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Abstract for an Invited Paper
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What are the physical principles that determine how enzymes really catalyze chemistry so magnificently efficiently (and why are they so hard to design)?

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The mechanisms of enzymes have been studied for many decades, but there remains basic disagreement as to how they achieve such extraordinary rate enhancements. This talk will focus on recent advances in our group aimed at answering just this question. Through advances in rare event quantum dynamics simulation, we have shown over the past decade that rapid protein motions, built into the protein matrix via evolution are central to the catalytic effect. Recently we have shown that in some cases, these motions modulate electrostatic fields at the active site, and this view harmonizes two divergent schools of thought on enzyme proficiency. We have applied these ideas to the concept of enzyme design and with our experimental collaborators have verified this new view of enzymatic action. These results also explain the relative lack of success of theoretical artificial enzyme design based on static structures. This work involved the development and application of new theoretical methods for the study of chemistry in such complex systems, and this talk will focus on method, application, and experimental verification.