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Heterogeneous helical propensity and its effects on dimerization and the stability of a model protein dimer YUBA BHANDARI, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, THEORETICAL BIOPHYSICS TEAM — We will present the results of Monte Carlo simulations of the dimerization and unfolding of a helical protein dimer. Using a three dimensional lattice model, we investigate the role of including sections of amino acids with strong alpha-helix propensity at different locations along the helices on the dimerization kinetics and the dimer stability. Specifically, we focus on the rate limiting steps in both folding and unfolding processes. We find that these processes can be optimized by tuning the ease of access through diffusion to the metastable intermediate state and its stability. The kinetics and thermodynamical stability is tuned by a combination of the locations of the amino acids with the high helical propensity and the salt bridges.

Yuba Bhandari
Department of Physics, Florida International University

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