

Program Schedule

3rd International Conference on Materials Genome (ICMG-III)

Organized by SRM University – AP, Andhra Pradesh

In association with

Asian Consortium on Computational Materials Science
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore
National Chemical Laboratory, Pune
Virginia Commonwealth University, USA
Indian Institute of Technology, Madras
Indian Institute of Technology, Bombay
TCG, Crest, Kolkata

22- 24 February 2024

22nd February, Thursday 2024 (Day - 1)

Venue: SRM Block, Mini Auditorium, Hall 1 and Hall 2 and Hall 3
All time are in IST

8.30 a.m. to - 9.30 a.m.: Registration, Mini Auditorium, SR Block, SRM University-AP

9.30 a.m. - 10.00 a.m.: Inaugural Session, Mini Auditorium, SR Block, SRM University-AP

**Lectures are in Mini Auditorium, Hall 1 (S 206), Hall 2 (S 207) and Hall 3 (S 201)
are on 2nd Floor of SR Block**

Morning Session: 10.00 a.m. – 1.00 p.m. Keynote Session

Session I

Session Chair: Prof. Ranjit Thapa & Dr. Pankaj Bhalla

10.00 a.m. – 10. 50 a.m.	Mini Auditorium	Invited Key Note Lecture 1	Prof. Puru Jena	Title: Cluster-based Energy Materials – A Paradigm shift in Design and Synthesis
20 Mins Break				
11:10 a.m. – 12:00 p.m.	Mini Auditorium	Invited Key Note Lecture 2	Prof. Bikas Chakrabarti	Title: FRACTURE STORY: A Personal Summary
12:05 pm – 12:55 pm	Mini Auditorium	Invited Key Note Lecture 3	Prof. G. P. Das	Title: Designing solid electrolytes for cheaper, safer and greener batteries

*45 mints lecture + 5 mints discussion

01. 00 p.m. – 2.00 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.00 p.m. – 5.45 p.m.: Three Parallel Sessions and One Symposium

Parallel Session I

Session Chair: Prof. Prasenjit Sen

2.00 p.m. – 2.30 p.m.	Mini Auditorium	Invited Lecture 4	Dr. Jun Zhou	Title: Emergent magnetic properties in electrenes
2.35 p.m. – 3:05 p.m.	Mini Auditorium	Invited Lecture 5	Dr. Karthik Rajendran	Title:
3.10 p.m. – 3.40 p.m.	Mini Auditorium	Invited Lecture 6	Dr. A. Lorenzo Mariano	Title: Spin-phonon interactions in single-molecule magnets: from theory to material design

Parallel Session I

Session Chair: Prof. Shen Lei and Dr. Debabrata Pramanik

4.00 p.m. – 4.30 p.m.	Mini Auditorium	Invited Lecture 7	Prof. Ranjit Thapa	Title: Electronic Descriptor then Predictive model using QM/ML Approach then Experimental Validation
4:35 p.m. – 5:05 p.m.	Mini Auditorium	Invited Lecture 8	Dr. Sharan Shetty	Title: Computational Study of CO ₂ Capture and Conversion: An Industrial Perspective
5:10 p.m. – 5.40 p.m.	Mini Auditorium	Invited Lecture 9	Prof. Prasenjit Sen	Title: Machine Learning assisted materials screening and design: Attempts at designing rare earth free permanent magnets

**25 mints lecture + 5 Questions > Invited Lecture*

Parallel Session II

Session Chair: Dr. Tanmoy Paul and Mr. E. S. Erakulan

2.00 p.m. – 2.30 p.m.	Hall 1	Invited Lecture 10	Dr. Debabrata Sarkar	Title: Ultra-thin Nanofibrous Membranes as high efficient and lightweight air filter
2.35 p.m. – 3:05 p.m.	Hall 1	Invited Lecture 11	Dr. Mahesh Kumar Ravva	Title: Computational Design and Performance Prediction of Organic Near-infrared Thermally Activated Delayed Fluorescent Molecules
3.10 p.m. – 3.40 p.m.	Hall 1	Invited Lecture 12	Dr. Uttam Kumar Ghorai	Title: Electrocatalytic Synthesis of Green Ammonia and Green Urea Using Metal Phthalocyanine Nanotubes: A Lab-to-Land Initiative

