S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR
Chemical and Biological Sciences

07th February,2024 **4.00 PM** **ONLINE / FERMION**

SPEAKER

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TITLE OF THE TALK

Understanding the retinal isomerization reaction using hybrid QM/MM simulations

ABSTRACT

Rhodopsins are membrane proteins that play a pivotal role in light perception across diverse life forms, converting light into chemical energy to facilitate various biological functions. These proteins, integral to processes like vision, also find application in optogenetics, a key aspect of biotechnology. The initial phase of rhodopsin activation involves light-triggered isomerization of the retinal chromophore from 11-cis to all-trans isomer in animal rhodopsins [1] and from all-trans to 13-cis in microbial rhodopsins [2]. However, despite their significance in light sensing, the atomistic insights of the photoisomerization mechanism remains elusive, primarily due to the lack of structural characterization of early intermediates during light-induced activation at physiological temperatures, particularly in the femtosecond to picosecond range. The investigation of photoisomerization in light-sensitive systems necessitates proper modeling of the reaction center (chromophore) within the protein environment. Moreover, an accurate depiction of electronic ground and excited states is crucial to decipher the photoactivation process. To address these challenges, we employ hybrid quantum mechanics and molecular mechanics (QM/MM) simulations to offer an atomic-level description of structural and electronic alterations in rhodopsins by utilizing multiconfigurational-based QM methodologies within QM/MM simulations, enabling the exploration of nonadiabatic excited state molecular dynamics [3] and spectroscopic characterization [2-3]. Through these approaches, we aim to shed light on unresolved aspects of rhodopsin activation mechanisms.

Reference
1. Gruhl, T.; Weinert, T.; Rodrigues, M. J.; Milne, C. J.; Ortolani, G.; Nass, K.; Nango, E.; Sen, S.; et al. Ultrafast structural changes direct the first molecular events of vision. Nature 2023, 615, 939–944.
2. Mous, S.; Gotthard, G.; Ehrenberg, D.; Sen, S.; et al. Dynamics and mechanism of a light-driven chloride pump. Science 2022, 375, 845–851.
3. Sen, S.; Borin, V. A.; Schapiro, I. Counterion assisted retinal isomerization of proteorhodopsin. (Manuscript under preparation).

HOST FACULTY

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