

**DETAILED SCHEDULE FOR**  
**ICMG-II**


**ACCMS Theme Meeting**

**24<sup>th</sup> March and 25<sup>th</sup> March , 2022**

**(Online)**

**(From 9:00 IST to 18:45 IST )**

**(Indian Standard Time)**

DAY	Session (IST)	In-Charge Dr. Kavita	In-charge -- Dr. Mahesh	In-charge -- Prof. Thapa	In-charge -- Dr. Amrit	 <b>SRM</b> In-charge -- Prof. Nanda UNIVERSITY AP Andhra Pradesh
<b>Special Address, Keynote – I &amp; Keynote - II</b>		<a href="https://srmapp.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09">https://srmapp.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09</a> Meeting ID: 996 8015 4107      Passcode: 593326 <b>Day – 24/03/2022, From 9:00 to 11:10 IST</b> <b>Day – 25/03/2022, From 9:00 to 10:35 IST</b> <b>Technical help -- Mr. Samadhan Kapse (<a href="mailto:samadhan_kapse@srmapp.edu.in">samadhan_kapse@srmapp.edu.in</a>)</b>				
<b>24/03/2022 &amp; 25/03/2022</b>	<b>Parallel Session</b>	<b>ZOOM -- I</b> <a href="https://srmapp.zoom.us/j/91704338086?pwd=QWVPajhiamdFa2INTDBWaHU4Sk9pdz09">https://srmapp.zoom.us/j/91704338086?pwd=QWVPajhiamdFa2INTDBWaHU4Sk9pdz09</a> Meeting ID: 917 0433 8086 Passcode: 766090	<b>ZOOM -- II</b> <a href="https://srmapp.zoom.us/j/97257931748?pwd=OUdJREtBYndoejdJTFIvUGZaYkcrZz09">https://srmapp.zoom.us/j/97257931748?pwd=OUdJREtBYndoejdJTFIvUGZaYkcrZz09</a> Meeting ID: 972 5793 1748 Passcode: 639964	<b>ZOOM -- III</b> <a href="https://srmapp.zoom.us/j/92126575594?pwd=dXhwS041QWJVOFRCWGRIVDBhdHpiQT09">https://srmapp.zoom.us/j/92126575594?pwd=dXhwS041QWJVOFRCWGRIVDBhdHpiQT09</a> Meeting ID: 921 2657 5594 Passcode: 643081	<b>ZOOM -- IV</b> <a href="https://srmapp.zoom.us/j/93946723832?pwd=UW9LNERMcZVUaTdza2VMVVBuWXFLZz09">https://srmapp.zoom.us/j/93946723832?pwd=UW9LNERMcZVUaTdza2VMVVBuWXFLZz09</a> Meeting ID: 939 4672 3832 Passcode: 758222	<b>ZOOM -- V</b> <a href="https://srmapp.zoom.us/j/92071066033?pwd=QUV2QjVCYUF2SjN0xN0xVNGJXMERJZz09">https://srmapp.zoom.us/j/92071066033?pwd=QUV2QjVCYUF2SjN0xN0xVNGJXMERJZz09</a> Meeting ID: 920 7106 6033 Passcode: 918792
	<b>Technical help</b>	Ms Anjana Tripathi ( <a href="mailto:anjana_tripathi@srmapp.edu.in">anjana_tripathi@srmapp.edu.in</a> )	Mr. Narad Barman ( <a href="mailto:narad_barman@srmapp.edu.in">narad_barman@srmapp.edu.in</a> )/ Mr. Deepak Gavali ( <a href="mailto:deepaksubhash_gavali@srmapp.edu.in">deepaksubhash_gavali@srmapp.edu.in</a> )	Mr. Samadhan Kapse ( <a href="mailto:samadhan_kapse@srmapp.edu.in">samadhan_kapse@srmapp.edu.in</a> )	Mr. E S Erakulan ( <a href="mailto:erakulan_es@srmapp.edu.in">erakulan_es@srmapp.edu.in</a> )/ Mr. Asif Iqbal ( <a href="mailto:asif_iqbal@srmapp.edu.in">asif_iqbal@srmapp.edu.in</a> )	Mr. Deepak Gavali ( <a href="mailto:deepaksubhash_gavali@srmapp.edu.in">deepaksubhash_gavali@srmapp.edu.in</a> )

