PLASTICITY OF ENZYME IN FUNCTION: EXPERIMENT AND THEORY

Tremendous advances have been made in recent decades, and has contributed to the understanding of the role of protein plasticity in the function of an enzyme, such as ligand binding, catalysis, allostery and even regulation of enzymatic activity by post-translational modification. Recent efforts are focused on the design of new enzymes by directed evolution and/or in silico, but most of these efforts result in lower activity than natural enzymes. The fundamental problems in obtaining greater enzyme activity are the role of protein dynamics in natural enzymes over designed enzymes and the incorporation of this knowledge into the enzyme design procedure. In this symposium, we will bring together experimentalists and computational enzymologists to discuss the current status of research on protein plasticity in enzyme action, conformational heterogeneity at different functional states, enzymatic catalysis and conformational changes, and how these new insights can be used to design novel enzymes. In the end, this symposium will identify important new directions and guide our research in enzymeology and enzyme design.

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ADVANCED IN NONLINEAR OPTICS AT INTERFACES

Interfaces are of fundamental importance in catalysis, energy storage and conversion, biological processes, environmental issues, and technological problems such as oil extractions. Understanding the molecular behaviors at interfaces is essential for both basic concepts and industrial applications. In the past decade, with the advent of novel nonlinear optical spectroscopy techniques, there have been developed and applied to reveal behavior of interfacial chemical systems on the molecular level. This progress deepens our fundamental understanding of interfacial chemistry and physics. This symposium will bring together both theoretical and experimental physical chemists who are interested in interfacial chemistry and physics.

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ADVANCED FORCE FIELDS (Virtual Only)

Simulations of complex materials with large numbers of atoms and for long times requires the use of force fields. Over the past decade, significant advances, including the use of machine learning techniques, have been made in the development of accurate force fields based on data from high level electronic structure calculations. QM/MM methods play an important role in modeling processes involving the breaking and formation of chemical bonds, and there is considerable interest in improving the quality of the force fields used in the embedding and in describing the interactions of complex systems. The presentation will discuss the development of force fields that can accurately describe bond breaking and formation without employing a QM/MM approach, but here too important advances have been made. The symposium will bring together researchers developing state-of-the-art force fields and those involved in developing simulation techniques that allow the efficient use of these force-fields on large-scale HPC- and GPU-based computer environments to allow more realistic simulation of chemical, biological, and material environments to allow more realistic simulation of chemical, biological, and material systems.

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SYNTHESIZING QUANTUM COHERENCE (Virtual Only)

Recent experimental and theoretical developments enliven our community to imagine the revolutionary possibilities that could be created by the capacity to design and realize coherent states that selectively deposit energy into specific reaction coordinates that may direct the subsequent electronic and vibronic dynamics. Directing molecular and nanostructured species in this way could upend conventional molecular intuition, which is largely grounded in thermodynamic and kinetic constraints. The capacity to design molecular coherences could thus enable the fine control of energy and charge migration, potentially freeing these processes from condensed-phase energy dissipation, and could lift some of the constraints of Boltzmann statistics, transforming our ability to manipulate the structure and dynamics of matter. The symposium will explore progress in molecular and nanoscale design and synthesis, electronic and electronic-vibronic spectroscopies, pulse-EPR spectroscopy, and theoretical/computational quantum dynamics that are being brought together to unlock the coherent flow of electronic excited states and of charges, along with their coherent spin-spin interactions, to realize novel quantum dynamical effects at the nanoscale.

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PHYSICAL CHEMISTRY PAPER SESSION

 Contributions from all areas of physical chemistry are highly encouraged for the poster session. If held in person, up to six awards will be given for exemplary work. To be eligible for the awards, the presenting author must be a graduate or undergraduate student at the time of the poster presentation and must be present during judging.