Program Schedule
ACCMS: International Conference on Materials Genome (ICMG-2020)
Organized by ***SRM University – AP***
In association with
Asian Consortium for Computational Materials Science
Jawaharlal Nehru Centre for Advanced Scientific Research
Institute of Mathematical Sciences
5- 7 February 2020

5th February, Wednesday 2020

Venue: Hall 3 and Hall 4, 4th Floor, Hall 1, 3rd Floor Admin Block

8.30 a.m. to - 9.30 a.m.: Registration, 4th Floor, Academic Block, SRM University

9.30 a.m. - 10.00 a.m.: Inaugural Session

Morning Session: 10.00 a.m. – 1.00 p.m.
Session I – Morning Lecture – Single Session
Session Chair: Prof. Udo Schwingeschlögl, KAUST, Saudi Arabia

10.00 a.m. – 10. 30 a.m.	Hall 3	Invited Lecture 1	Prof. Puru Jena, VCU, USA	Title: In Search of Metastable Forms of Carbon
10:35a.m – 11:05 a.m	Hall 3	Invited Lecture 2	Prof. Yoshiyuki Kawazoe, Tohoku University Japan	Title: Theoretical Materials Research in Past and Future
11.05 a.m. – 11.30 a.m.	Tea/Coffee Break 25 mints			

Session II A – Parallel: Materials Prediction, Database and Framework
Session Chair: Prof. Shobhana Narasimhan, JNCASR, India

11:30 a.m. – 12:00	Hall 3	Invited Lecture 3	Prof. G. P. Das, IIT KGP, India	Title: Computational design of low dimensional materials for energy applications
12:05p.m. – 12.35 p.m.	Hall 3	Invited Lecture 4	Prof. K. R. Lee, KIST, South Korea	Title: SimPL: A Framework for Web-based Materials Design Platform
12:40 a.m. – 01:10 p.m.	Hall 3	Invited Lecture 5	Prof. Lei Shen, NUS, Singapore	Title: 2DMatPedia: An open computational 2D materials database

Session II B – Parallel: Electronic Properties and Computational Design
Session Chair: Prof. Eunsang Kwon, Tohoku University, Japan

11:30 a.m. – 12:00	Hall 4	Invited Lecture 6	Prof. Udo Schwingeschlögl, KAUST, Saudi Arabia	Title: Valleytronics: A materials perspective
12:05p.m. – 12.35 p.m.	Hall 4	Invited Lecture 7	Prof. Amrita Bhattacharya, IIT Bombay, India	Title: Band engineering to enhance the thermoelectric figure of merit in half-Heusler alloys

12:40 a.m. – 01:10 p.m.	Hall 4	Invited Lecture 8	Prof. Swapan K. Ghosh, University of Mumbai, India	Title: Density functional theory in parameter space: A versatile tool for the investigation of dynamics of many-particle systems.

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Session II C – Parallel
Session Chair: Prof. Bikas K. Chakrabarti

11.30 a.m. – 12.15 a.m.	Hall-1, 3rd floor	Invited Lecture 9	Prof. Takahiro Hatano, Osaka University, Japan	Title: Complexity of Earthquake Time Series as Probed by Visibility Graph
12.20 a.m. – 01:05 p.m.	Hall-1, 3rd floor	Invited Lecture 10	Prof. Anuradha Banerjee, IIT Madras, India	Title: Micro-structural Aspects and Crushing Response of Bone

01. 10 p.m. – 2.00 p.m.: Lunch Break

Afternoon Sessions
Session IIIA – Parallel: Machine Learning for Materials - I
Session Chair: Prof. K. R. Lee

2.00 p.m. – 2.30 p.m.	Hall 3	Invited Lecture 11	Prof. Saurabh Ghosh, SRMIST, India	Title: Design of functional oxides guided by first-principles calculations and machine learning
2.35 p.m. – 3:05 p.m.	Hall 3	Invited Lecture 12	Prof. Hiroshi Mizuseki, KIST, South Korea	Title: Machine Learning on Band Gap Prediction of III-V Compound Semiconductor
3.10 p.m. – 3.40 p.m.	Hall 3	Invited Lecture 13	Prof. A. K. Singh, IISc, India	Title: Combined High-Throughput and Machine learning Approach for Prediction of Lattice Thermal Conductivity
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

Session IIIB – Parallel: Energy Materials
Session Chair: Prof. G.P. Das, IIT KGP, India

2.00 p.m. – 2.30 p.m.	Hall 4	Invited Lecture 14	Prof. Saswata Bhattacharya, IIT Delhi, India	Title: Role of defects in MAPbI3 to modulate optical absorption, and solar efficiency
2.35 p.m. – 3:05 p.m.	Hall 4	Invited Lecture 15	Prof. Prasenjit Ghosh, IISER Pune, India	Title: Theoretical investigations of a

				platinum–water interface using quantum-mechanics-molecular-mechanics based molecular dynamics simulations
3.10 p.m. – 3.40 p.m.	Hall 4	Invited Lecture 16	Prof. Prasenjit Sen, HRI, India	Title: New insights into old materials: Layered ternary tri-chalcogenides and Co-based clusters
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

