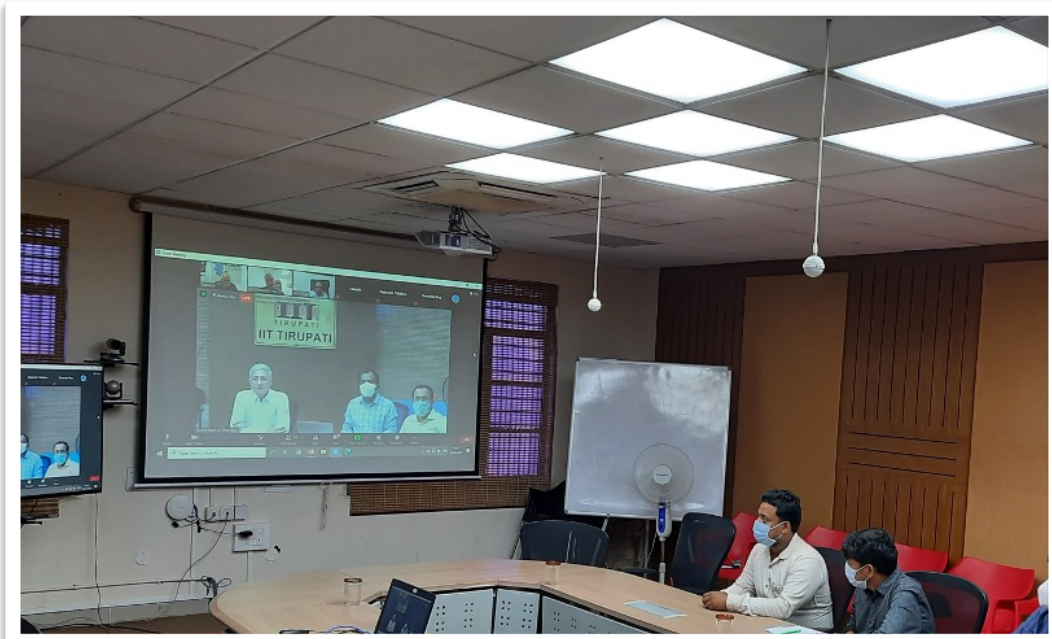
Statistical Mechanics in Chemistry and Biology (SMCB)

An online conference, 23-26 January 2021



Board Room, Temporary Campus, IIT Tirupati

The "*Statistical Mechanics in Chemistry and Biology (SMCB-2021)*" conference is jointly organised by IIT Tirupati, IISER Tirupati and IIT Goa over an online platform. The idea of this conference is conceived and nurtured by the country's legendary researcher in this domain **Prof. Biman Bagchi**, who is a National Science Chair Professor at IISc Bangalore. The coordinators for the pioneer event are **Dr. Rajib Biswas** (Asst. Prof. of Chemistry, IIT Tirupati), **Dr. Rakesh S. Singh** (Asst. Prof. of Chemistry, IISER Tirupati) and **Dr. Mantu Santra** (Asst. Prof. of Chemistry, IIT Goa). This was created to provide the young researchers a platform to discuss their research works.

DR. RAJIB BISWAS

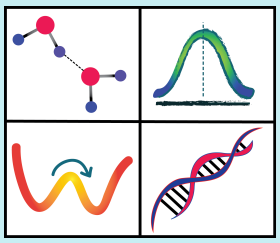
IIT Tirupati

DR. RAKESH S SINGH

IISER Tirupati

DR. MANTU SANTRA

IIT Goa

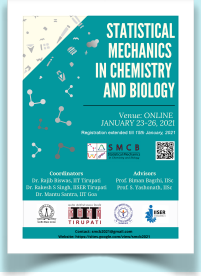


SMCB - 2021

Prof. Biman Bagchi
National Science Chair Professor, IISc Bangalore

Coordinators
Dr. Rajib Biswas
Dr. Rakesh S. Singh
Dr. Mantu Santra

Advisors
Prof. Biman Bagchi
Prof. S. Yashonath



Inauguration of SMCB-2021

Board Room, Temporary Campus, IIT Tirupati

The 4 days long online conference SMCB-2021 is formally inaugurated by Prof. K. N. Satyanarayana, Director, IIT Tirupati; Prof. K. N. Ganesh, Director, IISER Tirupati; Prof. C. P. Rao, HoD, Chemistry, IIT Tirupati, and Prof. K. Vijayamohanan Pillai, Chair, Chemistry, IISER Tirupati. The inaugural session was attended by near about 200 participants over ZOOM video conferencing platform.

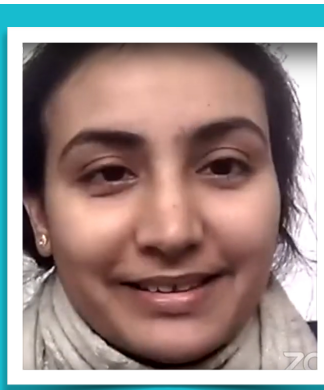
INAUGURATED BY

From Left: Prof. K. N. Satyanarayana (Director, IIT Tirupati); Prof. C. P. Rao (HoD Chemistry, IIT Tirupati); Prof. K. N. Ganesh (Director, IISER Tirupati); Prof. K. Vijayamohanan Pillai (Chair, Chemistry, IISER Tirupati)

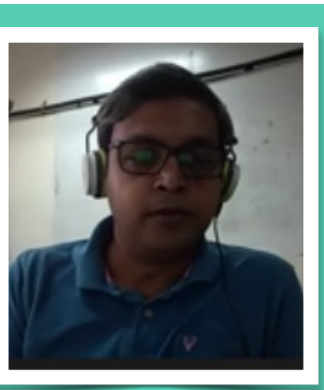
Glimpses of Inaugural Session

Chairpersons of the Technical Sessions

The conference has six technical sessions, comprise of 24 presentations by faculty members and 31 presentations by young research scholars.



