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DEPARTMENTAL SEMINAR
Chemical and Biological Sciences

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SPEAKER

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TITLE OF THE TALK

Understanding transition path dynamics for protein folding and unfolding

ABSTRACT

Recent experiments on transition path time distributions have raised intriguing questions. [1] The interpretation of the experiments indicates a small value of the fitted transition path barrier height as compared to the barrier height of the unfolded to folded transition. Also, the analyses of the experimental data using absorbing boundary conditions at the end points reveals long time tails that have thus far eluded quantitative theoretical interpretation. [2] A detailed investigation of the transition path time distribution using a diffusive model leads to the following conclusions. a. The available experimental data is not accurate enough to distinguish between functional forms of bell-shaped free energy barriers. b. Long time tails indicate the possible existence of a "trap" in the transition path region. Introduction of a well along the transition path leads to good fits with the experimental data provided that the transition path barrier height is $\sim 3k_BT$, substantially higher than the estimates of $\sim 1k_BT$ based on bell shaped functions. [3] It is also established that there is no need of introducing multi-dimensional effects, free energy barrier asymmetry and sub-diffusive memory kernels to explain the experimentally measured transition path time distribution. The central question of how many microstates are needed to justify modelling of the transition path dynamics in terms of an Smoluchowski equation has been addressed. [4] The numerical results for transition paths based on the diffusion equation are compared to the nearest neighbor Markov jump model. Comparison of the transition path time distributions indicates that one needs at least a few dozen microstates to obtain reasonable agreement between the two approaches. The Markov nearest neighbor model also shows good agreement with the experimentally measured transition path time distributions for a DNA hairpin and PrP protein.

References:

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