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ACCMS-Global Research Center, SRMIST, Chennai India

Webinar #4

Prof. Jer-Lai Kuo

Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica, Taiwan

Title: Exploring Structure-Property Relationship of Molecular Systems via *Ab Initio* Methods

30th November 2021, 10.00 am – 11.30 am IST

About speaker

Prof. Jer-Lai Kuo received B.Sc and M.Sc in Physics from National Taiwan University and Ph.D in Chemical Physics from Ohio State University. He did his post-doctoral research in University of Pennsylvania, USA. Currently, he is the Deputy Director in Institute of Atomic and Molecular Sciences (IAMS), Academia Sinica, Taiwan. Before joining IAMS in 2009, Prof. Kuo taught in Nanyang Technological University in Singapore. His research interests focus on the application and development of theoretical and computational tools to study a wide range of topics in Molecular and Material Research like Structure and Properties of H-bonded Clusters, First-Principles Studies of Bulk Materials, Application of Artificial Intelligence in Material Discovery/Design, and Order/Disorder Transitions in Ice. He has been as visiting and visiting adjunct professor in several institutes like INOMAR-Vietnam National University, TIFR, IIT Bombay and National Taiwan University. He has received a numerous accolades and awards like Presidential Pre-doctoral Fellowship from Ohio State University in 2002, Young Researcher Award from Nanyang Technological University-Singapore in 2008, Research Excellence Award from National Research Council of Thailand (NRCT) in 2013, Young Scholars' Creativity Award in 2013, Promising Scientist Award of CMOA from France in 2013, Mid-career award by ACCMS in 2016, Asia Special Lecture Award in Theoretical Chemistry from Chemical Society of Japan in 2019 and so on. He has published more than 190 papers with 7760 citations and h-index 48.

Abstract

The concept of potential energy surface (PES) plays an essential role in understanding the structure, properties and structure-property relationship of molecular systems. *Ab initio* methods are often the desirable choice to explore PES as no empirical parameters are used. But it is far from trivial to determine relevant geometries of molecular systems with floppy degrees of freedom. We develop a set of random/biased searching algorithms to help us to navigate through the energy landscape of alcohol in gas, liquid and solid phases. In experiments vibrational spectra are commonly used methods to extract structural information and harmonic frequencies derived from the curvatures around the minima is the standard method to analyze vibrational spectroscopy. However, vibrational motions of molecules are intrinsically “anharmonic”. In particular for molecules containing CH, NH, and OH bonds, experimental spectra often reveal more peaks in their vibrational spectra then the number of normal modes in their stretching modes. Such a general phenomenon is due to the vibrational coupling between X-H stretch fundamental and overtone of their bending modes, known as Fermi resonance. We have recently developed two *ab initio* anharmonic algorithms. Complex vibrational feature of functional group containing O-H, N-H and C-H due to Fermi Resonance has also been resolved with the assistance of our *ab initio* anharmonic schemes.

Registration is free.
Registration link: *https://tinyurl.com/9vh5c2ta*
Zoom meeting details will be shared with the registered participants.

Conveners:
Dr. V.J.Surya and Dr.S. Yuvaraj
ACCMS-GRC Center-in-Charges
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