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Brownian dynamics simulations of a five site model for a motor protein on a bead spring substrate NABINA PAUDYAL, MARAL ADELI KOUDEHI, JUTTA LUETTMER-STRATHMANN, University of Akron — Motor proteins play an important role in many biological processes. For example, kinesin molecules are responsible for the transport of vesicles in nerve cells and their malfunction has been linked to neurodegenerative diseases. Unfortunately, the complexity of motor proteins and their environment makes it difficult to model the detailed dynamics of molecular motors over long time scales. In this work, we develop a simple coarse-grained model for a motor protein on a bead-spring substrate under tension. In our model, different pair potentials describe interactions between substrate and motor, motor components and substrate components. The movement of motor proteins entails ATP hydrolysis. We have identified model parameters corresponding to protein and chain conformations of a walking protein. The next step is to construct the mechano-chemical states that couple positional and chemical degrees of freedom and simulate cargo transport in confined geometries.

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