

Abstract Submitted
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Toward Investigating Protein Folding Using the Combination of Computer Simulation and Spectroscopy WEI ZHUANG — Protein folding is an important problem that is attracting scientists from a wide range of disciplines. One of the major challenges comes from the gap between the experimental and the theoretical studies. We proposed a computational protocol of simulating the T-jump peptide unfolding experiments and the related transient IR and 2DIR spectra based on the Markov State Model (MSM) and Nonlinear Exciton Propagation (NEP) methods. MSMs partition the conformation space into a set of non-overlapping metastable states, and we can calculate spectra signal for each of these states using NEP method. Thus the overall spectroscopic observable for a given system is simply the sum of spectra of different metastable states weighted by their populations. Simulated spectra based on MSM have a much better agreement with the equilibrium experimental 2DIR spectra compared to MD simulations starting from the folded state. MSMs are also capable of simulating the unfolding relaxation dynamics upon the temperature jump. The agreement of the simulation using MSMs and NEP with the experiment provides a justification for our protocol as well as a physical insight underlying the spectroscopic observables.

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