Dr. Sangeeta Saini
Kurukshetra University

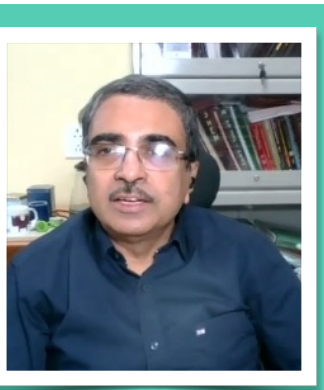


Dr. Sayan Bagchi
CSIR-NCL Pune

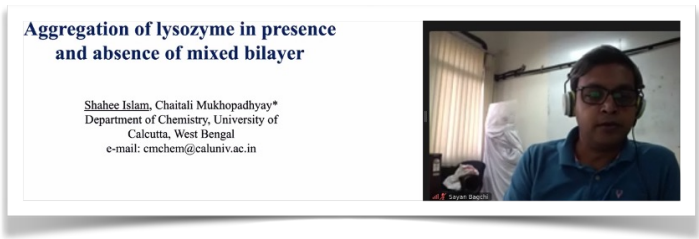
Dr. Hemant Kashyap
IIT Delhi

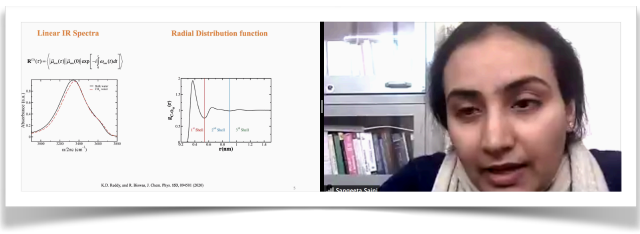
Dr. Manju Sharma
University of Hyderabad

