Computational Approaches to the Molecular Basis of Enzyme Catalysis – Reaction Coordinate Identification

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After decades of study, the mechanism by which enzymes accomplish their chemical rate enhancements (as much as a factor of 10^{12} over solution phase reactions) is still a topic of vigorous investigation. At least a partial answer to this problem is emerging, not from the biochemistry laboratory, but from computational methods. This talk will focus on transition path sampling and reaction coordinate identification via analysis of the stochastic separatrix in two very different enzymatic reactions. We present computational proof that in some enzymes, vibrational energy is channeled from the matrix of the protein to the reactive center via "promoting vibrations."