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Session IIIC - Parallel
Session Chair: Prof. Pinaki Chaudhuri

2.00 p.m. – 2.45 p.m.	Hall-1, 3rd floor	Invited Lecture 17	Prof. Lucas Goehring, Nottingham Trent University, UK	Title: Cohesive granular media
2.50 p.m. – 3:35 p.m.	Hall-1, 3rd floor	Invited Lecture 18	Prof. Arghya Das, IIT Kanpur, India	Title: Modelling and simulation of confined comminution in crushable granular materials
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

Session IVA – Parallel: Machine Learning for Materials - II
Session Chair: Prof. Puru Jena, VCU, USA

4.00 p.m. – 4.30 p.m.	Hall 3	Invited Lecture 19	Prof. Nguyen, Duc M, CCFE, UK	Title: First-principles modelling of radiation induced segregation in multi-component systems: From defective Hamiltonian to machine-leaning based smart energy model
4:35 p.m. – 5:05 p.m.	Hall 3	Invited Lectures 20	Dr. DLVK Prasad, IIT Kanpur, India	Title: An MGI approach to free energy landscape of compositional alloys

Session IVB – Parallel: Energy
Session Chair: Prof. Shiv Khanna, VCU, USA

4.00 p.m. – 4.30 p.m.	Hall 4	Invited Lecture 21	Prof. Eunsang Kwon, Tohoku University, Japan	Title: Crystal Structure and Application of Lithium-Cation Endohedral [C60] Fullerene
4:35 p.m. – 4.55 p.m.	Hall 4	YRP1	M. V. M Jyothirmai, SRM IST	Searching of suitable cationic dopants for

				CZTS/Se using First-Principles study
5:00 p.m. – 5.20 p.m.	Hall 4	YRP2	Dr. Paramita Banerjee, JNCASR, India	Title: Exploring the Efficiency of Carbon Nanostructures for Hydrogen Storage and Oxygen Reduction Reaction

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Session IVC - Parallel
Session Chair: Prof. Takahiro Hatano

4.00 p.m. – 4:45p.m.	Hall-1, 3rd floor	Invited Lecture 22	Prof. R. Rajesh, IMSc, India	Title: Shock propagation in a dilute medium
4:50 p.m. – 5.15 p.m.	Hall-1, 3rd floor	YRP 3	Dr. Chandreyee Roy, IMSc, Chennai, India	Title: Brittle to quasi-brittle transition in a compound fiber bundle

Buses will start at 5:30 p.m to Hotels

7.30 p.m. – 9.30 p.m.: Dinner for Participants in the venue and Speakers in the Hotels

6th February, Thursday 2020

Venue: Hall 3 and Hall 4, 4th Floor and, Hall 1, 3rd Floor, Admin Block

Session VI
Morning Session: 9.00 a.m. – 1.00 p.m.
Session Chair: Prof. Yoshiyuki Kawazoe, Tohoku University, Japan

9.30 a.m. – 10:00 a.m.	Hall 3	Invited Lecture 23	Prof. Ferenc Kun	Title: Discrete element modelling of the compressive failure of porous rocks
10:05 a.m. – 10.35 a.m.	Hall 3	Invited Lecture 24	Prof. Shiv Khanna, VCU, USA	Title: Transforming Redox Properties of Clusters Using Ligands to Create Super Dopants for Two-Dimensional Semiconductors and to Synthesize Nano p- n-junctions
10.35 a.m. – 10:50 a.m.	Tea/Coffee Break 15 mints			

Session VII-A Parallel: Catalyst and Descriptor
Session Chair: Prof. Ranjit Thapa, SRM University - AP

10.50 a.m. – 11:20 a.m.	Hall 3	Invited Lecture 25	Prof. Shobhana Narasimhan, JNCASR, India	Title: Simple Yet Successful Descriptors for Self-Assembly on Surfaces

11.25 p.m. – 11:55 p.m.	Hall 3	Invited Lecture 26	Prof. Hisato Yasumatsu, Tokyo Tech. Japan	Title: Low-temperature and highly-selective catalysis of NO reduction and CO oxidation on platinum cluster disk bound to silicon substrate
12.00 p.m. – 12.30 p.m.	Hall 3	Invited Lecture 27	Prof. Nurbosyn U. Zhanpeisov, Tohoku University, Japan	Title: Theoretical DFT Study on Modified Oxides and Gold Structures
12:35 p.m. – 01:05 p.m.	Hall 3	Invited Lecture 28	Prof. M. Ali Haider, IIT Delhi, India	Title: Rational Catalyst Design Augmented with DFT, Machine Learning and Ab-Initio Microkinetic Modeling