<b>Keynote = (40+5) Mins</b>	<b>Oral = (10+3) Mins</b>
<b>Invited Talk = (20 +5) Mins</b>	<b>Poster = (5+3) Mins</b>

*Date -- 24/03/2022*

**Zoom -- <https://srmmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09>**

**Chair -- Prof. Tanusri Saha Dasgupta**

<b>Time</b>	<b>Type</b>	<b>Speaker/ Presented By</b>	<b>Title</b>
<i>09:00 - 9:15 IST</i>	<i>Inauguration</i>		
<i>09:15 - 9:45 IST</i>	<i>Special Address I</i>	<i>Prof. Yoshiyuki Kawazoe</i> New Industry Creation Hatchery Center, Tohoku University, Japan	<i>Reliable Ab initio Simulation for Materials Design Fundamentally Better than Present Day Standard for Materials Genome</i>
<i>09:50 - 10:20 IST</i>	<i>Special Address II</i>	<i>Prof. Umesh Waghmare</i> JNCASR, India	<i>Predictive Models for Innovative Design of Materials using Quantum Mechanics and Machine Learning</i>
<i>10:25 - 11:10 IST</i>	<i>Keynote I</i>	<i>Prof. Jian Tao Wang</i> University of Chinese Academy of Sciences, China	<i>Pressure Induced Structural Phase Transitions in Layered <math>\text{EuSn}_2\text{As}_2</math> Compounds</i>



Date -- 24/03/2022 Theme – Machine Learning for Materials

Zoom – I -- <https://srmapp.zoom.us/j/91704338086?pwd=QWVPa2hiamdFa2lNTDBWahU4Sk9pdz09>

Session In-charge -- Dr. Kavita

Chair: Dr. Kavita Joshi

Time	Keynote	Speaker/ Presented By	Title
11:30 - 11:55 IST	<i>Invited Speaker - 1</i>	<i>Dr. Jun Zhou,</i> IMRE Singapore	<i>Machine learning assisted development of 2D MatPedia</i>
12:00 - 12:25 IST	<i>Invited Speaker – 2</i>	<i>Prof. Abhishek Singh</i> IISc, Bangalore, India	<i>Exploring machine learning based models to predict materials' properties</i>
12:30 - 12:55 IST	<i>Invited Speaker – 3</i>	<i>Dr. Tanushri Saha Dasgupta,</i> S N Bose centre for basic sciences, India	<i>Machine Learning Approach of Design of New Materials with Targeted Properties</i>

**Lunch Break : From 13:00 to 14:30**

**Chair -- Dr. Sandip De**

14:30 - 14:55 IST	<i>Invited Speaker – 4</i>	<i>Prof. Darwin Putungan</i> University of Philippines, Philippines	<i>Machine learning-assisted Ab-initio Random Structure Searching (AIRSS): Preliminary application to Sodium-VS 2 system for NIBs</i>
15:00 - 15:25 IST	<i>Invited Speaker – 5</i>	<i>Dr. Maaouia Souissi</i> Brunel University, United Kingdom	<i>Applied Machine Learning and DFT for alloys, additive manufacturing and beyond ...</i>
15:30 - 15:55 IST	<i>Invited Speaker – 6</i>	<i>Dr. Amrita Bhattacharya ,</i> Indian Institute of Technology, Bombay, India	<i>Combining Machine Learning with high throughput first principles calculations to analyse the charge and heat transport in thermoelectric solid</i>
15:45 - 16:00 IST			

**Tea Break : From 16:00 to 16:30**



Date -- 24/03/2022

Theme – Machine Learning for Materials

Zoom – I -- <https://srmap.zoom.us/j/91704338086?pwd=QWVPajhiamdFa2lNTDBWakpndz09>

Session In-charge -- Dr. Kavita

Chair -- Prof. Ankita Katre

16:30 - 16:55 IST	<i>Invited Speaker – 7</i>	<i>Dr. Prsenjit Sen</i> HRI, Allahabad, India	<i>Machine Learning assisted hierarchical screening: A strategy for designing novel magnetic materials</i>
17:00 - 17:25 IST	<i>Invited Speaker – 8</i>	<i>Dr. Tuhin Khan,</i> CSIR-IIP, India	<i>In-silico Design of Novel Catalytic Materials using ab-initio Microkietic Modeling Augmented with Machine Learning</i>
17:30 - 17:45 IST	<i>Invited Speaker – 9</i>	<i>Dr. Prasanna Bhalchandran</i> University of Virginia, USA	<i>Adaptive Learning, Model Interpretability and Bayesian Inference for Accelerating Materials Design</i>

