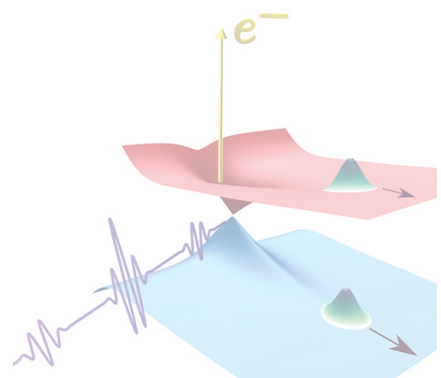
IISER KOLKATA

INTERSECTION OF THEORY AND COMPUTATION IN CHEMISTRY (ITCC)

1st July, 2022

IISER Kolkata



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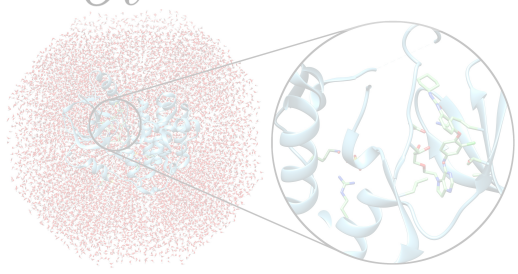


भारतीय विज्ञान शिक्षा और अनुसंधान संस्थान, कोलकाता

Indian Institute of Science Education and Research, Kolkata

... towards excellence in science

From Convenors' Desk

We are pleased to organize the first Intersection of Theory and Computation in Chemistry (ITCC) conference at Indian Institute of Science Education and Research (IISER) Kolkata. The idea of this meeting originates from the fact that Kolkata has a strong legacy of Theoretical Chemistry and therefore, emerging theoretical chemists of Kolkata region should meet annually to discuss their ongoing research.

In the last few decades, Theoretical and Computational Methods have emerged as powerful, modern-day methods for the study of molecules, nanomaterials and biomolecular systems. Complementary development of theoretical methods and applications are expected to expand their collective predictive abilities and scope of applications. The one-day ITCC Conference at IISER Kolkata aims to bring together researchers in overlapping domains for invigorating interactions.

We hope all the participants will enjoy the talks and the discussions will be fruitful.

With warm regards,

Ashwani and Neelanjana

Speakers

Prof. Arun Yethiraj (University of Wisconsin-Madison)

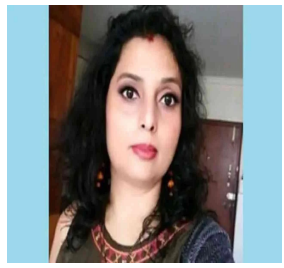
Prof. Ayan Datta (IACS Kolkata)

Prof. Manoranjan Kumar (SNBNCBS Kolkata)

Prof. Neha Agnihotri (NIT Jamshedpur)

Prof. Suman Chakrabarty (SNBNCBS Kolkata)

Speakers



Prof. Vidya Avasare (Parashurambhau College, Pune)

Prof. Divya Nayar (IIT Delhi)

Prof. Sangita Sen (IISER Kolkata)

Prof. Asis Jana (Sister Nivedita University, Kolkata)

Program Schedule

Inauguration

Venue: G06 Lecture Hall Complex

9:00-9:40	Registration
9:40-9:45	Welcome Address, Ashwani K. Tiwari, Convener ITCC
9:45-9:50	Welcome Address, C. Malla Reddy, HoD, DCS
9:50-10:00	Welcome Address, Sourav Pal, Director, IISER Kolkata

Session 1

Chairperson	**Neelanjana Sengupta**
10:00-10:45	Arun Yethiraj Machine learning for phase diagrams of complex fluids
10:45-11:15	Manoranjan Kumar Application of Hybrid ED/DMRG in Frustrated Spin-1/2 Systems
11:15-11:45	Divya Nayar An overview of crowding effects on fibrillar self assembly using molecular simulations