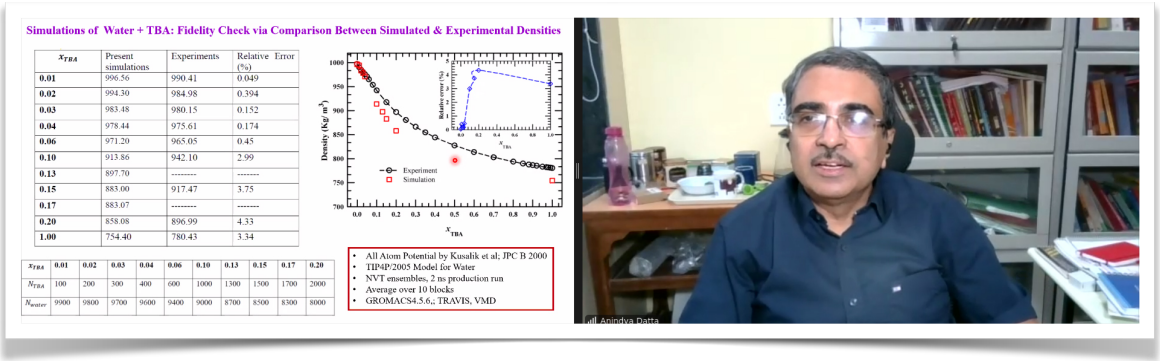
Dr. Sandip Paul
IIT Guwahati



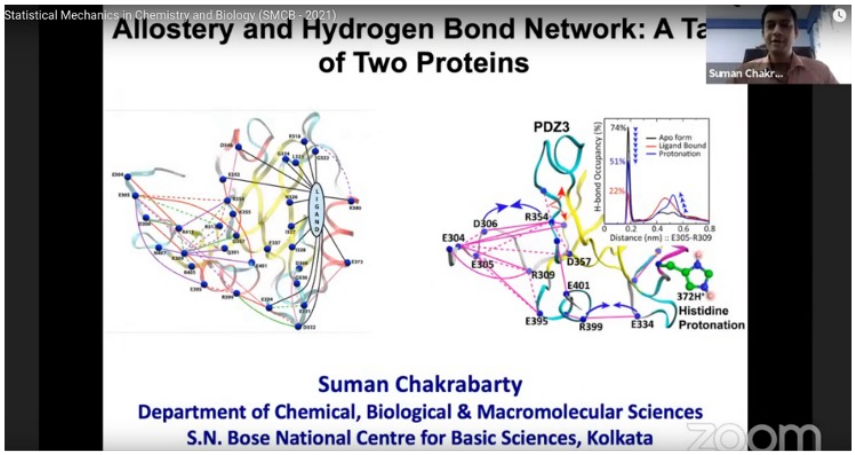
Prof. Anindya Datta
IIT Bombay

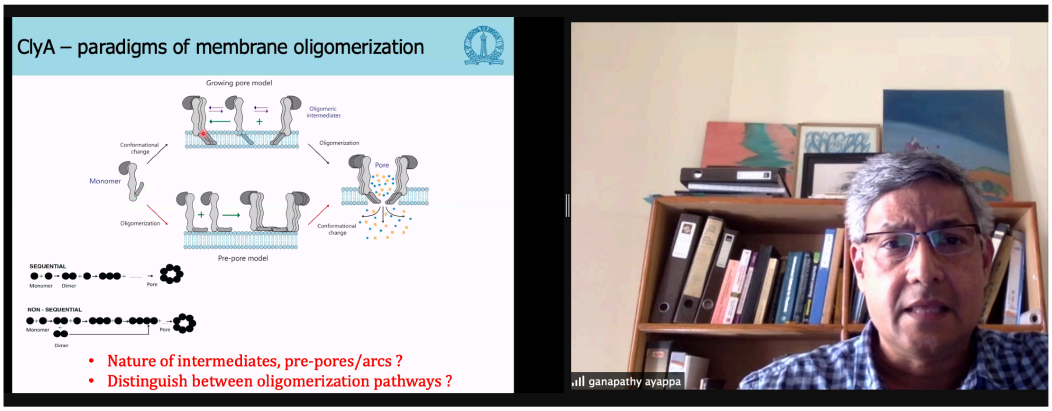


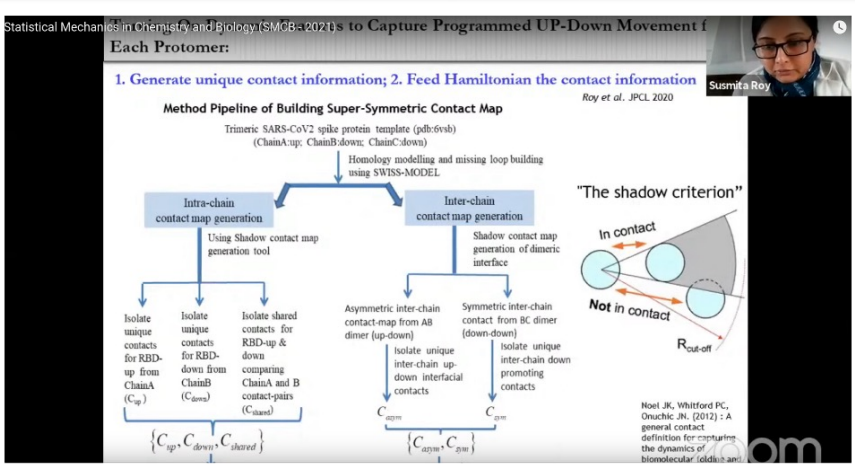




Glimpses of the Technical Sessions



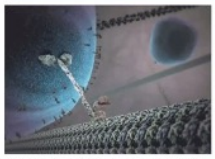


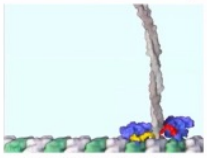


Understanding HIV invasion mechanism and designing efficient inhibitor through computational techniques

Prabal K. Maiti
Centre for Condensed Matter Theory
Dept. of Physics, Indian Institute of Science (IISc)
Bangalore, India.

Motor proteins walking on the cellular track





Features:

Perhaps the most important entity in living cell. Walks on microtubule or actin filament while carrying important cellular cargos. Converts chemical energy of ATP/GTP hydrolysis to produce mechanical energy.

Questions:

- What are the different states in the mechanochemical cycle?
- How two heads coordinate between them to produce a long distance walk?
- How multiple motors work as a team?
- Molecular mechanism of ATP/GTP hydrolysis in motor proteins?
- How specific mutations of motor proteins lead to disease or small molecule binding lead to anesthesia?

A statistical Approach to Understand Bacterial Cytoplasm

Jagannath Mondal
TIFR Hyderabad

tifr TIFR Centre for Interdisciplinary Sciences

SMCB Statistical Mechanics in Chemistry and Biology

urface Complementarity in Proteins
sing Unsupervised Learning and
obust Curvature Measure

SMCB-Jan 2021

Arnab Mukherjee
Chemistry Department
IISER PUNE

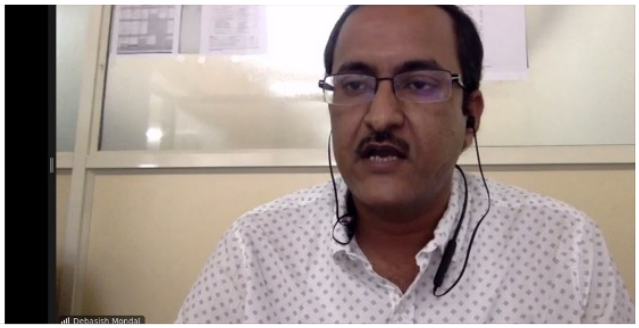
Noise-induced symmetry breaking of self-regulators: Nonequilibrium transition towards homochirality