**ZOOM -- <https://srmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09>**

*Chair -- Prof. Youshiyuki Kawazoe*

18:00 - 18:45 IST	<b>Keynote II</b>	<i>Prof. Jun Hee Lee,</i> UNIST, South Korea	<i>Atomic semiconductor of ultimate- density via flat phonon bands</i>
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Date -- 24/03/2022

Theme – OER/HER/ORR



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Zoom II – <https://srmap.zoom.us/j/97257931748?pwd=OUdJREtBYndoejdJTFVLaUkxZWpYd0pDZ0pRd0pR>

Session In-charge -- Dr. Mahesh

Chair -- Prof. Ryoji Sahara & Dr. Jatis Kumar Dash

Time	Keynote	Speaker/ Presented By	Title
<b>Inauguration</b>			
11:30 - 11:55 IST	<i>Invited Speaker – 10</i>	<i>Prof. Sang Uck Lee,</i> Hanyang University, South Korea	<i>Theoretical Strategies and Methodologies for Investigating Electrocatalytic Reactions (HER/OER/ORR/IRR) on Nanostructures</i>
12:00 - 12:25 IST	<i>Invited Speaker – 11</i>	<i>Dr. Mehmet Emin Kilic,</i> Korea Institute of Science and Technology, South Korea	<i>Two-Dimensional Group-IV Carbides for Nanoelectronics and Photocatalytic Water Splitting</i>
12:30 - 12:55 IST	<i>Invited Speaker - 12</i>	<i>Prof. Chandra Sekhar Rout,</i> Jain University, India	<i>MXene Based Hybrid Materials for Energy Conversion and Storage Applications</i>
<b>Lunch Break : From 13:00 to 14:30</b>			
<b>Chair: Prof. Ranjit Thapa</b>			
14:30 - 14:55 IST	<i>Invited Speaker – 13</i>	<i>Dr. Yeoh Keat Hoe,</i> Universiti Tunku Abdul Rahman, Malaysia	<i>Two-dimensional NbSe<sub>2</sub>/g-ZnO van der Waals heterostructures as a water splitting photocatalyst: A first-principles study</i>
15:00 - 15:25 IST	<i>Invited Speaker – 14</i>	<i>Prof. Ashwani Tiwari,</i> IISER Kolkata, India	<i>Dynamics of H<sub>2</sub>O Dissociation on Metal Surfaces</i>
15:30 - 15:45 IST	<i>Invited Speaker - 15</i>	<i>Prof. Ryoji Sahara</i> National Institute of Materials Science, Japan	<i>Mechanisms of oxidation of pure and Si-segregated Ti surfaces</i>
<b>Tea Break : From 16:00 to 16:30</b>			

Date -- 24/03/2022

Theme – OER/HER/ORR



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Zoom II – <https://srmap.zoom.us/j/97257931748?pwd=OUdJREtBYndoejdJTFVlZz09Zz09Zz09>

Session In-charge -- Dr. Mahesh

Chair -- Chair: Prof. Sang Uck Lee

Time	Keynote	Speaker/ Presented By	Title
16:30 - 16:55 IST	<i>Invited Speaker – 16</i>	<i>Prof. Gunther Andersson</i> Flinders University, Australia	<i>Electronic Structure of Titania Surfaces Modified by Metal Clusters for Applications in Photocatalysis</i>
17:00 - 17:25 IST	<i>Invited Speaker – 17</i>	<i>Dr. Uday Narayana Maiti,</i> Indian Institute of Technology Guwahati, India	<i>Heterostructures as efficient electrocatalysts for water splitting</i>
17:30 - 17:45 IST	<i>Invited Speaker – 18</i>	<i>Dr. Uttam Kumar Ghorai,</i> Ramakrishna Mission Vidyamandira, India	<i>Electrochemical ammonia synthesis through nitrogen reduction reaction on metal phthalocyanine nanostructures</i>

**ZOOM -- <https://srmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZ1RmljZz09>**

Chair -- Prof. Youshiyuki Kawazoe

18:00 - 18:45 IST	<b>Keynote II</b>	<i>Prof. Jun Hee Lee,</i> UNIST, South Korea	<i>Atomic semiconductor of ultimate-density via flat phonon bands</i>
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Date -- 24/03/2022