11:45-12:00 TEA BREAK

Session 2

Chairperson	**Debashree Ghosh**
12:00-12:30	Ayan Datta Pseudo Jahn-Teller Distortions in Two - Dimensional Atomically Thin Monolayers
12:30-13:00	Neha Agnihotri Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells
13:00-13:30	Suman Chakrabarty How do proteins talk to each other? A molecular thermodynamic view

13:30-14:30 LUNCH BREAK

Session 3

Chairperson	Biman Jana
14:30 - 15:00	Vidya Avasare Computational Catalysis in the Quest of Robust Catalysts
15:00 - 15:30	Sangita Sen Spin And Orbital Effects in Non-Uniform Magnetic Fields
15:30 - 16:00	Asis Jana Computational Microscopy of Viruses
16:00 - 17:00	Felicitation of Prof Sourav Pal (Chair, Prof. Satrajit Adhikari)
17:00 - 17.05	Vote of Thanks by Prof. Neelanjana Sengupta

17:05-17:30 HIGH TEA

End of the Conference

Abstracts

Machine learning for phase diagrams of complex fluids

Arun Yethiraj

Department of Chemistry, University of Wisconsin, Madison
E-mail: yethiraj@chem.wisc.edu

Machine learning (ML) has become an important tool in computational chemistry. This work describes the use of supervised and unsupervised ML methods to obtain the phase diagram of complex fluids from computer simulations. A convolutional neural network approach, based on a grid interpolation of particle positions, successfully predicts the phase behavior of off-lattice systems, e.g., the Widom-Rowlinson mixture and symmetric polymer blends. The method is too computationally intensive, however, for more complex polymeric systems. A deep neural network approach, based on structural and thermodynamic input from computer simulations predicts the phase diagram of polymers in ionic liquids. The disadvantage of supervised methods is that they require some knowledge of the phase diagram for training purposes. Unsupervised methods based on principal component analyses can predict the phase diagram of off-lattice systems, without any prior knowledge. The method is, however, sensitive to the choice of the input features. ML methods are therefore an attractive route to obtaining phase diagrams via computation, but physical insight plays an important role in their implementation.

Application of Hybrid ED/DMRG in Frustrated Spin-1/2 Systems

Manoranjan Kumar

S N Bose National Centre for Basic Sciences Kolkata
E-mail: manoranjan.kumar@bose.res.in

We study the quantum phase diagram and low temperature magnetic properties of a frustrated spin-1/2 one dimensional system. In this talk we show that the frustration in the system can induce various kinds of exotic phases. It is well known that study of magnetic properties of a frustrated system at low temperature is not reliable. In this presentation we will also try to show that the hybrid exact diagonalization/density matrix renormalization group method is a reliable numerical method to calculate the low temperature properties of these systems .

An overview of crowding effects on fibrillar self-assembly using molecular simulations

Divya Nayar

Department of Materials Science and Engineering, IIT Delhi
E-mail: divyanayar@mse.iitd.ac.in

Macromolecular crowding effects are ubiquitous inside a living cell and are expected to modulate biomolecular structure and dynamics.[1] The role of such an environment in regulating self-assembly, protein folding and aggregation remains elusive. The traditional view highlights that crowded milieu induces compaction or self-assembly in biomolecules. A new view has emerged that indicates that the crowded environment may either promote or oppose protein folding.[2,3] Additionally, the emerging view indicates that the widely accepted size (entropic) effects of large-sized macromolecular crowders may not be sufficient to explain the collapse or self-assembly of proteins inside a living cell.[4-6] Molecular dynamics simulations can be an effective tool to obtain a microscopic view of the underlying mechanisms by which a crowded environment induces or prevents biomolecular self-assembly. However, there are challenges associated with the accurate modeling of such systems at the molecular level.[7] Therefore, it becomes imperative to ask the following questions: (a) does a crowded environment always lead to self-assembly or collapse of biomolecules? (b) can we understand the role of intermolecular attractions in a more explicit way (c) what are the thermodynamic driving forces underlying such effects? (d) can the current molecular simulation models accurately model a crowded environment? My talk will provide an overview of the strategy to answer the above questions for an interesting system, pseudo-isocyanine chloride dyestuff, that is known to self-assemble into fibril-like aggregates, like those formed by amyloid-forming intrinsically disordered proteins.[8] Interestingly, experiments have indicated that the crowded environment can promote or inhibit the aggregation of these dye molecules depending upon the chemical nature of the crowders, making it an interesting system for designing molecular sensors for crowding effects on self-assembly processes in the living cell.[8]

