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Five-site model for a walking motor protein JUTTA LUETTNER-STRATHMANN, MARAL ADELI KOUDEHI, NABINA PAUDYAL, Department of Physics, The 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, pair potentials describe interactions between substrate and motor, motor components, and substrate components. The movement of motor proteins entails ATP hydrolysis, which is modeled in terms of mechano-chemical states that couple positional and chemical degrees of freedom. We apply the model to simulate cargo transport and the pulling of a chain molecule by a motor-protein walker.

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