Theme – CO<sub>2</sub> to value added products / CO Oxidation

Zoom III – <https://srmmap.zoom.us/j/92126575594?pwd=dXhwS041QWJVOFRCWGRVbHhlcjZlZDZkdz09>



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Session In-charge -- Prof. Ranjit Thapa

Chair -- Prof. Hisato Yasumatsu

Time	Type	Speaker/ Presented By	Title
11:30 - 11:55 IST	<i>Invited Speaker – 19</i>	<i>Prof. Siriporn Jungstuwong</i> , Ubon Ratchathani University, Thailand	<i>Encouraging metal-free catalyst reactivity with a synergistic effect on phosphorus and nitrogen co-doped graphene for catalyzed CO-oxidation reaction</i>
12:00 - 12:25 IST	<i>Invited Speaker – 20</i>	<i>Prof. Kaito Takahashi</i> , Academia Sinica, Taiwan	<i>Can we understand CO<sub>2</sub> electroreduction activity of 3d-transition metal atom doping on ZnO monolayers from their oxidation state?</i>
12:30-12:55 IST	<i>Invited Speaker – 21</i>	<i>Dr. Ramendra Sundar Dey</i> Institute of Nano Science & Technology, India	<i>Next-generation smart nanomaterials for electrochemical oxygen and nitrogen reduction reaction</i>

**Lunch Break : From 13:00 to 14:30**

**Chair -- Prof. Siriporn Jungstuwong**

14:30 - 14:55 IST	<i>Invited Speaker – 22</i>	<i>Prof. Hisato Yasumatsu</i> , Toyota Technological Institute, Japan	<i>Highly-durable low-temperature catalysis driven by uni-sized Pt clusters supported on SiC substrate</i>
15:00 - 15:25 IST	<i>Invited Speaker – 23</i>	<i>Prof. Asim Bhaumik</i> , Indian Association for the Cultivation of Sciences, India	<i>Utilization of CO<sub>2</sub> as feedstock for the synthesis of valuable chemicals</i>

**Tea Break : From 16:00 to 16:30**



Date -- 24/03/2022

Theme – CO<sub>2</sub> to value added products / CO<sub>2</sub> Conversion

Zoom III – <https://srmapp.zoom.us/j/92126575594?pwd=dXhwS041QWJVOFRWGRVlbnRhdHhpbjQ1OT09>



Session In-charge -- Prof. Ranjit Thapa

Chair -- Prof. Kaito Takahashi

Time	Keynote	Speaker/ Presented By	Title
16:30 - 16:55 IST	<i>Invited Speaker – 25</i>	<i>Dr. Prasenjit Ghosh,</i> IISER, Pune- India	<i>Role of intrinsic C-vacancies in CH<sub>4</sub> activation and C-C coupling: The case of Ti<sub>2</sub>C</i>
17:00 - 17:25 IST	<i>Invited Speaker – 26</i>	<i>Dr. Sushant Kumar,</i> Indian Institute of Technology, Patna, India	<i>CO<sub>2</sub> reduction and N<sub>2</sub> fixation on transition-metal-doped MIL-88A (Fe)</i>
17:30 - 17:45 IST	<i>Invited Speaker – 27</i>	<i>Dr. Sebastian C. Peter,</i> JNCASR, Bangalore, India	<i>Rationally designed Intermetallics as Efficient Catalysts for the Selective Conversion of CO<sub>2</sub> to Methanol at Low Energy Input</i>

**<https://srmapp.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09>**

Chair -- Prof. Youshiyuki Kawazoe

18:00 - 18:45 IST	<i>Keynote II</i>	<i>Prof. Jun Hee Lee,</i> UNIST, South Korea	<i>Atomic semiconductor of ultimate-density via flat phonon bands</i>
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Date -- 24/03/2022 Theme – Thermoelectric Materials

Zoom IV – <https://srmmap.zoom.us/j/93946723832?pwd=UW9LNERMczVUaTdza2VMVVBaWXPFLZz09>



Session In-charge -- Dr. Amrita Bhattacharya

Chair -- Dr. Amrita Bhattacharya

Time	Keynote	Speaker/ Presented By	Title
16:30 - 16:55 IST	<i>Invited Speaker – 33</i>	<i>Prof. Qian Wang,</i> Peking University, China	<i>Recent Advances in Pentagon-Based 2D Materials</i>
17:00 - 17:25 IST	<i>Invited Speaker – 34</i>	<i>Prof. Nurbosyn Zhanpeisov,</i> Tohoku University, Japan	<i>Theoretical DFT Study on Metal-Organic Frameworks for Hydrogen Storage</i>
17:30 - 17:45 IST	<i>Invited Speaker – 35</i>	<i>Prof. Keivan Esfarjani,</i> University of Virginia, USA	<i>High Entropy Alloy</i>