Debasish Mondal

Department of Chemistry
Indian Institute of Technology Tirupati

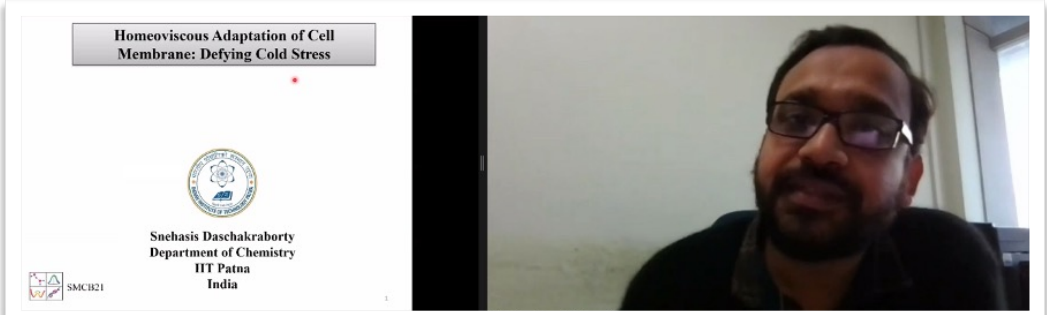
TIRUPATI

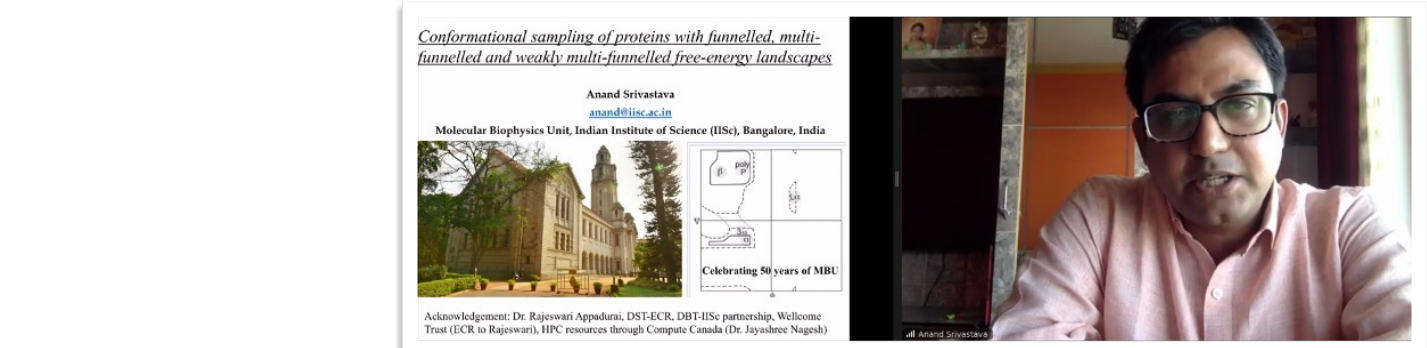
SMCB2021, 24th January, 2021

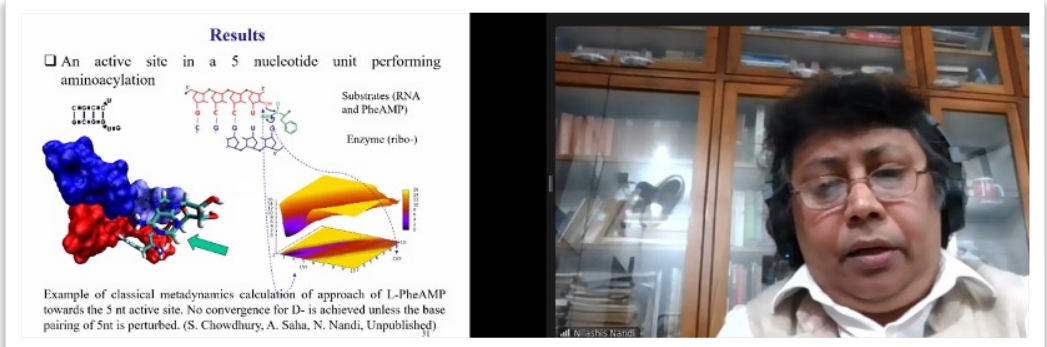



Activity and crowding, two major players in single probe dynamics
Rajarshi Chakrabarti
Department of Chemistry
Indian Institute of Technology Bombay
Statistical Mechanics in Chemistry and Biology (SMCB), 23-26 January 2021


Thank You
Save water ...
Drink Pure Water. Stay Healthy.
Anyone who can solve the problems of water will be worthy of two Nobel prizes - one for peace and one for science
.... John F. Kennedy
So why waiting , start now to design a nanomembrane , give it to the experimentalist and solve the water problem
Dr. Sk. Musharaf Ali

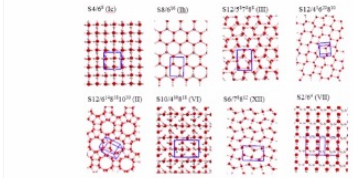

Homeoviscous Adaptation of Cell Membrane: Defying Cold Stress
Snehasis Daschakraborty
Department of Chemistry
IIT Patna
India
SMCB21


Conformational sampling of proteins with funnelled, multi-funnelled and weakly multi-funnelled free-energy landscapes
Anand Srivastava
anand@iisc.ac.in
Molecular Biophysics Unit, Indian Institute of Science (IISc), Bangalore, India
Celebrating 50 years of MBU
Acknowledgement: Dr. Rajeswari Appadurai, DST-ECR, DBT-IISc partnership, Wellcome Trust (ECR to Rajeswari), HPC resources through Compute Canada (Dr. Jayashree Nagesh)
Anand Srivastava


Results
An active site in a 5 nucleotide unit performing aminoacylation
Substrates (RNA and PheAMP)
Enzyme (ribo-)
Example of classical metadynamics calculation of approach of L-PheAMP towards the 5 nt active site. No convergence for D- is achieved unless the base pairing of 5nt is perturbed. (S. Chowdhury, A. Saha, N. Nandi, Unpublished)

Polymorphism

❖ Phenomenon of existing in multiple crystal structures



Ice has 18 known crystalline structures

Thermodynamic Anomalies and Ice Nucleation in Deeply Stretched Water

Rakesh S. Singh

Indian Institute of Science Education and Research
Tirupati

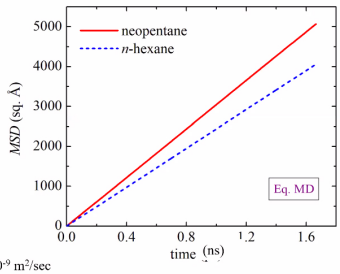
IISER TIRUPATI

SMCB-2021

Finding the correspondence between real time and mc step

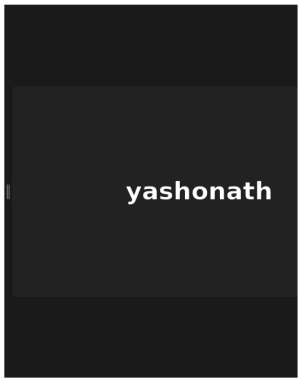
Eq. MD Simulations

- A system of equimolar mixture of neopentane and *n*-hexane in zeolite NaY at a loading of 1mpc is simulated with equilibrium molecular dynamics at 300K temperature.
- The timestep is 1fs.
- The system is equilibrated for 1ns, and then production ran for 5ns.
- The system dimension is 2x2x2.



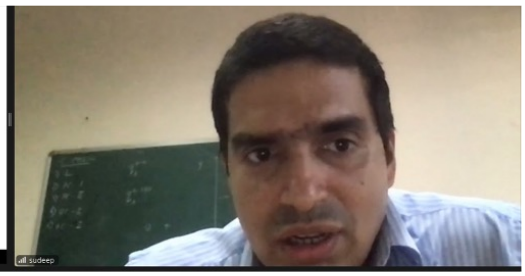
$D^{MD}_{neopentane} = 5.07 \times 10^{-9}$ m^2/sec

$D^{MD}_{n\text{-}hexane} = 4.06 \times 10^{-9}$ m^2/sec



Examining the origin of two-step crystal nucleation from vapor phases using molecular theory for non-classical nucleation

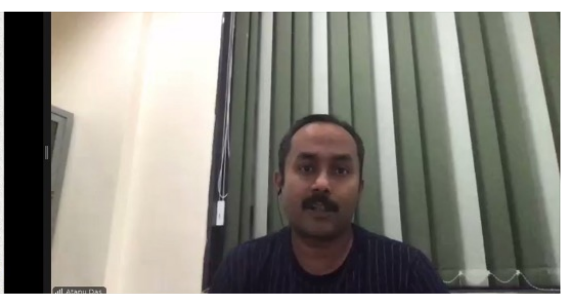
Sudeep N. Punnathanam
Department of Chemical Engineering,
Indian Institute of Science, Bengaluru