Session VII-B Parallel: Metal oxides, Perovskites and Magnetic Materials
Session Chair: Prof. Nurbosyn U. Zhanpeisov, Tohoku University, Japan

10.50 a.m. – 11:20 a.m.	Hall 4	Invited Lecture 29	Prof. Kersti Hermansson, Uppsala University, Sweden	Title: e-Chemistry of metal oxides – molecule interfaces: data or insights?
11.25 p.m. – 11:55 p.m.	Hall 4	Invited Lecture 30	Prof. B. R. K. Nanada, IIT Madras	Title: Recreating Metal out of Insulators and Insulators out of Metals in Oxide Heterostructures
12.00 p.m. – 12.30 p.m.	Hall 4	Invited Lecture 31	Prof. Subodh Kumar De, IACS, India	Title: Magnetic Properties of Nd_2CoIrO_6 Double Perovskite
12:35 p.m. – 01:05 p.m.	Hall 4	Invited Lecture 32	Prof. Hena Das, Tokyo Institute of Technology, Japan	Title: Exploring the potential of Quadruple perovskites for fast lithium-ion transport

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Session VII-C Parallel
Session Chair: Prof. Purusattam Ray

11:00 a.m. – 11:45 a.m.	Hall-1, 3rd floor	Invited Lecture 33	Prof. Sujata Tarafdar, Jadavpur University, India	Title: An Interesting Application of Desiccation Crack Networks in Technology
11:50 a.m. – 12:35 p.m.	Hall-1, 3rd floor	Invited Lecture 34	Prof. Akio Nakahara, Nihon University, Japan	Title: Controlled crack patterns produced by memory effect of paste

12:40 p.m. – 13:05 p.m	Hall-1, 3rd floor	YRP4	Dr. Subhadeep Roy, NTNU, Norway	Title: Effective rheology of two-phase flow in porous media: dependence on system disorder

01. 05 p.m. – 2.10 p.m.: Lunch Break

Session VIII-A Parallel: Materials Informatics and Storage
Session Chair: Prof. Ryo Maezono, JAIST , Japan

2.10 p.m. – 2.40 p.m.	Hall 3	Invited Lecture 35	Prof. Kenta Hongo, JAIST, Japan	Title: Computational materials design from materials simulations to informatics
2.45 p.m. – 3:05 p.m.	Hall 3	YRP5	Dr. Mudit Dixit, LPU, India	Title: Elucidating the origin of capacity fading of Ni-rich layered oxide-based positive electrode materials for Li-ion batteries
3.10 p.m. – 3.30 p.m.	Hall 3	YRP6	Dr. Aaditya Manjanath, Academia Sinica, Taiwan	Title: Excitation energies from thermally-assisted-occupation density functional theory: Theory and computational implementation
3:35 p.m. – 3:45 p.m.	Hall 3	Oral1	Dr. Tong Yang, NUS, Singapore	Title: High-Throughput Screening Of Single Transition Metal Atoms Anchored On Mos2 Monolayer For Nitrogen Fixation

Session VIII-B Parallel
Session Chair: Prof. Nguyen, Duc M, Culham Centre for Fusion Energy, UK

2.10 p.m. – 2.40 p.m.	Hall 4	Invited Lecture 36	Dr. Mahesh Kumar Ravva, SRM-AP	Title: Theoretical design and development of new macrocycle organic materials for organic electronic applications
2.45 p.m. – 3:15 p.m.	Hall 4	Invited Lecture 37	Prof. Vannajan Sanghiran Lee, University of Malaya,	Title: Quasiparticle energies of ground state and excited state

			Malaysia	of metal clusters using all-electron mixed basis of plane waves (PWs) and atomic orbitals (AOs)
3:15 p.m – 3: 45 p.m	Hall 4	Invited Lecture 38	Prof. V. Subramanian, CLRI, India	Title: Computational Evaluation of Donor-Bridge-Acceptor (D-B-A) Motifs for High Performance Optoelectronic Device Applications
3.45 p.m. – 4:.05 p.m.	Hall 4	YRP7	Dr. Kanchan Ulman, NUS, Singapore	Title: Understanding the chemical enhancement mechanism of 2D substrate enhanced Raman Spectroscopy (2D-SERS)

