

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Multistate coarse-grained molecular dynamics for modelling the catalytic cycle of allosteric enzyme. WENFEI LI, WEI WANG, Department of Physics, Nanjing University, Nanjing 210093, P. R. China, SHOJI TAKADA, Department of Biophysics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan — Biological functions of proteins are often related to their conformational dynamics, therefore, the intrinsic energy landscape. Adenylate kinase (AK), which catalyzes the reversible conversion from ATP and AMP to ADP, has widely been used as a model system of allosteric enzyme to study the role of conformational dynamics in protein functions. However, the underlying mechanism on the interplay between enzymatic turnover and conformational dynamics is not fully understood. In this work we constructed a multistate coarse-grained molecular dynamics model within the framework of the energy landscape theory, with which we have been able to simulate the full catalytic cycle of the AK. Our results demonstrated the tight coupling between the substrate exchange and lid open/closing motions, and their contributions to the final turnover rate. Particularly, we revealed how typical physiochemical factors, such as substrate concentrations, temperatures, and mechanical force, modulate the multistate allosteric motions of the protein and the pathways of the catalytic cycle.

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Date submitted: 11 Nov 2016

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