MAR16-2015-005127

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Unraveling protein catalysis through neutron diffraction.

DEAN MYLES, Neutron Science Directorate, Oak Ridge National Laboratory, Oak Ridge, TN. 37831

Neutron scattering and diffraction are exquisitely sensitive to the location, concentration and dynamics of hydrogen atoms in materials and provide a powerful tool for the characterization of structure-function and interfacial relationships in biological systems. Modern neutron scattering facilities offer access to a sophisticated, non-destructive suite of instruments for biophysical characterization that provide spatial and dynamic information spanning from Angstroms to microns and from picoseconds to microseconds, respectively. Applications range from atomic-resolution analysis of individual hydrogen atoms in enzymes, through to multi-scale analysis of hierarchical structures and assemblies in biological complexes, membranes and in living cells. Here we describe how the precise location of protein and water hydrogen atoms using neutron diffraction provides a more complete description of the atomic and electronic structures of proteins, enabling key questions concerning enzyme reaction mechanisms, molecular recognition and binding and protein-water interactions to be addressed. Current work is focused on understanding how molecular structure and dynamics control function in photosynthetic, cell signaling and DNA repair proteins. We will highlight recent studies that provide detailed understanding of the physiochemical mechanisms through which proteins recognize ligands and catalyze reactions, and help to define and understand the key principles involved.