Parallel Session II

Session Chair: Dr. E Varathan

4.00 p.m. – 4.30 p.m.	Hall 1	Invited Lecture 13	Dr. Chiranjib Majumder	Title: 'Atom-by-Atom' design of catalyst using Density Functional theory
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4:35 p.m. – 5:05 p.m.	Hall 1	Invited Lecture 14	Dr. Ujjwal Pal	Title: Prospective Ultrathin 2D-Materials for Large-Scale Solar to Hydrogen
5:10 p.m. – 5:40 p.m.	Hall 1	Invited Lecture 15	Dr. Abir De Sarkar	Title: DFT perspectives on valleytronics, piezoelectricity and flexible piezo-spintronics in selected functional 2D materials

*25 mints lecture + 5 Questions > Invited Lecture

Parallel Session III

Session Chair: Prof. Dilip Kanhare

2.00 p.m. – 2.30 p.m.	Hall 2	Invited Lecture 16	Dr. Jatis Kumar Dash	Title: TBA
2.35 p.m. – 3:05 p.m.	Hall 2	Invited Lecture 17	Prof. Phan Bach Thang	Title: Electrocatalytic activity and thermal properties of Metal-organic frameworks for Lithium-ion batteries, Hydrogen evolution reaction, Oxygen evolution reaction and Thermoelectric conversion
3.10 p.m. – 3.40 p.m.	Hall 2	Invited Lecture 18	Dr. D. H. Nagaraju	Title: Nanostructured Electrode Materials for High Energy Density Symmetric and Asymmetric Supercapacitors

Parallel Session III

Session Chair: Dr. Awadhesh Narayan and Dr. Baswanth Oruganti

4.00 p.m. – 4.30 p.m.	Hall 2	Invited Lecture 19	Prof. Dilip Kanhare	Title: Machine-Learned Potential Energy Surfaces for clusters of Sodium and Aluminium Clusters with Density Functional Accuracy: Applications to Melting
4:35 p.m. – 5:05 p.m.	Hall 2	Invited Lecture 20	Dr. Pankaj Bhalla	Title: Light-induced Nonlinear Spin Hall Current in Single-layer WTe ₂

*25 mints lecture + 5 Questions > Invited Lecture

SYMPOSIUM : Collective Phenomena in Disordered Systems

Afternoon Session: 2.00 p.m. – 5.45 p.m.

Session chair: Prof. Purusattam Ray

2.00 p.m. – 2.50 p.m.	Hall 3	Invited Lecture 21	Dr. Lucas Goehring	Title: Cohesive Granular Media
2.55 p.m. – 3.45 p.m.	Hall 3	Invited Lecture 22	Dr. Tapati Dutta	Title: Real disordered dynamical systems locked in topological signatures

**45 mints lecture + 5 mints discussion*

10 Mints Break

Session chair: Dr. Tapati Dutta

4.00 p.m. – 4.50 p.m.	Hall 3	Invited Lecture 23	Dr. Jordi Baro	Title: Avalanches at the arcade: understanding the statistics of avalanches and aftershock production in mean-field models.
4.55 p.m. – 5.45 p.m.	Hall 3	Invited Lecture 24	Dr. Abhik Basu	Title: Mobility-induced order in active XY spins on a substrate

Evening Session: 6.00 p.m. – 7.30 p.m.: Cultural Program, Main Auditorium, X Lab
7.30 p.m. – 9.30 p.m.: Dinner, In front of SR Block

Bus will leave to Red Fox Hotel at 9:30 p.m

23rd February, Friday 2024 (Day - 2)

Venue: Mini Auditorium, Hall 1 (S 206), Hall 2 (S 207) and Hall 3 (S 201)

Morning Session: 9.20 a.m. – 1.05 p.m.

Session Chair: Prof. Kavita Joshi and Dr. Pranab Mandal

9.20 a.m. – 10:00 a.m.	Mini Auditorium	Invited Key Note Lecture 25	Prof. Yoshiyuki Kawazoe	Title: Parameter-free and Predictable Molecular Dynamics Simulation
10.05 a.m. – 10:45 a.m.	Mini Auditorium	Invited Key Note Lecture 26	Prof. Swapan Pati	Title: Computational Modeling of Thermoelectricity and Mobility in Semiconductors

10:45 a.m. – 11.00 a.m. : Tea/Coffee Break 15 mints

Parallel Sessions and One Symposium

Parallel Session I

Session Chair: Dr. Debabrata Sarkar

11:00 a.m. – 11:30	Mini Auditorium	Invited Lecture 27	Prof. Shen Lei	Title: High-Throughput Computational Discovery and Intelligent Design of Two- Dimensional Functional Materials for Various Applications
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11.35 a.m. – 12.05 p.m.	Mini Auditorium	Invited Lecture 28	Dr. Anirban Mukerjee	Title: Quantum Computational chemistry protocols for porting Density functional approximation onto Quantum Processing units
12.05 a.m. – 12.35 p.m.	Mini Auditorium	Invited Lecture 29	Prof. Priya Johari	Computational Search for Potential Anode Materials for Li-ion Batteries
12:40 a.m. – 1:05 p.m.	Mini Auditorium	YSS	Dr. Tanmoy Paul	Title: Novel Na-ion Battery Cathodes Prediction using Machine Learning and Density Functional Theory Approach