FRACTMEET 2020
Session VIII-C Parallel
Session Chair: Prof. Sujata Tarafdar

2.10 p.m. – 2.55 p.m.	Hall-1, 3rd floor	Invited Lecture 39	Prof. Parag Tandaiya, IIT Bombay, India	Title: Mechanics and Mechanisms of Deformation and Failure in Heterogeneous Amorphous Alloys: Insights from Continuum Simulations of Porous BMGs and ex-situ BMG Composites
3.00 p.m. – 3:25 p.m.	Hall-1, 3rd floor	YRP8	Prof. Srutarshi Pradhan, NTNU, Norway	Predicting the collapse point of materials under stress
3:30p.m.-4:15p.m.	Hall-1, 3rd floor	Invited lecture 40	Prof. Bikas K. Chakrabarti, SINP, India	Title: Kolmogorov Dispersion for Turbulence & Statistics of Fracture in the Fiber Bundle Model

Evening Session: 4.00 p.m. – 6.00 p.m.: Poster session with Tea/coffee
Venue: Atrium

7.30 p.m. – 9.30 p.m.: Banquet Dinner
Bus will start at 6:30 P.M to venue for Banquet Dinner, Please wear the conference ID card

7th February, Friday 2020

Morning Session: 9.00 a.m. – 1.00 p.m.
Session IX a
Session Chair: Prof. Jungsuttiwong Siriporn

9.30 a.m. – 10.00 a.m.	Hall 3	Invited Lecture 41	Prof. Ranjit Thapa, SRM-AP	Title: Electronic Descriptor for carbon catalyst using QM/ML approach
10:05 a.m – 10:35 a.m	Hall 3	Invited Lecture 42	Prof. Ryo Maezono, JAIST, Japan	Title: Ab initio Quantum Monte Carlo method; Role in Materials Genome
10.35 a.m. – 10.50 a.m.	Tea/Coffee Break 15 mints			

Session X-A Parallel: Energy, Plasmonic and ML
Session Chair: Prof. Kenta Hongo

10.50 a.m. – 11:20 a.m.	Hall 3	Invited Lecture 43	Prof. Tanmay Basak, IIT Madras, India	Title: Analysis of heat flow visualization and thermodynamic efficiency during thermal convection in cavities with distributed solar heaters
11.25 a.m. – 11:55 a.m.	Hall 3	Invited Lecture 44	Prof. MAJIDI Muhammad Aziz, Universitas Indonesia	Title: Controlling plasmonic characteristics through confinement and correlation effects
12:00 p.m – 12:10 p.m	Hall 3	Oral 2	Dr. Kavita Joshi, NCL, India	Title: Combining DFT With ML To Study Size Specific Interactions Between Metal Clusters And Adsorbates
12:15 p.m – 12:25 p.m	Hall 3	Oral 3	Mr. Amrish Kumar, IIT Delhi, India	Title: Rational Design Of Single Atom Catalysts Based On Cu, Ag And Au Alloys Using Machine Learning Approaches

Session X-B Parallel: Chemical and Thermal Analysis
Session Chair: Prof.Vannajan Sanghiran Lee

10.50 a.m. – 11:20 a.m.	Hall 4	Invited Lecture 45	Prof. Kothandaraman Ramanujam, IIT Madras, India	Title: Catalysis on the surface of nanotubes having confined solvent media
11:25 p.m. – 11:55 p.m.	Hall 4	Invited Lecture 46	Prof. JUNGSUTTIWONG, Siriporn, URU, Thailand	Title: Theoretical and Mechanistic Studies on Catalysis of Carbon Dioxide Hydrogenation to Formic Acid on Pt

				doped Boron Nitride Nanosheets
12:00 p.m – 12: 10 p.m	Hall 4	Oral 4	Dr. Sujith Kalluri, SRM University -AP	Title: Thermal analysis of Myristic - Layric acid –Fe2O3 composite as nano-enhanced organic phase change material
12:15 p.m – 12:25 p.m	Hall 4	Oral5	Dr. V. Arivindan, Thiagarajar College of Engineering, India	Title: First Principles Study Of Structural, Electronic, Magnetic And Elastic Properties Of The Mn2-X-Sb (X= Co, Fe) Inverse Heusler Alloys

FRACTMEET 2020
Session X-C Parallel
Session Chair: Prof. Lucas Goehring

11.00 a.m. – 11:45 a.m.	Hall-1, 3rd floor	Invited Lecture 47	Prof. V. Madhurima, Central Uni. Tamil Nadu, India	Title: Lubrication Driven Hierarchical Self-Assembly of Droplets
11.50 p.m. – 12:35 p.m.	Hall-1, 3rd floor	Invited Lecture 48	Prof. Smarajit Karmakar, TIFR Hyderabad, India	Title: Yielding at bulk and Nanoscale amorphous solids
12:40 p.m – 01:25 p.m	Hall-1, 3rd floor	Invited Lecture 49	Prof. Koushik Vishwanathan, IISc Bangalore, India	Title: Stick-slip in soft polymers: Elasticity, adhesion and slow wave propagation

Closing Remarks: 12:45 p.m to 01:15 p.m

Lunch 01:15 to 02:15 p.m.

Half Day Tour 2:30 to 6:00 p.m.
Dinner in the respective accommodation places