References:

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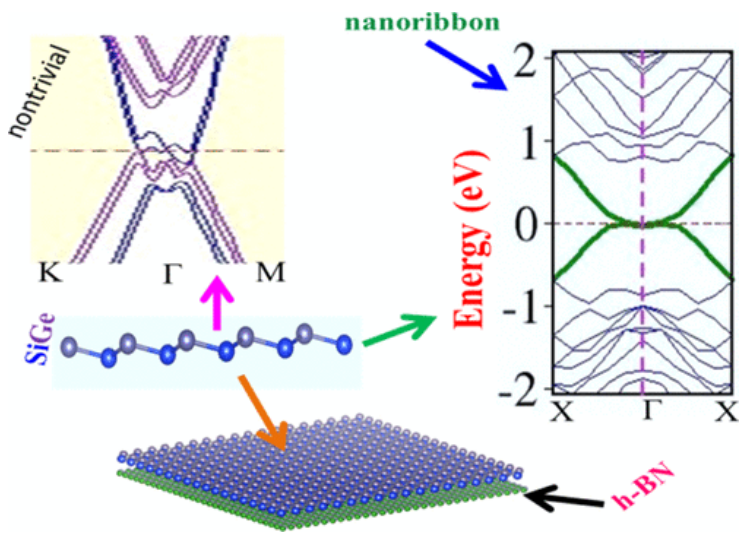
Pseudo Jahn-Teller Distortions in Two - Dimensional Atomically Thin Monolayers

Ayan Datta

School of Chemical Sciences, Indian Association for the Cultivation of Science (IACS), Kolkata – 700032, INDIA
E-mail: spad@iacs.res.in

Graphene has emerged as one of the most fascinating areas of research in condensed matter and materials science. Apart from graphene, several other 2D analogues like silicene, phosphorene, MXenes, MoS 2 , germanene have been recently isolated and characterized. One unifying theme among these new materials is that unlike graphene, they are non-planar. The mode and measure of the buckling (puckering) from planarity depends on the local electronic structure. The effects of such ripples are manifold particularly in its local reactivity to halogens and hydrogens along the more ~sp 3 atoms. Pseudo Jahn-Teller (PJT) distortions is shown as a central unifying concept that explains the overall structural preferences of these systems. The extent of buckling also leads to interesting and emerging phenomenon like phase-transitions into Topological Insulators from normal semi-metal due to spin-orbital coupling (SOC). The effect of PJT in bestowing structural diversity and novel electronic and spin phases in 2D-monoatomic layers will be discussed in this lecture.



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Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells

Neha Agnihotri*

Department of Physics
National Institute of Technology, Jamshedpur-831014, India
E-mail: neha.phy@nitjsr.ac.in