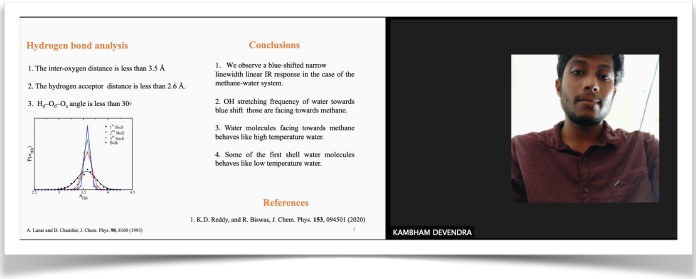


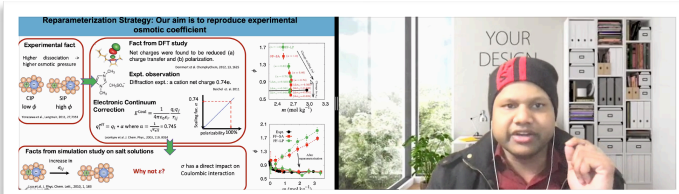
Structural Polymorphism Driven Thermodynamic Variability Effectively Predicts Disease Phenotype

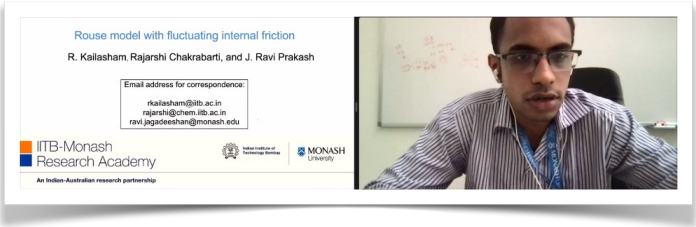
National Chemical Laboratory

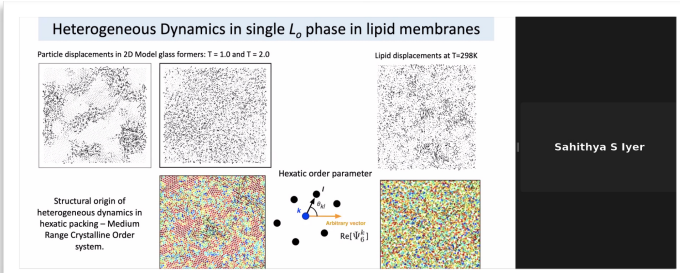
Statistical Mechanics in Chemistry and Biology 23rd – 26th Jan, 2021



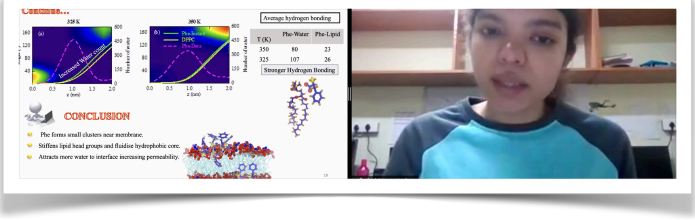

Hydrogen bond analysis
1. The inter-oxygen distance is less than 3.5 Å
2. The hydrogen acceptor distance is less than 2.6 Å.
3. H_d-O_d-O_a angle is less than 30°
Conclusions
1. We observe a blue-shifted narrow linewidth linear IR response in the case of the methane-water system.
2. OH stretching frequency of water towards blue shift those are facing towards methane.
3. Water molecules facing towards methane behaves like high temperature water.
4. Some of the first shell water molecules behaves like low temperature water.
References
1. K.D. Reddy, and R. Biswas, J. Chem. Phys. 153, 094501 (2020)
A. Lasar and D. Chandler, J. Chem. Phys. 98, 8160 (1993)
KAMBHAM DEVENDRA

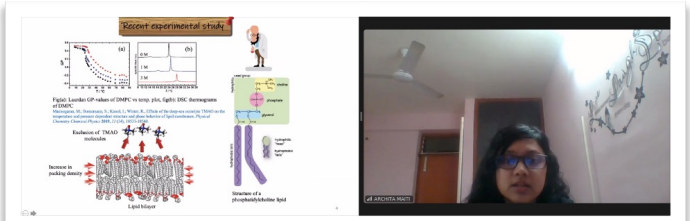

Reparameterization Strategy: Our aim is to reproduce experimental osmotic coefficient
Experimental fact
Fact from DFT study
Expt. observation
Electronic Continuum Correction
Facts from simulation study on salt solutions
Why not ε?
YOUR DESIGN

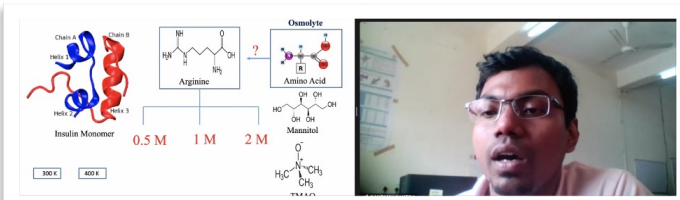

Rouse model with fluctuating internal friction
R. Kailasham, Rajarshi Chakrabarti, and J. Ravi Prakash
Email address for correspondence:
rkailasham@iitb.ac.in
rajarshi@chem.iitb.ac.in
ravi.jagadeeshan@monash.edu
IITB-Monash Research Academy
An Indian-Australian research partnership
MONASH University

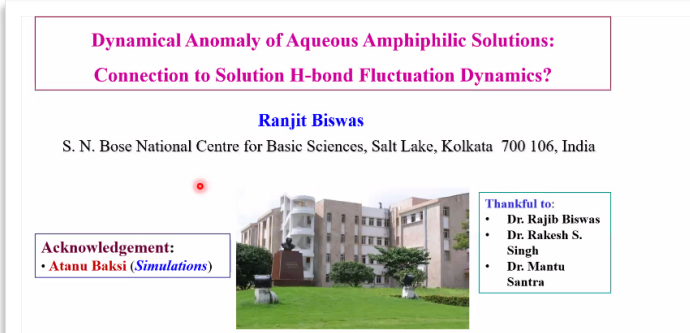

Heterogeneous Dynamics in single L_o phase in lipid membranes
Particle displacements in 2D Model glass formers: T = 1.0 and T = 2.0
Lipid displacements at T=298K
Structural origin of heterogeneous dynamics in hexatic packing – Medium Range Crystalline Order system.
Hexatic order parameter
Sahithya S Iyer


