Scientific Programme (CTTC-2024)

वैज्ञानिक कार्यक्रम (सीटीटीसी – 2024)

DAE-BRNS Symposium on Current Trends in Theoretical Chemistry

सैद्धांतिक रसायन शास्त्र में समसामयिक विचारधाराओं पर पऊवि बीआरएनएस संगोष्ठी

Bhabha Atomic Research Centre, Mumbai, India

September 26 – 28, 2024

भाभा परमाणु अनुसंधान केंद्र, मुंबई – 400085, भारत

सितंबर 26 – 28, 2024

Day -1, 26th September 2024 (Thursday)		
Time		
8:30 – 9:30	***Registration***	
9:30 – 10:30	***Inaugural Function & Keynote address by the Chief Guest***	
10:30 – 11:00	***High Tea***	
11:00 – 12:20	***Plenary Session 1*** **Session Chair: Prof. A. K. Tyagi**	
11:00 – 11:40	**PL-1: Prof. Sourav Pal, Ashoka University** *Accurate methods for shape resonance and decay processes in molecules*	
11:40 – 12:20	**PL-2: Prof. Rajeev Ahuja, IIT Ropar** *Computational Materials Science and Its Applications in The Area of Materials for Energy*	
12:20 – 13:20	***Session 1*** **Session Chair: Prof. Awadhesh Kumar**	
12:20 – 12:50	**Perspective Talk - 1**	**Prof. Prabal K. Maiti, IISc, Bangaluru** *2-TIPS and ordering in various active matter systems*
12:50 – 13:20	**Perspective Talk - 2**	**Prof. Sanjoy Bandyopadhyay, IIT Kharagpur** *Interfacial Properties of Biomolecules in Aqueous Ionic Liquid Solution*
13:20 – 14:00	***Lunch Break***	
14:00 – 15:45	***Session 2*** **Session Chair: Prof. A. C. Bhasikuttan**	
14:00 – 14:30	**Perspective Talk - 3**	**Prof. Ashok Arya, BARC, Mumbai** *Efficient screening of single phase forming low-activation high entropy alloys*
14:30 – 15:00	**Perspective Talk – 4**	**Prof. Suman Chakrabarty, S N Bose National Centre for Basic Sciences, Kolkata** *Exploration of Free Energy Landscape of Complex Molecular Systems: Dynamics to Thermodynamics and Back*
15:00 – 15:30	**Perspective Talk - 5**	**Prof. Dilip K. Maity, BARC, Mumbai** *Hydration of metal ions and molecules*
15:30 – 15:45	**LT-1**	**Prof. Anoop Ayyappan, Digital University Kerala** *Exploring Boron Group Nanoclusters for Catalytic Activity*
15:45 – 16:00	**Technical Talk-1**	**Netweb Technologies**
16:00 – 16:15	***Tea Break***	
16:15 – 18:15	***Session 3*** **Session Chair: Prof. S. R. Gadre & Co-Chair: Prof. V. Subramanian**	
16:15 – 16:45	**Perspective Talk - 6**	**Prof. Gour P. Das, TCG CREST, Kolkata** *Quo Vadis DFT:a Perspective*
16:45 – 17:15	**Perspective Talk - 7**	**Prof. Pratim K. Chattaraj, BIT Mesra** *Global Optimization of Atomic Clusters: A Soft Computing Perspective*
17: 15 –17:45	**Perspective Talk – 8**	**Prof. Alok K. Samanta, Former BARC, Mumbai** *A new approach to a Generalized Smoluchowski Equation*
17: 45 –18:15	**Perspective Talk - 9**	**Prof. Chandra N. Patra, BARC, Mumbai** *Large Molecules in Solution: Multiscale Modeling and Simulation*
18:15 – 19:00	**Session Chair: Prof. J. P. Mittal**	
18:15 – 19:00	**Evening Lecture**	**Prof. Swapan K. Ghosh, UM-DAE CEBS, Mumbai**
19:30 Onwards		**Banquet Dinner**