Dye-sensitized solar cells (DSSCs) have appeared as a most promising alternative to traditional silicon-based solar cells. They are utilizing different components for light-harvesting and transport functions. Thus, we have the freedom to fine-tune each component individually to optimize their overall power conversion efficiency. Predictive modeling simulations have been performed, in which the properties of a system were simulated before time-consuming laboratory synthesis and characterization of the material. At the same time, computer simulations offer crucial insight into hitherto inaccessible experimental observations. Organic dye-sensitizers are essential components of the DSSCs. A comprehensive theoretical study of the dye's spectroscopic properties, including excitation energies, allows us to design and screen potential sensitizers for DSSCs. Density functional theory (DFT) and time-dependent density functional theory (TDDFT) approaches have been employed to estimate the optoelectronic properties of sensitizers. This study has revealed that the longest wavelength electronic transitions are characterized by fully allowing one electron highest occupied molecular orbital to the lowest unoccupied molecular orbital promotions, and extend well into the usable region of the near-infrared portion of the solar spectrum. Charge transfer indices reveal the electron density distribution in the molecular system. The absorption spectra are panchromatic in nature with strong near-infra-red absorptions. It has been proposed that the substituted derivatives of porphyrins are worthy of consideration as dye-sensitizers for efficient DSSCs.

How do proteins talk to each other? A molecular thermodynamic view

Suman Chakrabarty

S. N. Bose National Centre for Basic Sciences, Kolkata
E-mail: sumanc@bose.res.in

Cell signaling involves a fascinatingly complex network of interacting protein molecules, where information might flow through molecular recognition, protein-protein interactions or long range communication within a single/multi-domain protein (allostery). In this talk, we shall demonstrate how simple ideas from molecular thermodynamics and computer simulations can lead to meaningful mechanistic information about such complex processes.

Some representative test cases will be discussed to elucidate that internal re-distribution of electrostatic interactions in terms of re-wiring and rearrangement of hydrogen bonded network can play a significant role in the long range signal propagation in proteins including *dynamic allostery*.[1] We speculate the existence of a *universal response network* in signalling proteins which may respond to different kinds of external stimuli/perturbations.[2] Finally, we shall discuss the molecular thermodynamic basis of "phosphorylation code" in release of specific partners selectively in RhoGDI-RhoA type of protein complexes.[3] While biology is all about specific details, we hope to arrive at some generalisations in terms of the molecular thermodynamics of long range signal propagation in the above systems. During this talk, we shall raise many questions, and hopefully answer a few!

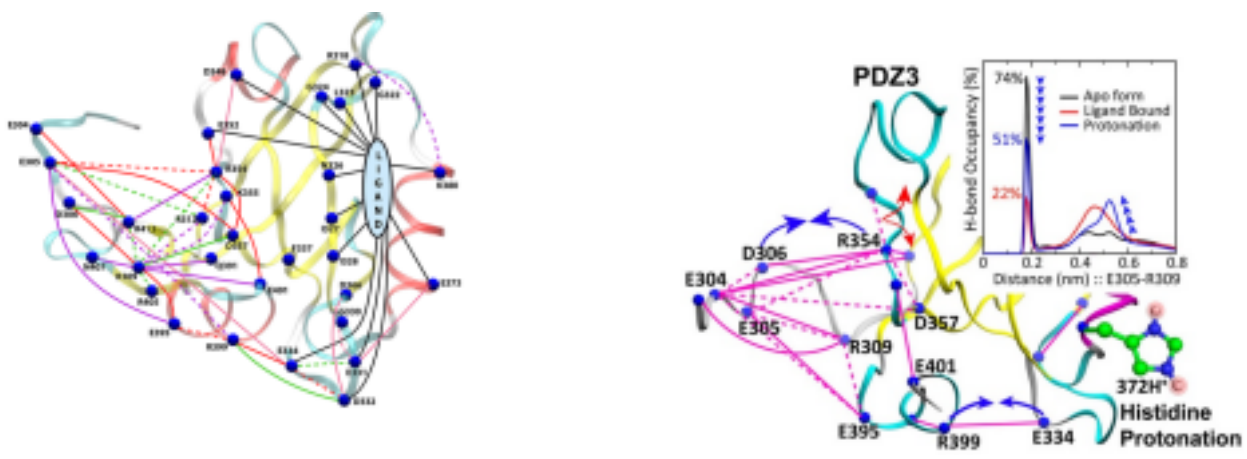

Figure: Universal response network in PDZ domain protein: ligand binding (left) and protonation of H372 (right)

