Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Colloquium

Uncovering the Signal Transduction Mechanisms in Light-Oxygen-Voltage Sensitive Receptors by electron and nuclear magnetic resonance

Songi Han

Northwestern University, IL

How proteins transduce environmental signals such as light, stress or magnetic field vectors into responses, including mechanical and fluorescence, that activates subsequent actions remains a central and elusive question in biology. Flavin containing photoreceptors are central to environmental signal entrainments across all kingdoms of life. However, elucidating their mechanisms require advanced physical chemistry tools including nuclear and electron spin magnetic resonance spectroscopy, optical excitation and detection methods, control over the optical-spin interface, fundamentals of spin physics and insight into the structural and dynamical property of water at the interface to proteins.

I will present studies of the molecular basis of blue light activation of a light-oxygen-voltage (LOV) sensitive avena sativa protein (AsLOV2) that gives rise to concerted water movement to induce conformational extensions. Using electron and nuclear magnetic resonance spectroscopy, along with atomistic molecular dynamics simulations at high pressure, we find that activation, whether initiated by blue light or high pressure, is accompanied by selective expulsion of low-entropy, tetrahedrally coordinated “wrap” water from hydrophobic regions of the protein. These findings suggest that interfacial water serves as functional constituents to help reshape the protein’s free energy landscape during activation. Our study highlights hydration water as an active medium with the capacity to drive long-range conformational changes underlying protein mechanics and offers a new conceptual understanding for engineering externally controllable protein actuators for biomedical studies to smart materials. I will also present ongoing studies of LOV protein variants that are fluorescent in a magnetic field dependent fashion, allowing for optically detected magnetic resonance (ODMR). At the core of mechano- or magneto-sensitive LOV proteins is an excited triplet state formed upon light activation of flavin mononucleotides that serve as a central, spin state-dependent, molecular switch whose action we intend to elucidate and control by advanced magnetic resonance methods.

Friday, Jul 11th 2025

11:30 Hrs (Tea / Coffee 11:15 Hrs)

Auditorium, TIFRH