Vibrational energy relaxation in proteins

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When a protein is excited by ligand binding, ATP attachment, or laser pulses, there occurs vibrational energy relaxation (VER). Energy initially "injected" into a localized region flows to the rest of the protein and surrounding solvent. VER in large molecules (including proteins) itself is an important problem for chemical physics. Even more significant is the challenge to relate VER to fundamental reaction processes, such as a conformational change or electron transfer of a protein, associated with protein function. The development of a accurate understanding of VER in proteins is an essential step toward the goal of controlling protein dynamics.

Here VER of a selected mode in cytochrome c is studied using two theoretical approaches. One is the equilibrium simulation approach, with quantum correction factors, and the other is the reduced model approach, which describes the protein as an ensemble of normal modes interacting through nonlinear coupling elements. Both methods result in similar estimates of the VER time (sub picosecond) for a CD stretching mode in the protein at room temperature. The theoretical predictions are in accord with the experimental data of Romesberg's group. A perspective on future directions for the detailed study of time scales and mechanisms for VER in proteins is presented.