References:

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2. A. Kumawat and S. Chakrabarty*, J. Phys. Chem. Lett., 2020, 11, 9026.
3. Unpublished data

Computational Catalysis in the Quest of Robust Catalysts

Vidya D. Avasare

Department of Chemistry, Parashurambhau College, Pune Maharashtra 411030 India
Department of Chemistry, Ashoka University, Sonipat, Haryana 131029 India
E-mail: avasarevidya7@gmail.com

Catalyst is the magic wand and has transformed many synthetic protocols beyond the imagination. There is always a scope to design and develop a robust catalyst. The development of a completely new catalysts and the experimental validation is an arduous task and it would be difficult to invest in the development of a 'newfangled' catalyst. Computational drug design has enormously impacted the field of medicinal chemistry. Now, it is a widely accepted, user-friendly, precise, less laborious, and cost-effective method in drug development. On a similar line, the computationally designed catalysts would be useful to perform the targeted synthesis under desired conditions. This would be tremendously beneficial to academia as well as industry. It would be important to understand, how the same ligand with different metals or the same metal with different ligands plays a crucial role in the performance of the catalyst prior to the experimental. The density functional theory (DFT) is a very powerful tool to get insight into catalytic performance.

Recently, we have been designing various catalysts to perform carbon dioxide hydrogenation. 1-3 These findings could be useful in understanding the significance of fine-tuning of ligands on catalytic performance and enhancing turnover frequency (TOF) to get desired results in carbon dioxide hydrogenation.

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[2] S. V Parmar, V. Avasare, S. Pal, *Front. Chem.* (2021) (doi.org/10.3389/fchem.2021.778718)
[3] V. Avasare, S. Virani, D. Das, S. Pal *J. Phy. Chem. C* (2021) (doi.org/10.1021 acs.jpcc.1c05918).

Spin And Orbital Effects in Non-Uniform Magnetic Fields

Sangita Sen[1], Erik Tellgren[2]

[1] Indian Institute for Science Education and Research, Kolkata
[2] Hylleraas Centre for Quantum Molecular Sciences, University of Oslo, Norway
E-mail: sangita.sen@iiserkol.ac.in

The direct interaction of the spin of an electron comes into play in the presence of an external magnetic field during variational optimisation of the orbitals of an electronic system. While the role of a uniform field is relatively easy to understand the presence of a position dependent field can complicate matters. In this presentation we try to analyse various aspects of the interplay of spin and orbital interactions on electronic states.

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[3] S. Sen and E. I. Tellgren, *J. Chem. Theory Comput.* 17, (2021) 1480.

Computational Microscopy of Viruses

Asis Jana

Sister Nivedita University, Kolkata
E-mail: jana.asis@gmail.com

All-atom molecular dynamics (MD) simulations, sometimes termed a “computational microscope” have emerged as a powerful tool for studying viral systems. We performed a series of atomically detailed simulations to study the molecular details of cell entry in non-enveloped viruses. Apart from this, we have investigated over the last year SARS-COV-2 induced amyloid formation as a way to explain some of the long-term effects troubling COVOID-19 survivors. For instance, symptoms of “Long COVID” and the Multisystem Inflammatory Syndrome in adults (MIS-A) resemble Serum Amyloid A (SAA) amyloidosis, and SAA overproduction is a symptom of COVID-19. Similarly, various case studies have hinted at a correlation between COVID-19 and the onset of Parkinson’s disease. However, the molecular mechanisms that underlie this process remain unknown and are particularly challenging to address using current experimental techniques. For this reason, we have performed long all-atom molecular dynamic simulations to study whether amyloidogenic regions in SARS-COV-2 proteins can initiate and modulate aggregation of SAA and α-synuclein, which are responsible for SAA amyloidosis and Parkinson disease, respectively. Our simulations agree with experimental observations and reveal nanoscopic details regarding SARS-COV-2 induced amyloid formation.