**ZOOM -- <https://srmmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZ1RmljZz09>**

Chair -- Prof. Youshiyuki Kawazoe

18:00 - 18:45 IST	<i>Keynote II</i>	<i>Prof. Jun Hee Lee,</i> UNIST, South Korea	<i>Atomic semiconductor of ultimate-density via flat phonon bands</i>
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Date -- 24/03/2022

Theme – High Entropy Alloy



Zoom V – <https://srmmap.zoom.us/j/92071066033?pwd=QUV2QjVCYUF2SjN0xVNGJAMERJZZ09>

Session In-charge -- Prof. B. R. K. Nanda

Chair -- Prof. Gandham Phanikumar

Time	Type	Speaker/ Presented By	Title
11:30 - 11:55 IST	<i>Invited Speaker – 36</i>	<i>Prof. Hiroshi Mizuseki</i> Korea Institute of Science and Technology, South Korea	<i>3d-transition-metal-based HEAs by high-throughput sampling based on first-principles calculations</i>
12:00 - 12:25 IST	<i>Invited Speaker – 37</i>	<i>Prof. Talgat M. Inerbaev,</i> Novosibirsk State University, Russia	<i>Effect of doping on electronic structure and magnetostriction in FeGa alloys</i>
12:30 - 12:55 IST	<i>Invited Speaker - 38</i>	<i>Prof. Duc Nguyen Manh,</i> United Kingdom Atomic Energy Authority, United Kingdom	<i>Integrated first-principles approach for modelling microstructure evolution in multi-component alloys under irradiation</i>

***Lunch Break ----- End for Session V***

**<https://srmmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09>**

***Chair -- Prof. Youshiyuki Kawazoe***

18:00 - 18:45 IST	<i>Keynote II</i>	<b><i>Prof. Jun Hee Lee,</i></b> UNIST, South Korea	<b><i>Atomic semiconductor of ultimate-density via flat phonon bands</i></b>
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*Date -- 25/03/2022*

*Zoom link -- <https://srmap.zoom.us/j/99680154107?pwd=d0VLTvRYclBSdUxtUGE5MmZlRmljZz09>*

*Session In-charge -- Dr. Kavita*

*Chair -- Prof. G. P. Das*

<b>Time</b>	<b>Type</b>	<b>Speaker/ Presented By</b>	<b>Title</b>
<i>09:00 - 9:45 IST</i>	<i>Keynote III</i>	<i>Prof. D D Sarma</i> IISC Bangalore, India	<i>What is so interesting about <math>A_{1-y}B_yPbX_3</math> (<math>A/B = MA, FA, Cs</math> and <math>X = I, Br, Cl</math>)</i>
<i>09:50 - 10:35 IST</i>	<i>Keynote IV</i>	<i>Prof. Kaoru Ohno</i> Yokohama National University, Japan	<i>Extended Kohn-Sham theory applicable to arbitrary excited eigenstates</i>



*Date -- 25/03/2022      Theme – Machine Learning for Materials*

*Zoom I -- <https://srmap.zoom.us/j/91704338086?pwd=QWVPajhiamdFa2lNTDBWaHU4Sk9pdz09>*

*Session In-charge -- Dr. Kavita*

*Chair -- Prof. Prasenjit Sen*

<b>Time</b>	<b>Type</b>	<b>Speaker/ Presented By</b>	<b>Title</b>
<i>11:00 - 11:25 IST</i>	<i>Invited Speaker – 39</i>	<i>Dr. Kavita Joshi , CSIR- NCL, Pune, India</i>	<i>Exploring machine learning based models to predict materials properties</i>
<i>11:30 - 11:55 IST</i>	<i>Invited Speaker – 40</i>	<i>Prof. Jer Lai Kuo, Academia Sinica, Taiwan</i>	<i>Exploring Chemical and Physical Space of Carbohydrates by Quantum Chemistry assisted by Machine Learning Methods</i>
<i>12:00 - 12:25 IST</i>	<i>Invited Speaker – 41</i>	<i>Prof. Kenta Hongo, JAIST, Japan</i>	<i>Computational materials design from materials simulations to informatics</i>
<i>12:30 - 12:55 IST</i>	<i>Invited Speaker - 42</i>	<i>Dr. Sandip De, BASF, Germany</i>	<i>Datadriven Catalysis Research: High throughput experiments and high throughput simulations</i>

