Recent multidimensional vibrational experiments on peptides and proteins have provided a wealth of new information on the conformational dynamics of these systems. To study the correlations between spectra and peptide dynamics and to obtain a microscopic understanding of the phenomena, molecular dynamics (MD) simulations of various small peptides in aqueous solution have been performed. From these simulations, time-dependent correlation functions reflecting vibrational dephasing, energy transfer and energy relaxation are computed and compared to experiment. Furthermore, nonequilibrium MD simulations of laser-induced peptide dynamics are presented, which allow us to study the folding and unfolding of small peptides in atomistic detail. Analyzing the free energy landscape, various conformational states as well as pathways of helix nucleation are identified and discussed.

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