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Molecular Motor-Cargo systems: Modeling energetics of the kinesin with different approaches

Motor proteins, sometimes referred to as mechanoenzymes, are a group of proteins that maintain a large part of intracellular motion. Being *enzymes*, they undergo chemical reactions leading to energy conversion and changes of their conformation. Being *mechano*, they use the (chemical) energy to perform mechanical work, leading to the phenomena of motion. Series of novel experiments, e.g. single molecule observations, were performed to gain the knowledge about the performance of chemical states of the molecular motors as well as their dynamics in presence or absence of an external force.

At the same time, many theoretical models were proposed, offering deeper insight into the small-world (nanoworld) dynamics. They can be divided into three main categories: chemical models, ratchet models and molecular dynamics models. Chemical models focus on the Markovchain, kinetic description of the reaction cycles responsible for the mechanical transitions. Ratchet models are mostly based on sets of Langevin equations and treat the kinesin dimer as two linked Brownian particles moving in a periodic potential. Molecular dynamics models approach the problem from the low level dynamics of single or grouped molecules, based on information obtained from crystallographical data.

We show that by combining those complementary approaches one can gain deeper understanding of the dynamics and chemistry of the motor proteins. As a working example, we choose kinesin and dynein — motor proteins responsible for bidirectional transport of organelles and vesicles using microtubular tracts.

References

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