

Abstract Submitted
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The Speed Limit of Protein Folding: Alpha-Helix Initiation Modeled and Observed¹ MILO LIN, OMAR MOHAMMED, AHMED ZEWAİL², Physical Biology Center for Ultrafast Science and Technology, California Institute of Technology — As a primary event of protein folding, alpha-helix initiation is the starting point of macromolecular complexity. In this work, an analytic coarse-grained model which predicts the initiation rate as a function of temperature, is presented. Helix initiation was measured via ultrafast temperature-jump fluorescence refolding experiments on two penta-peptides, and the measured rates agreed well with those of the model. In addition, the temporal separation of rate-limiting diffusion from fast annealing stipulated by the model was confirmed via ensemble-converging all-atom molecular dynamics simulations, which reproduced both the diffusion and the picosecond annealing processes and rates observed experimentally. Some of these results were published in: Mohammed OF, Jas GS, Lin MM, Ma H, Zewail AH (2009) Primary peptide folding dynamics observed with ultrafast temperature jump. *Angew Chem* 48: 5628-5632.

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