STATISTICAL MECHANICS IN CHEMISTRY AND BIOLOGY(SMCB)-2021
Fluctuation transduction guides protein-RNA target recognition
Binding Progress
Activated Domain Fluctuation
Deactivated Domain Fluctuation
Fluctuation Transduction
IISER KOLKATA


CONCLUSION
Phe forms small clusters near membrane.
Stiffens lipid head groups and fluidize hydrophobic core.
Attracts more water to interface increasing permeability.
Average hydrogen bonding
Stronger Hydrogen Bonding


Recent experimental study
Lipid bilayer
Structure of a phosphatidylcholine lipid

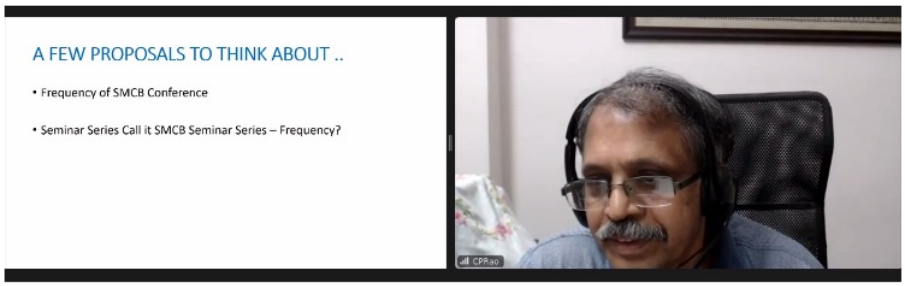

Chain A
Chain B
Helix 1
Helix 2
Helix 3
Insulin Monomer
Arginine
Osmolyte
Amino Acid
Mannitol
0.5 M
1 M
2 M
300 K
400 K

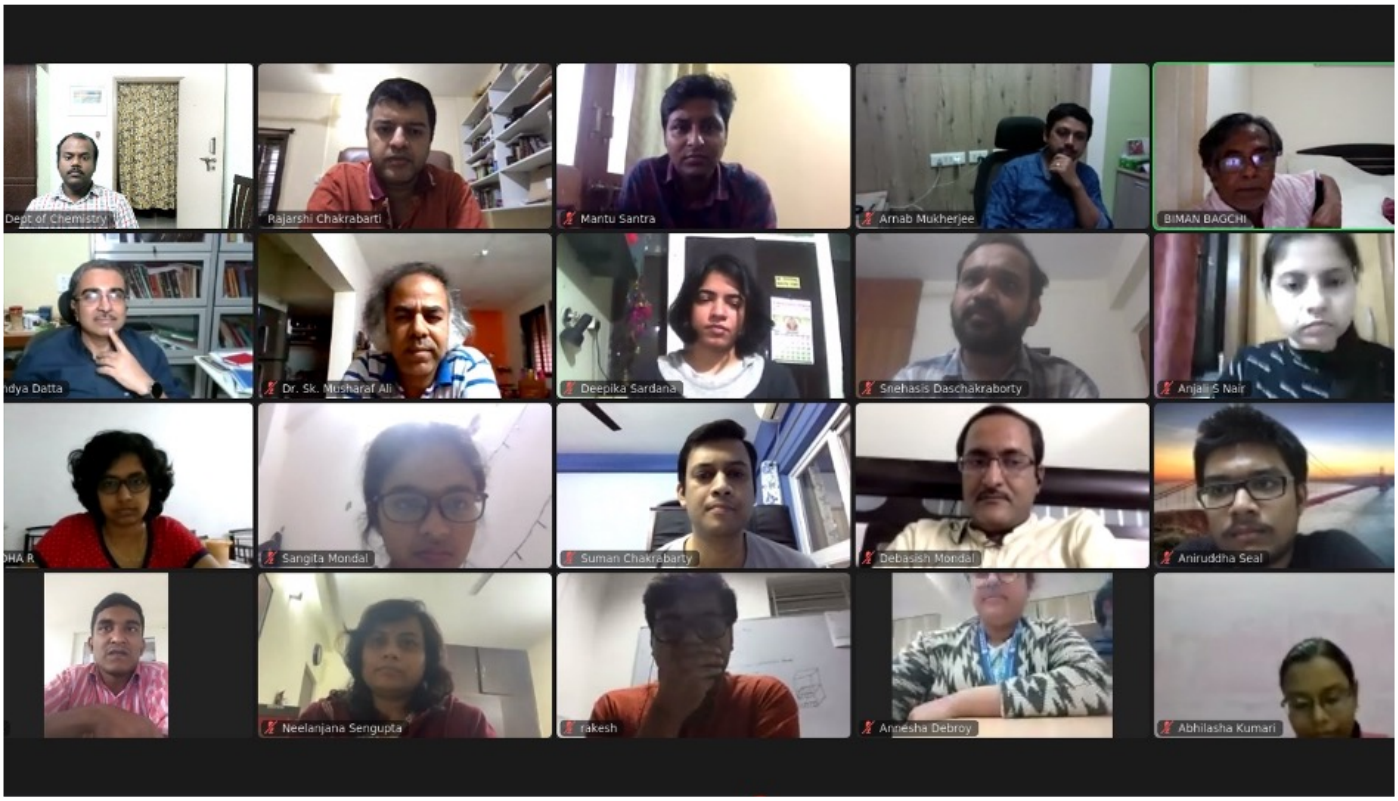

Dynamical Anomaly of Aqueous Amphiphilic Solutions:
Connection to Solution H-bond Fluctuation Dynamics?
Ranjit Biswas
S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700 106, India
Acknowledgement:
• Atanu Baksi (Simulations)
Thankful to:
• Dr. Rajib Biswas
• Dr. Rakesh S. Singh
• Dr. Mantu Santra
Focus: Anomaly in Solute-Centered Relaxation Dynamics in Aqueous Solutions
Method:
Molecular Dynamics Simulations


Ranjit Biswas


A FEW PROPOSALS TO THINK ABOUT ..
• Frequency of SMCB Conference
• Seminar Series Call it SMCB Seminar Series – Frequency?


