation at the interface of cell's interaction with the extracellular matrix. Another example of potential molecular systems taking part in mechanotransduction is the nuclear pore complex that controls the nucleocytoplasmic transport, regulating gene expression and protein synthesis. In this talk, I will present some of our recent efforts aimed at better understanding of the molecular players involved in cellular mechanotransduction, focused on these two particular molecular complex systems, namely the focal adhesions and the nuclear pores. A series of molecular dynamics investigations will be presented to explore the potential mechanosensing and mechanotransduction functions of key molecules involved in focal adhesion formation. Using state-of-the-art molecular dynamics modeling and simulation techniques, the molecular mechanics of these proteins, their force-induced activation, and changes in their molecular conformation and binding partnership will be discussed. I will also present our "biological breadboard" platform for programmable, addressable adhesion/detachment of the cell to gold surfaces modified with a thiol-functionalized RGD peptide. Finally, I will present recent modeling efforts to explore the function of the nuclear pores and the relationship between biochemical factors and mechanical behavior of cargo being transported across the nuclear pore.

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IMETUM E.126 **Boltzmannstr. 11, 85748 Garching**

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