***Lunch Break : From 13:00 to 14:30***



Date -- 25/03/2022

Theme – Computational Aided Discov

Zoom II – <https://srmap.zoom.us/j/97257931748?pwd=OUdJREtBYndoejdJTFIvUGZaYkcrZz09>

Session In-charge -- Dr. Mahesh

Chair -- Prof. Ranjit Nanda

Time	Type	Speaker/ Presented By	Title
11:00 - 11:25 IST	<i>Invited Speaker – 43</i>	<i>Dr. Saswata Bhattacharya,</i> IIT Delhi, India	<i>Charged Defects in TiO2 Anatase: A Comparative Study of Hybrid DFT, GW and BSE to Explore Optical Properties</i>
11:30 - 11:55 IST	<i>Invited Speaker – 44</i>	<i>Dr. Saurabh Ghosh,</i> SRM Institute of Science and Technology, India	<i>Engineering multifunctionality at oxide interfaces by structural mode coupling</i>
12:00 - 12:25 IST	<i>Invited Speaker – 45</i>	<i>Dr. Momoji Kubo,</i> Tohoku University, Japan	<i>Large-Scale Molecular Dynamics Simulations on Chemical-Reaction-Induced Wear Processes of Diamond-like Carbon Films</i>
12:30 - 12:55 IST	<i>Invited Speaker – 46</i>	<i>Prof. Hannes Raebiger,</i> Yokohama National University, Japan	<i>Structural deformation in Mxenes: Charge-density waves and electriles</i>

**Lunch Break : From 13:00 to 14:30**

*Date -- 25/03/2022*

*Theme – Solar Cell*



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*Zoom III -- <https://srmap.zoom.us/j/92126575594?pwd=dXhwS041QWJVOFRWGRIVDBhdHpjQT09>*

*Session In-charge -- Prof. Ranjit Thapa*

*Chair -- Prof. Nurbosyn Zhanpeisov*

<b>Time</b>	<b>Type</b>	<b>Speaker/ Presented By</b>	<b>Title</b>
<i>11:00 - 11:25 IST</i>	<i>Invited Speaker – 47</i>	<i>Prof. Khian-Hooi Chew,</i> University of Malaya, Malaysia	<i>Suppression of Oxidation in Perovskites CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> by Lithium-ion Endohedral Fullerenes Li<sup>+</sup>@C<sub>60</sub></i>
<i>11:30 - 11:55 IST</i>	<i>Invited Speaker – 48</i>	<i>Dr. Safakath Karuthedath,</i> KAUST, Saudi Arabia	<i>Charge Generation in Emerging Non- fullerene Organic Solar Cells</i>
<i>12:00 - 12:25 IST</i>	<i>Invited Speaker – 49</i>	<i>Prof. Vijay Kumar,</i> Shiv Nadar University, India	<i>2D halide perovskites and rare-earth doping for solar energy and optoelectronic applications</i>
<i>12:30 - 12:55 IST</i>	<i>Invited Speaker – 50</i>	<i>Dr. Vaishali Shah,</i> University of Pune, India	<i>Ab initio investigations of green cesium tin halide quantum dots for photovoltaic applications</i>

***Lunch Break : From 13:00 to 14:30***



*Date -- 25/03/2022*

*Theme – NRR*

*Zoom IV -- <https://srmap.zoom.us/j/93946723832?pwd=UW9LNERMcZVUaTdza2VMVVBuWXFLZz09>*

*Session In-charge -- Dr. Amrita Bhattacharya*

*Chair -- Dr. Prasenjit Ghosh*

<b>Time</b>	<b>Type</b>	<b>Speaker/ Presented By</b>	<b>Title</b>
<i>11:00 - 11:25 IST</i>	<i>Invited Speaker – 51</i>	<i>Prof. Hung – Lung Chou</i> National Taiwan University of Science and Technology, Taiwan	<i>Electrocatalytic Reduction of NO<sub>3</sub><sup>-</sup> to Ultrapure Ammonia on {200} Facet Dominant Cu Nanodendrites: Experiment and DFT study</i>
<i>11:30 - 11:55 IST</i>	<i>Invited Speaker - 52</i>	<i>Dr. Kothandaraman Ramanujam</i> Indian Institute of Technology, Madras	<i>A Manmade Nitrogen Cycle: Electrochemical Nitrogen Reduction Reaction With Nanostructured Catalysts</i>
<i>12:00-12:25IST</i>	<i>Invited Speaker -53</i>	<i>Dr. Manzoor Ahmad Dar</i> Islamic University of Science and Technology	