*25 mints lecture + 5 Questions > Invited Lecture

01. 05 p.m. – 2.15 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.15 p.m. – 5.45 p.m.:

Parallel Session I

Session Chair: Dr. Ananth Govind Rajan

2.15 p.m. – 2.45 p.m.	Mini Auditorium	Invited Lecture 30	Dr. Srinivasu Kancharlapalli	Title: Computational High-Throughput Screening of Metal Organic Frameworks for Separation and Storage Gas Mixtures
2.50 p.m. – 3:20 p.m.	Mini Auditorium	Invited Lecture 31	Dr. Satadeep Bhattacharjee	Title: Computational Design of Hydrogen Storage Materials: Integrating Density Functional Theory and Data Analytics
3.25 p.m. – 3.40 p.m.	Mini Auditorium	Oral1	Li Yifan	Title: A machine learning framework based on Local environment descriptors for adsorption energy prediction.
3:40 p.m – 3:55 p.m	Mini Auditorium	Oral2	Ashwini Verma	Title: Machine Learning-Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage

Parallel Session II

Session Chair: Dr. Srinivasu Kancharlapalli

11:00 a.m. – 11:30	Hall 1	Invited Lecture 32	Prof. Asim Bhaumik	Title: Porous Nanomaterials for CO2 Storage and Fixation Reactions
11.35 a.m. – 12.05 p.m.	Hall 1	Invited Lecture 33	Dr. Abhijit Chattopadhyay	Title: Sustainable material innovation using generative material design - a digital twin
12.10 a.m. – 12.40 p.m.	Hall 1	Invited Lecture 34	Dr. Annapureddy V.	Title: Are Lead-Free Piezoelectric Materials Suitable for Energy Storage and Energy Harvesting in Integrated Wearable Systems?

*25 mints lecture + 5 Questions > Invited Lecture

01. 05 p.m. – 2.15 p.m.: Lunch Break, In front of SR Block

Parallel Session II

Session Chair: *Dr. Manjusha Shelke*

2.15 p.m. – 2.45 p.m.	Hall 1	Invited Lecture 35	Dr. Ramendra Sundar Dey	Title: Understanding the Rules of Electrochemical Nitrogen Reduction to Ammonia
2.50 p.m. – 3:20 p.m.	Hall 1	Invited Lecture 36	Dr. Brahmananda Chakraborty	Title: 2D Nanomaterials for Hydrogen Storage and Electro-chemical Energy Storage: Computational Design using DFT & MD Simulations
3:25 p.m. – 3:40 p.m.	Hall 1	Oral3	Kshitij Srivastava	Title: Defect-mediated NaBH ₄ as solid-state electrolytes

SYMPOSIUM : Collective Phenomena in Disordered Systems

Morning Session: 10.00 a.m. – 1.00 p.m.

Session chair: *Dr. Geza Odor*

10.00 a.m. – 10.50 a.m.	Hall 3	Invited Lecture 37	Prof. Neelima M. Gupte	Title: Synchronization on Simplicial complexes
11.00 a.m. – 11.50 a.m.	Hall 3	Invited Lecture 38	Prof. Takahiro Hatano	Title: Triggering of unstable slip of granular matter by weak acoustic waves

**45 mints lecture + 5 mints discussion*

11:50 p.m. – 12.00 p.m.: 10 Mins Break

12.00 p.m. – 12.50 p.m.	Hall 3	Invited Lecture 39	Dr. Ferenc Jarai-Szabo	Title: Avalance statistics on different scales
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01. 00 p.m. – 2.00 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.00 p.m. – 3.45 p.m.

