

Conference on Recent Advances in
DYNAMICS AT THE INTERFACE OF CHEMISTRY AND BIOLOGY (DICB-2019)
February 18-20, 2019

Organized by: Solid State and Structural Chemistry Unit
Venue: Faculty Hall, Main Building, Indian Institute of Science, Bengaluru

Monday, February 18, 2019

09:00 – 09:15 Welcome Address, Chair, SSCU

09:15 – 09:45 Inauguration by Bharat Ratna Professor C.N.R. Rao, FRS

Chair: A J Bhattacharyya

09:45 – 10:20 M. L. Klein, Temple University

Title: Nature's Way of Sensing Pain and How to Survive as Dean of Science

10:20 – 10:50 **Break**

10:50 – 11:25 Gregory A. Voth, University of Chicago

Title: Overcoming the Multiscale Challenge for Biomolecular Systems

11:25 – 11:50 Srabani Taraphdar, IIT-Kharagpur

Title: Reaction Coordinate, Free Energy and Rate of an Enzyme Catalysed Reaction

11:50 – 12:10 Manju Sharma, Central University, Hyderabad

Title: Prenucleation Behaviour of Active Pharmaceutical Ingredients

12:10 – 12:30 Rakesh Singh, Johns Hopkins University

Title: Thermodynamic anomalies in deeply stretched water

12:30 – 02:00 **Lunch break**

Chair: S. Natarajan

02:00 – 02:25 S. Umamathy, IISER-Bhopal

Title: Structure and dynamics from stimulated Raman Spectroscopy

02:25 – 02:50 Ranjit Biswas, SNBNCBS, Kolkata

Title: Ethanol and Water Azeotrope: A Combined Fluorescence Spectroscopic and Computer Simulation Study

02:50 – 03:15 Govardhan Reddy, SSCU-IISc

TBA

03:15 – 03:45 **Break**

Chair: Swapan Pati

03:45 – 04:20 Yoshitaka Tanimura, Kyoto University

Title: Low-Temperature Quantum Fokker-Planck and Smoluchowski Equations: Applications to Nonlinear Spectroscopies

04:20 – 04:40 Arnab Mukherjee, IISER-Pune

Title: Understanding Internal Friction Using Simple Model Systems

04:40 – 05:00 Nilashish Nandi, Kalyani University

Title: Inhibition of Seryl tRNA Synthetase by Seryl Nucleoside Moiety of Albomycin Antibiotic

05:00 – 05:20 Prashant Jose, IIT, Mandi

Title: Relation between local density and density relaxation in glass transition: A molecular dynamics simulation study

5.20 - 7.30 **Poster Session**

7.30 – 09:00 *Dinner in The Main Guest House Lawns*

Tuesday, February 19, 2019

Chair : Sriram Ramaswamy

09:00 – 9:35 Graham Fleming, University of California Berkeley

Title: Recent Studies of Old Problems

9:35 – 10:00 Amalendu Chandra, IIT-Kanpur

Title: Free Energy Landscapes and Reaction Pathways of Transamination Process at the Active Site of an Aminotransferase Enzyme in Aqueous Medium

10:00 – 10:20 Biman Jana, IACS

Title: Function and Folding of Antifreeze protein: A remarkable story of unusual hydration

10:20 – 10:50 **Break**

Chair: N. Sathyamurthy

10:50 – 11:25 Shinji Saito, Institute for Molecular Science, Okazaki

Title: Circadian rhythm of Kai system: A reaction model considering reactions and conformational changes

11:25 – 11:50 Prabal Maiti, Physics-IISc

Title: Structure, dynamics and thermodynamics of confined water

11:50 – 12:15 Sarika Bhattacharyya, National Chemical Laboratory, Pune

Title: The role of pair correlation function in the dynamical transition predicted by the mode coupling theory

12:15 – 12:35 Sangeeta Saini, Kurukshetra University

Title: Mechanistic investigation into CO oxidation catalyzed by gold nanocluster

12:35 – 02:00 **Break**

Chair: A. K. Ganguli

02:00 – 02:35 Arun Yethiraj, University of Wisconsin-Madison

Title: Polymers in ionic liquids

02:35 – 02:55 Suman Chakraborty, SNBNCBS

Title: A molecular thermodynamic view of biomolecular recognition and signaling

02:55 – 03:20 Sanjoy Bandyopadhyay, IIT-Kharagpur

Title: Exploring the microscopic properties of intrinsically disordered proteins in aqueous environment

03:20 – 03:45 **Break**

Chair: S. Ramakrishnan

03:45 – 04:20 P. Demontis, Universita di Sassari

Title: Multiscale simulation of adsorption and diffusion in microporous materials

04:20 – 04:40 Mantu Santra, SNBNCBS, Kolkata

Title: Mathematical modeling of bacterial proteostasis and protein damage

04:40 – 05:00 Neelanjana Sengupta, IISER-Kolkata

Title: Modulation of peptide aggregation and water flow through nanochannels

05:00 – 05:30 **High Tea**

05:30 – 06:30 Felicitation Function in honor of *Professor Biman Bagchi*

07:30 pm onwards Conference Banquet, JVH Lawns

Wednesday, February 20, 2019

Chair: S. Chadrsekaran

09:00 – 9:35 Horacio Corti, Ciudad Universitaria, Buenos Aires

Title: An experimental approach to the structure and dynamics of glassy, supercooled and confined water and aqueous solutions

09:35 – 10:10 Kazuhiko Seki, AIST, Tsukuba

Title: Theoretical study on fundamental kinetic processes in photoelectric conversion

10:10 – 10:35 Sobhan Sen, Jawaharlal Nehru University

Title: New Insight of Location Dependent Polarity, Energy Transfer and Solvation Dynamics at Lipid/Water Interfaces

10:35 – 10:55 Rajesh Murarka, IISER-Bhopal

Title: Towards Understanding the Effect of Lipid Composition on Membrane-bound α -Synuclein

10:55 – 11:30 **Break**

Chair: Srikant Sastry

11:30 – 11:55 Parbati Biswas, University of Delhi

Title: How do Proteins Misfold?

11:55 – 12:15 Rajarshi Chakraborty, IIT-Mumbai

Title: Dynamics of Polymer in Active Bath

12:15 – 12:35 Rajib Biswas, IIT-Tirupati

Title: In Silico Spectroscopy and Structure-Spectrum Correlations of Aqueous Systems

12:35 – 12:55 Vivek Tiwary, IISc

Title: Robust Quantum Coherences in Bacterial Photosynthetic Antennas and Vibronic Decoherence

12:55 - 02:00 **Lunch**

Chair: Kankan Bhattacharyya

02:00 – 02:25 S. Yashonath

Title: A new and conceptually different approach for separation of mixtures

02:25 – 03:05 Biman Bagchi, IISc

Title: Spatial and Temporal Evolution of Molecular Motion

03:05 – 03:20 **Concluding Session**