

ACCMS-Global Research Center SRMIST, Chennai India



Webinar #29



July 30th 2024,

11.30 am - 1.00 pm

Indian Standard

Time

Prof. Vannajan Sanghiran Lee,

Department of Chemistry, Center of Quantum Information Science and Technology (QIST) University of Malaya, Malaysia

Exploring DNA Dynamics: Title: **Energy Landscapes and Molecular Simulations**

Registration link https://tinyurl.com/3w7w9n2r *Zoom details will be shared with the registered participants

Short biography

Prof. Dr. Vannajan Sanghiran Lee, with a BSc in Chemistry from Chiang Mai University, Thailand (1994), and a PhD in Pharmaceutical Sciences and Physical Chemistry from the University of Missouri-Kansas City, USA (2001), is a distinguished researcher specializing in molecular modeling and simulations. She currently serves as the head of the Center of Excellence in Quantum Information Science and Technology (QIST). Dr. Lee received the 2023 UNESCO Woman of Influence for Science and Technology award for her contributions to sustainable development through her research.

Abstract

DNA dynamics have been investigated through energy landscapes and molecular simulations, employing various advanced computational techniques. Time-dependent density functional theory (TD-DFT) is utilized to model energy landscapes and electronic properties of DNA, providing insights into stability and transitions among conformations. Molecular dynamics simulations and Monte Carlo methods are employed to study DNA behavior under diverse physiological and experimental conditions. Additionally, plasma simulations explore the effects of plasma interactions on DNA, revealing potential mechanisms for plasma-induced DNA damage. These combined approaches enhance our understanding of DNA dynamics, damage pathways, and genetic stability in biological systems.

Panelist



Prof. Kaoru Ohno Yokohama National University Japan













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