BIMAN BAGCHI


A FEW PROPOSALS TO THINK ABOUT ..
• Frequency of SMCB Conference
• Seminar Series Call it SMCB Seminar Series – Frequency?
CPRao


Dept of Chemistry
Rajarshi Chakrabarti
Mantu Santra
Arnab Mukherjee
BIMAN BAGCHI
Dr. Sk. Musharaf Ali
Deepika Sardana
Snehasis Daschakraborty
Anjali S Nair
Sangita Mondal
Suman Chakrabarty
Debasish Mondal
Aniruddha Seal
Neelanjana Sengupta
Annesha Debroy
Abhilasha Kumari


Arijit Mondal
Bikramjit Sharma
Mantu Santra
Aniruddha Seal
Snehasis Daschakraborty
Deepika Sardana
Anand Srivastava
Madhav Ranganathan
Saumyak Mukherjee
Dr. Sk. Musharaf Ali
Sangram Prusty
Sangeeta Saini
Sayantan Mondal
Atanu Das
Ranjit Biswas
Srijan Chatterjee
Neelanjana Sengupta
Kajal Kumbhakar
keshav garg
Shreya
SARMISTHA SARKAR
M Sahil
Tanushree Das
Annesha Debroy
Prashant Pandey


Jagannath Mondal
Rajarshi Chakrabarti
Bhupendra
Arnab Mukherjee
Arijit Mondal
Bikramjit Sharma
Mantu Santra
Aniruddha Seal
Snehasis Daschakraborty
Deepika Sardana
Anand Srivastava
Madhav Ranganathan
Saumyak Mukherjee
Dr. Sk. Musharaf Ali
Sangram Prusty
Sangeeta Saini
Sayantan Mondal
Atanu Das
Ranjit Biswas
Srijan Chatterjee
Neelanjana Sengupta
Kajal Kumbhakar
keshav garg
Shreya
SARMISTHA SARKAR


Zoom Dept of Chemistry
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Rajarshi Chakrabarti
Mantu Santra
Arnab Mukherjee
Saumyak Mukherjee
BIMAN BAGCHI
Anindya Datta
Dr. Sk. Musharaf Ali
Deepika Sardana
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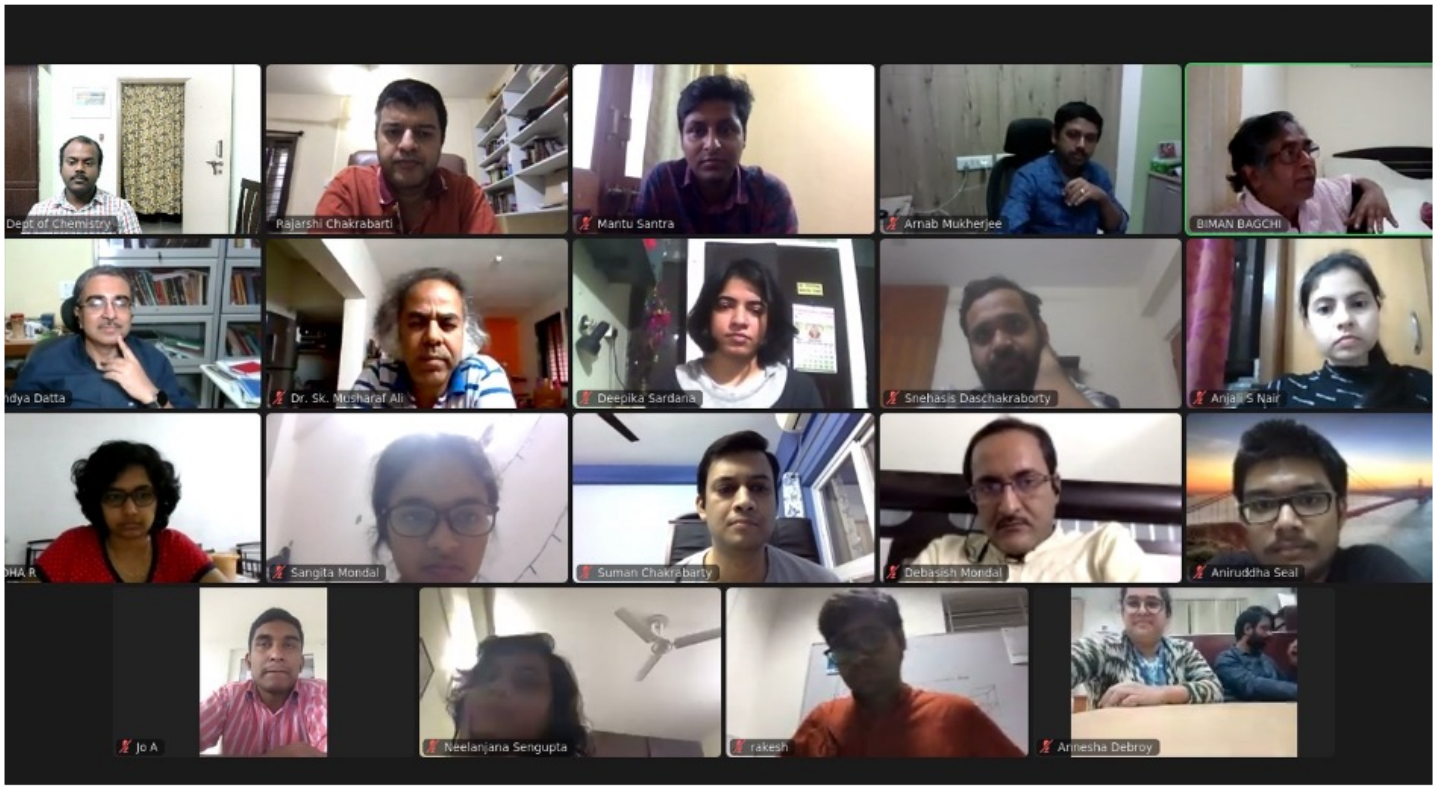
Anjali S Nair
CPRao
Anand Srivastava
GADHA R
Sangita Mondal
Suman Chakrabarty
Debasish Mondal
Aniruddha Seal
Jo A
Neelanjana Sengupta
Abhilasha Kumari
rakesh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Snehasis Daschakraborty
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Arnesha Debroy


