

SEMINAR ANNOUNCEMENT

TUESDAY, 25.02.2014
4:00 PM S.T. IN ROOM NC 2/99

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"Ligand migration through heme protein cavities, protein dynamics, and solvent coupling: insights from laser flash photolysis and molecular dynamics simulations"

Abstract: The presence of cavities and tunnels in the interior of proteins, in conjunction with the structural plasticity arising from the coupling to the thermal fluctuations of the protein scaffold, has profound consequences on the pathways followed by ligands moving through the protein matrix. In this perspective we discuss how quantitative analysis of experimental rebinding kinetics from laser flash photolysis, trapping of unstable conformational states by embedding proteins within the nanopores of silica gels or sugar glasses, enhancing the viscosity by cosolvents, and molecular simulations can synergistically converge to gain insight into the migration mechanism of ligands. We show how the evaluation of the free energy landscape for ligand diffusion, based on the outcome of computational techniques, can assist the definition of sound reaction schemes, leading to a comprehensive understanding of the broad range of chemical events and time scales that encompass the transport of small ligands in heme proteins.

Interested persons are cordially invited to attend!