

# Chemical Sciences Division

## Condensed Phase and Interfacial Chemical Physics

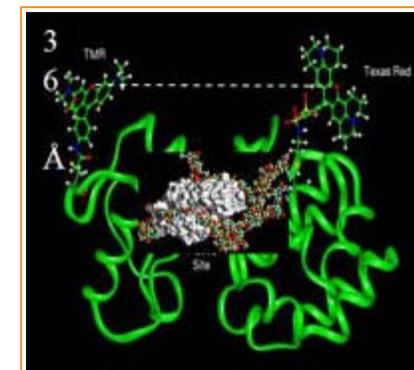
The Chemical Sciences Division's program in condensed phase and interfacial chemical physics supports research that is nationally and internationally recognized for providing a fundamental understanding of molecular processes in condensed phases. This research addresses fundamental uncertainties in thermal and non-thermal (i.e., radiation) chemistry, interfacial molecular and ionic transport (key to subsurface contaminant transport and to separations processes), and other processes in complex systems related to energy use, environmental remediation, and waste management.

Research in this area is focused on structures and processes of molecular and nanoscale systems in complex environments such as condensed phases and interfaces. We study model systems to better understand natural systems and guide the development of new materials and approaches for clean and efficient energy use. Another central feature is the development of new experimental and theoretical methods with broad applications to research in the natural sciences.

The program in condensed phase and interfacial chemical physics consists of both theoretical and experimental elements. We conduct fundamental research on

- interactions of atoms, molecules, and ions with photons and electrons in all states of matter
- the use of model systems and unique methods to understand chemical processes on surfaces, in condensed media, and at interfaces
- first-principle calculations and advanced methods for modeling and simulations closely coupled with experiments to extend our understanding of chemical reactivity from the molecular scale to collective phenomenon in complex systems.

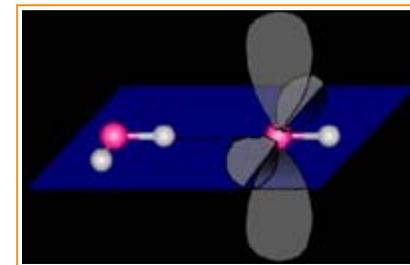
A unique aspect of PNNL's theoretical and computational program is the strategy used to address complex molecular systems. Rather than relying on empirical data to build models for simulating these systems, our approach builds upon highly accurate first-principle calculations (e.g., ab initio electronic structure calculations) on prototype systems to develop models (e.g., molecular interaction potentials) used in simulations of complex molecular systems such as liquid/liquid and liquid/solid interfaces. Many of these problems are not amenable to standard computational tools, so increases in computational capacity are not sufficient to solve the



PNNL achieved simultaneous observation of single-molecule enzymatic reaction turnovers and the correlated conformational hinge-bending motion trajectories. This image shows single-pair fluorescence resonant energy transfer was used in probing T4 lysozyme hinge-bending motions and its enzymatic reaction of hydrolyzing polysaccharides of E Coli B cell wall, and MD simulation of T4 lysozyme conformational change under substrate binding. We obtained detailed information on the dynamics, mechanism, and energy landscape of the T4 lysozyme enzymatic reaction by combining single-molecule enzymatic dynamics and molecular dynamics simulations.

problems of interest. Therefore, another unique aspect of our research is the integration of computational tool development with applications to targeted problems.

The experimental Chemical Physics Program provides a molecular-level understanding of chemistry at complex interfaces by 1) implementing a multi-investigator approach to provide the breadth of expertise and capability required for investigation of complex interfacial chemical processes and 2) developing state-of-the-art research and analytical methods for characterizing complex materials of the types found in natural systems. Model systems are used to support detailed understanding and modeling of complex interfaces. Liquid/liquid and liquid/solid interfaces are constructed one molecule at a time to provide structures whose chemistry is understood and visualized at a level of detail and certainty not afforded by studies of naturally occurring, inhomogeneous systems. Both thermal processes and those activated by photons or electrons are studied. In a similar fashion, isolated ions are solvated by the addition of one solvent molecule at a time providing a detailed understanding of this process. Single-molecule imaging and spectroscopy are also used to provide data free from natural inhomogeneities. Advanced theory and modeling methods are used to model and interpret these results, providing a molecular-level understanding of interfacial chemistry in complex natural systems.



In one example of PNNL's study of interfacial chemistry, we are studying the molecular interactions of OH radicals with water because the effects of electronic states on the radicals' molecular interactions can affect their solvation structure, transport properties, and reactivity.

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