Session chair: *Dr. Takahiro Hatano*

2.00 p.m. – 2.50 p.m.	Hall 3	Invited Lecture 40	Prof. Géza Ódor	Title: Improving power-grid systems via topological changes or how self-organized criticality can help stability
2.55 p.m. – 3.45 p.m.	Hall 3	Invited Lecture 41	Dr. Subhadeep Roy	Title: Effective rheology of two-phase flow through porous media

**45 mints lecture + 5 mints discussion*

Evening Session: 4.00 p.m. – 5.45 p.m.: Poster session with Tea/Soft drinks in front of SR Block

7.30 p.m. – 9.30 p.m.: Banquet Dinner by Vice Chancellor, SRM University -AP

Bus will start at 6:00 P.M to venue for Banquet Dinner, please wear the conference ID card

24th February, Saturday 2024 (Day - 3)

Venue: Mini Auditorium, Hall 1 (S 206), Hall 2 (S 207) and Hall 3 (S 201)

Morning Session: 9.30 a.m. – 1.00 p.m.

Parallel Session I

Session Chair: *Prof. Priya Johari*

9.30 a.m. – 10.00 a.m.	Mini Auditorium	Invited Lecture 42	Dr. Kavita Joshi	Title: Understanding catalytic activity through electronic structure
10:05 am. – 10.35 a.m.	Mini Auditorium	Invited Lecture 43	Dr. Ananth Govind Rajan	Title: Predicting Defect Topologies in 2D Materials By Combining First-Principles Calculations and Machine Learning
10:40 p.m. – 11.10 p.m.	Mini Auditorium	Invited Lecture 44	Dr Uday Narayan Maiti	Title: Crystallization selective growth of metallic nanoclusters on graphitic layers for efficient water splitting
11:15 p.m. – 11:45 p.m.	Mini Auditorium	Invited Lecture 45	Dr. Debabrata Pramanik	Title: Understanding thermodynamic and kinetic properties of complex biomolecular systems employing molecular dynamics simulation
11:50 p.m. – 12:10 p.m.	Mini Auditorium	Oral 4	Mr. E. S. Erakulan	Title: Site Specific Descriptor for Metals to Predict Oxygen Evolution Reaction Activity on Single Atom Catalysts
12:25 p.m. – 12:35 p.m.	Mini Auditorium	Oral 5	Dr. Sheik Haseena	Title: Application of Newly Designed Y-series Non fullerene Acceptors for High-Efficient Organic Solar Cells

*25 mints lecture + 5 Questions > Invited Lecture

Parallel Session II

Session Chair: *Dr. Satadeep Bhattacharjee*

9.30 a.m. – 10.00 a.m.	Hall 1	Invited Lecture 46	Dr. Awadhesh Narayan	Title: Berry curvature dipole and non-linear Hall effect in two-dimensional materials
10:05 am. – 10:35 a.m.	Hall 1	Invited Lecture 46	Dr. Manjusha Shelke	Title: Regulating Lithium Metal Plating/Stripping via 3D Host Materials
10:40 p.m. – 11.10 p.m.	Hall 1	Invited Lecture 47	Dr. Pralok Kumar Samanta	Title: Modelling Excited State Properties and Processes in Multi-Resonant OLED Emitters
11:15 p.m. – 11:45 p.m.	Hall 1	Invited Lecture 48	Dr. E Varathan	Title: Theoretical Actinide Molecular Science: Macrocyclic Complexes
11:50 p.m. – 12:10 p.m.	Hall 1	Oral 6	Mr. Mukaddar S K	Title: 16.35 % efficient Cs ₂ GeSnCl ₆ based heterojunction solar cell with hole-blocking SnO ₂ layer: DFT and SCAPS-1D simulation
12:25 p.m. – 12:35 p.m.	Hall 1	Oral 7	Khusnul Yakin	Title: Mechanism of Proton Transfer at Poly (acrylic acid)-Imidazole

SYMPOSIUM : Collective Phenomena in Disordered Systems

Morning Session: 10.00 a.m. – 1.00 p.m.

Session chair: Prof. Bikas K. Chakrabarti

10.00 a.m. – 10.50 a.m.	Hall 3	Invited Lecture 49	Dr. Purusattam Ray	Title: Nucleation and Growth of Damage in Disordered Systems
11.00 a.m. – 11.50 a.m.	Hall 3	Invited Lecture 50	Dr. Parongama Sen	Title: Disorder and polarisation induced by extreme switches in kinetic exchange models of opinion dynamics.

**45 mints lecture + 5 mints discussion*

11:50 a.m. – 12:00 p.m. : 10 Mints Break

12.00 p.m. – 12.50 p.m.	Hall 3	Invited Lecture 51	Dr. Supravat Dey	Title: Role of cilia activity and surrounding viscous fluid on properties of emergent waves
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Closing Session 12:45 to 1:15 P.M

Lunch 01:15 pm to 2:15 p.m.

Half Day Tour 2:00 to 6:00 p.m.