*Lunch Break : From 13:00 to 14:30*

25-Mar-2022

Poster Session (Parallel) 14:30-15:30 IST



<b>Time</b>	<b>ZOOM -- I Judges: Dr. Amrita Bhattacharya</b>	<b>ZOOM -- II Judges: Prof. Yoshiyuki Kawazoe and Dr. Sabyasachi Mukhopadhyay</b>	<b>ZOOM -- III Judges: Prof. G. P. Das and Dr. Pranab Mandal</b>	<b>ZOOM -- IV Judges: Prof. Ranjit Nanda and Dr. Siddartha Ghosh</b>
14:30 - 14:40 (IST)	<i>Sheena Agarwal</i> CSIR NCL PUNE	<i>Samadhan Kapse</i> SRM University-AP	<i>Meema Bhati</i> CSIR NCL PUNE	<i>Rajeev Ranjan</i> IISER Pune
14:40 - 14:50 (IST)	<i>Dr. Manoj Kumar Sinha</i> SRM University-AP	<i>Erakulan E.S.</i> SRM University-AP	<i>Shweta</i> CSIR NCL PUNE	<i>Vineet Kumar Pandey</i> IISER Pune
14:50 - 15:00 (IST)	<i>Kurapati Kalyan</i> SRM University-AP	<i>Unmesh Mondal,</i> Indian Institute of Science Education and Research	<i>Anjana Tripathi</i> SRM University-AP	<i>Tratiya Darshan Kamleshbhai</i> Faculty of Engg. & Tech., Atmiya University, Rajkot
15:00 - 15:10 (IST)	<i>Aradhana Tiwari</i> MNNIT Allahabad	<i>Narad Barman</i> SRM University-AP	<i>Asif Iqbal</i> SRM University-AP	<i>Shrabani paul,</i> The University of Burdwan
15:10 - 15:20 (IST)	<i>Darin Joseph</i> SRM Institute of science and technology	<i>Nikhil C</i> IIT Madras	<i>Abhijitha V G,</i> IIT Madras	<i>Deepak Subhash Gavali</i> SRM University-AP
15:20 - 15:30 (IST)	<i>Thong May Han</i> Department of Physics, University of Malaya	<i>Mohammed Abzal</i> SRM University-AP	<i>Gowsalya R</i> SRM Institute of science and technology	--

**POSTER = (5+3) Mins : Please Prepare a presentation for 5 mins**

25-Mar-22

Oral Session (Parallel) 16:00-17.45 IST

Oral = (10+3) Mins



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Andhra Pradesh

<b>Time</b>	<b>ZOOM I (parallel) In-charge -- Dr. Kavita Chair -- Ms. Shweta Mehta</b>	<b>ZOOM II (parallel) In-charge -- Dr. Mahesh Chair -- Anjana Tripathi</b>	<b>ZOOM III (parallel) In-charge -- Prof. Thapa Chair -- Mr. Samadhan Kapse</b>
16:00 - 16:15 IST	<i>Vishesh Dharaiya</i>	<i>Paramita Banerjee</i>	<i>Harshan Reddy Gopidi</i>
16:15 - 16:30 IST	<i>Malav Shah</i>	<i>Manish Kumar</i>	<i>Tetsuya Nakamura</i>
16:30 - 16:45 IST	<i>Deepika Gill</i>	<i>Jessiel Siaron Gueriba</i>	<i>Preeti Bhumla</i>
16:45 - 17:00 IST	<i>Manjari Jain</i>	<i>Jesni M Jacob</i>	<i>Pernapati Nagaraja</i>
17:00 - 17:15 IST	<i>Sheik Haseena</i>	<i>Sairathna choppella</i>	<i>Sai Lakshmi Janga</i>
17:15 - 17:30 IST	<i>Mizuho Yokoi</i>	<i>Arunima Singh</i>	<i>Sarika</i>
17:30 - 17:45 IST	--	<i>H Seshagiri Rao</i>	<i>V. Aravindan</i>