Molecular Simulations of Transport through Bacterial Nanopores

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Channels in the outer membrane of Gram-negative bacteria provide essential pathways for the controlled and unidirectional transport of ions, nutrients and metabolites into the cell. At the same time the outer membrane serves as a physical barrier for the penetration of noxious substances such as antibiotics into the bacteria. In this presentation the simulation of ion and substrate transport across such bacterial channels is investigated [1,2]. To this end we do employ molecular dynamics simulations and will, for example, model the transport of ions. Due to electroosmosis this ion transport can have a significant on the translocation of neutral substrates such as cyclodextrins [3].

The transport of neutral as well as charged substrates and especially antibiotics molecules through membrane pores will be discussed. Moreover, an example of a pore in an asymmetric lipopolysaccharide membrane will be reported as well.

Since the determination of free energy surfaces for substrate translocation using MD simulations is computationally very demanding, we developed a hybrid scheme of Brownian dynamics which can account for atomic details of a selected set of atoms. The basics of this scheme will be outlined briefly [4].

References

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