Day -2, 27th September 2024 (Friday)				
Time				
8:30 – 9:30	***Registration***			
9:30 – 10:15	***Plenary Session 2*** **Session Chair: Prof. A. K. Samanta**			
9:30 – 10:15	**PL-3**	**Prof. Swapan K. Ghosh, UM-DAE CEBS, Mumbai** *Density functional theory : A versatile tool for modelling Chemistry across the length scales*		
10:15 – 11:15	**Session 4** **Session Chair: Prof. Pratim K Chattaraj**			
10:15 – 10:45	**Perspective Talk – 10**	**Prof. Satrajit Adhikari, IACS Kolkata** *The effect of surface temperature on molecule-surface scattering processes*		
10:45 – 11:15	**Perspective Talk – 11**	**Prof. Nisanth N. Nair, IIT Kanpur** *Exploring Rugged Energy Landscapes of Enzymatic Reactions*		
11:15 – 11:30	***Tea Break***			
11:30 – 13:10	***Session 5*** **Session Chair: Prof. Y. K. Bhardwaj & Prof. C. Majumder**			
11:30 – 12:00	**Perspective Talk – 12**	**Prof. Amalendu Chandra, IIT Kanpur** *Terahertz Spectroscopy of Aqueous Systems using Polarizable Models*		
12:00 – 12:30	**Perspective Talk – 13**	**Prof. Biman Jana, IACS Kolkata** *Optimizing Collective Variable for Linear Hydrophobic Polymer Collapse and Protein Folding Transitions: Crucial Role of Hydration*		
12:30 – 12:50	**ST-1**	**Prof. Arup K. Pathak, BARC, Mumbai** *Uranyl Ion Binding to Human Serum Albumin: Influence of Fatty Acid*		
12:50 – 13:10	**ST-2**	**Prof. Mahesh Sundararajan, BARC, Mumbai** *Theory Driven Experiments for Small Molecule Activation*		
13:10 – 14:00	**Lunch Break**			
14:00 – 15:30	***Poster Session & Tea* (Categories: A to F)** **Session Chairs: Prof. V. Sudarsan & Prof. S. Sahoo** **(Members: Profs. R. Acharya, Y. Sajeev, B. Modak, S. Nath, S. N. Achary, J. Jose, R. Mahesh, J. Mohanty, M. C. Rath, C. A. Betty)**			
15:30 – 17:15	***Session 6*** **Session Chair: Prof. S. M. Yusuf**			
15:30 – 16:00	**Perspective Talk – 14**	**Prof. Ranjit Biswas, S N Bose National Centre for Basic Sciences, Kolkata** *Liquid Phase of Deep Eutectics: Enthalpy versus Entropy*		
16:00 – 16:30	**Perspective Talk – 15**	**Prof. Sk. Musharaf Ali, BARC, Mumbai** *Dehydration Induced Selective Ion Trapping by Topology Constrained Atomically Thin Graphene-Crown Membranes*		
16:30 – 17:00	**Perspective Talk – 16**	**Prof. B. V. R. Tata, GITAM University, Vizag** *Unusual Dynamics, Phase Behavior and Yielding of Dense Stimuli Responsive Microgel Glasses: Experiments and Simulations*		
17:00 – 17:15	**Technical Talk 2**	**Wiley Publishers**		
17:15 – 18:35	***Parallel Session 1*** **Session Chair: Prof. A. Sen & Prof. J. Jose**		***Parallel Session 2*** **Session Chair: Prof. S. Mazumder & Prof. B. Goyal**	
17:15 – 17:35	**ST-3**	**Prof. Sandeep Nigam, BARC, Mumbai** *Computational Chemistry and Experiment: So Close, Yet So Far* *Sandeep Nigam*	**ST-7**	**Prof. Kailas D. Sonawane, Shivaji University, Kohlapur** *Understanding antibiotic resistance : A major public health problem*
17:35 – 17:55	**ST-4**	**Prof. Snehasis Daschakraborty, IIT Patna** *Photoswitchable Lipids in Liposomal Membrane: From Fundamentals to Applications*	**ST-8**	**Prof. G. Gopakumar, IGCAR, Kaplakkam** *Density Functional Theory Studies on the Separation and Recovery of Lanthanides and Actinides*
17:55 – 18:15	**ST-5**	**Prof. Divya Nayar, IIT Delhi** *Living Cell Soup: Biomolecular Self-Assembly to Nanomaterial Design*	**ST-9**	**Prof. Paritosh Modak, BARC, Mumbai** *Elemental Solids under High Pressure: A Case Study on Elemental Calcium*
18:15 – 18:35	**ST-6**	**Shri Pritam P. Shete, BARC, Mumbai** *Introduction to Large Language Models: From Foundation to Real World Applications*	**ST-10**	**Prof. Neetu Goel, Punjab University** *First Principle Tailoring of Metal Porphyrins for Electrocatalysis*
18:35 –18:45	**Tea Break**			
18:45 – 19:30	**Cultural Programme**			
19:30 Onwards	**Dinner**			