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Saumyak Mukherjee
BIMAN BAGCHI
Anindya Datta
Dr. Sk. Musharaf Ali
Deepika Sardana
Snehasis Daschakraborty
Anjali S Nair
CPRao
Anand Srivastava
GADHA R
Sangita Mondal
Suman Chakrabarty
Debasish Mondal
Aniruddha Seal
Jo A
Neelanjana Sengupta
Abhilasha Kumari
rakesh


Zoom Dept of Chemistry
Ranjit Biswas
Rajarshi Chakrabarti
Mantu Santra
Arnab Mukherjee
Saumyak Mukherjee
BIMAN BAGCHI
Anindya Datta
Dr. Sk. Musharaf Ali
Deepika Sardana
Snehasis Daschakraborty
Anjali S Nair
CPRao
Anand Srivastava
GADHA R
Sangita Mondal
Suman Chakrabarty
Sangram Prusty
Debasish Mondal
Aniruddha Seal
Jo A
Neelanjana Sengupta
Abhilasha Kumari


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JURITI RAJBANGSHI
Snehasis Daschakraborty
Sayantan Mondal
Anjali S Nair
CPRao
Kajal Kumbhakar
Anand Srivastava
Hemant Kashyap
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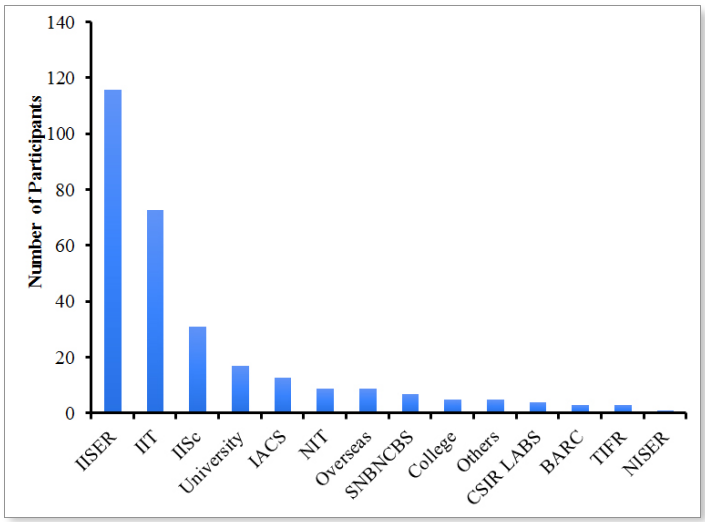
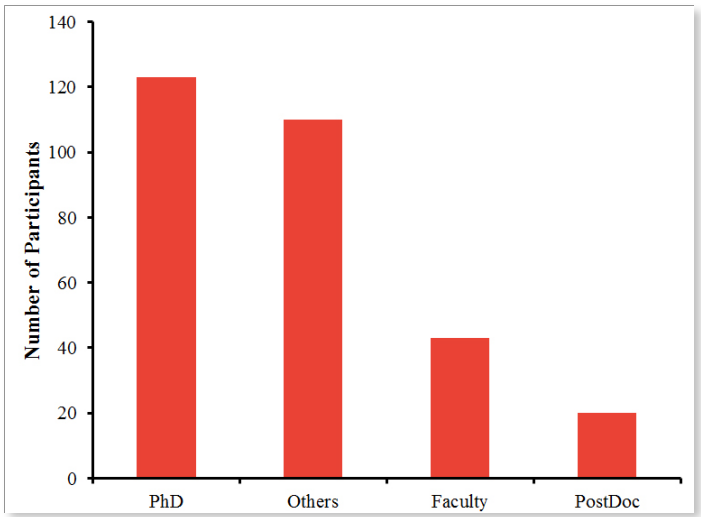
Suman Chakrabarty
Sangram Prusty
Debasish Mondal
Aniruddha Seal
SARMISTHA SARKAR
Jo A
Neelanjana Sengupta

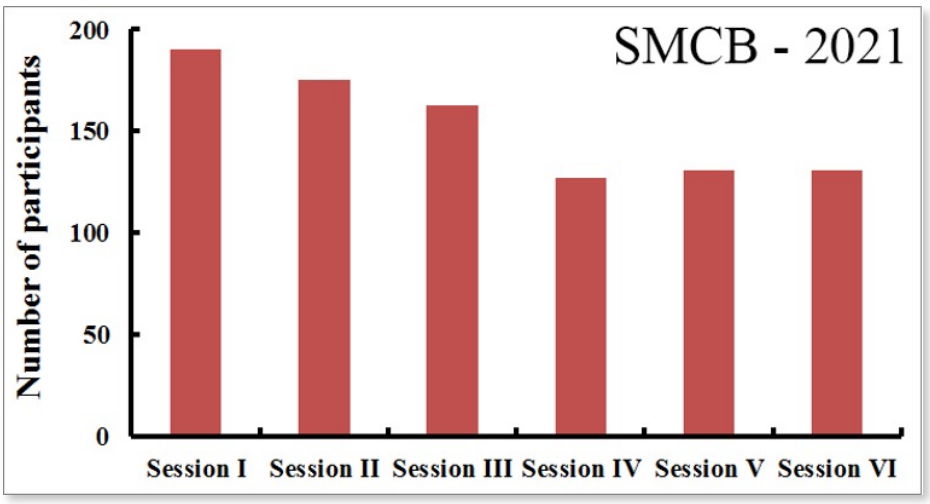
Statistics

The conference has received overwhelming responses from the community. More than 300 participants registered for the conference across the country and a few from overseas as well.





Details of registered participants.



Total number of participants attended at least one full talk in each session.

Thank You!