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Protein Dynamics and Enzyme Catalysis: New results from Theory and Experiment

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This talk will focus on recent work identifying enzymes in which rapid protein dynamics are central to the function of chemical catalysis. These motions, on a picosecond timescale, are part of the complex system's reaction coordinate, and so reaction does not occur without them. We also show evidence that such motions is are not simply part of a largely isotropic milieu, but rather special directions in the protein matrix. Theoretical results are coupled to recent experiments that show unequivocally that rapid protein dynamics are not just concomitant with reaction, but are causative. Disruption of these dynamics through mass changes, with no change in the potential energy of the system results in mis-timings of necessary promoting vibrations, and slows the rate of on enzyme chemistry. This is a new paradigm for enzyme function, and perhaps eventually for enzyme design.