Day -3, 28th September 2024 (Saturday)				
Time				
09:30 – 11:40	***Session 7*** **Session Chair: Prof. T. K. Ghanty**			
09:30 – 10:00	**Perspective Talk – 17**	**Prof. R. B. Sunoj, IIT Bombay** *Molecular Machine Learning Approaches to Chemical Catalysis*		
10:00 – 10:30	**Perspective Talk – 18**	**Prof. Deva Priyakumar, IIIT Hyderabad** *Generative Artificial Intelligence in Molecular Science Research*		
10:30 – 11:00	**Perspective Talk – 19**	**Prof. Ram K. Roy , BITS-Pilani** *In Search of Mechanism of Aggregation Induced Emission: A Theoretical Study*		
11:00 – 11:20	**ST-11**	**Prof. Biswarup Pathak, IIT Indore** *Development of Artificially Intelligent Nanopores for HighThroughput Seque*		
11:20 – 11:40	**ST-12**	**Prof. Arnab Mukherjee, IISER Pune** *Reinforcement Learning Helix Disrupting Mutation*		
11:40 – 11:55	***Tea Break***			
11:55 – 12:55	***Parallel Session 3*** **Session Chair: Shri K. Bhanja & Prof. M. K. Ravva**		***Parallel Session 4*** **Session Chair: Prof. M. Manna & Prof. A. Chand**	
11:55 – 12:10	**LT-2**	**Prof. Achintya K. Dutta, IIT Bombay** *Relativistic Coupled Cluster Method Beyond Diatomic Molecules*	**LT-6**	**Prof. Padmesh A., IIT Palakkad** *Sub-Pico-Newton Forces and The Folding-Unfolding of Trpzip2 B-Hairpin*
12:10 – 12:25	**LT-3**	**Prof. Kaushik Talukdar, Bhattadev University, Bajali** *Relativistic Coupled-Cluster Study of Molecules for Precision Experiments*	**LT-7**	**Prof. Mudit Dixit, CLRI, Chennai** *Accelerating Materials Discovery for Catalysis and Electrochemical Energy Storage*
12:25 – 12:40	**LT-4**	**Prof. Prakash M. SRM University, Chennai** *Electrode/Electrolyte-Based Interface Models for CO2 Catalysis: A First Principle Study*	**LT-8**	**Prof. Brindaban Modak, BARC, Mumbai** *Tuning Intrinsic Defects through Dopant Engineering*
12:40 – 12:55	**LT-5**	**Prof. Tijo J. Vazhappilly, BARC, Mumbai** *Computational Modeling Of Materials for Energy Applications*	**LT-9**	**Prof. Harish Srinivasan, BARC, Mumbai** *Modeling, Theory, And Simulation in Soft Condensed Matter (F) Nature of Universal Subdiffusion Crossover in Molecular Glass-Formers*
12:55 – 13:40	**Lunch Break**			
13:40 – 15:10	***Session :*** **Poster Session & Tea (Categories: G-J)** **Session Chairs: Prof. H. P. Upadhyaya & Prof. A. K. Pathak** **(Members: Profs. R. Mishra, M. Pai, S. Varma, M. Kumbhakar, R. Ganguly, P. Mathi, A. Sen, M. Manna, S. Mahesh, Tijo J.)**			
15:10 – 16:55	***Session 8*** **Session Chairs: Prof. Chandra N. Patra & Prof. N. Choudhury**			
15:10 – 15:40	**Perspective Talk – 20**	**Prof. Gopalan Rajaraman, IIT Bombay** *Role of Molecular Modelling in the Design and Development of Molecular Nano Magnets*		
15:40 – 16:10	**Perspective Talk – 21**	**Prof. Ranjan Mittal, BARC, Mumbai** *Phonons and Thermodynamic Behaviour of Novel Compounds: A Perspective from Neutron Scattering Experiments and Ab-initio Simulations*		
16:10 – 16:40	**Perspective Talk – 22**	**Prof. Rajarshi Chakrabarti, IIT Bombay** *Phase separation in active systems: insights from computer simulations*		
16:40 – 16:55	**Technical Talk 3**	**ACS Publishers**		
16:55 – 17:40	***Poster Awards & Concluding Session***			
19:30 Onwards	***Dinner***			

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