

## ACCMS-ICMG 2020-Poster/Oral presentation

ACCMS-ICMG-006 <b>P-01</b>	DEEPAK S. GAVALI	SRM UNIVERSITY - AP	First-Principles Identification Of Si/Graphite Hetrostructure As Anode Material For Li-Ion Battery
ACCMS-ICMG-009 <b>P-02</b>	SURASREE SADHUKHAN	IIT GOA	Study Of Electronic Structure And Magnetic Properties Of Substituted T Graphene Using First Principles Formalism
ACCMS-ICMG-011 <b>P-03</b>	M.J.SWAMYNADHAN	SRMIST	Hydrogenation Of Quinoline To 1,2,3,4-Tetrahydrquinoline Using Metallic Clusters Supported By Carbon Based Low Dimensional Materials
ACCMS-ICMG-014 <b>P-04</b>	DR. KAZUHITO SHIDA	SRM UNIVERSITY, AP AMARAVATI	A Simplified Method For Irreversible Monte Carlo
ACCMS-ICMG-016 <b>P-05</b>	M V JYOTHIRMAI	SRM IST	Searching Of Suitable Cationic Dopants For CZTS/Se Using First-Principles Study
ACCMS-ICMG-017 <b>P-06</b>	AAFREEN FATHIMA	SRM IST	Design Of Polar Metals In BTO/Metal/BTO Hetero-Structures
ACCMS-ICMG-018 <b>P-07</b>	ATHULYA SURENDRAN P	SRMIST-KATTANKULATHUR	Combined Computational And Experimental Investigation On Chemical Fixation Of CO <sub>2</sub> And Catalytic Transfer Hydrogenation Of Ethyl Levulinate To $\gamma$ -Valerolactone Using Water-Tolerant DUT-Series Metal-Organic Frameworks
ACCMS-ICMG-019 <b>P-08</b>	SHAIK KHAJA MUSWAREEN	ACHARYA NAGARJUNA UNIVERSITY	Impact On The Spectroscopic Properties Of Cdo-Fepo <sub>4</sub> Nanocomposites With Varying Dopant Concentrations Of V <sub>2</sub> O <sub>5</sub>
ACCMS-ICMG-020 <b>P-09</b>	MANOJ PRAJAPAT	BARKATULLAH UNIVERSITY	Quenching Of Magnetic Ordering By Nb And Ru Doping In Srcoo <sub>3-<math>\Delta</math></sub> Systems
ACCMS-ICMG-021 <b>P-10</b>	BOKINALA MOSES ABRAHAM	UNIVERSITY OF HYDERABAD	Computational Study Of Green Primary Explosive Potassium 4,4'-Bis(Dinitromethyl)-3,3'-Azofurazanate Under High Pressure.

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ACCMS-ICMG-022 <b>P-11</b>	KAVITA THAKKAR	CSIR- NATIONAL CHEMICAL LABORATORY	Comparative Study Of CO <sub>2</sub> Activation On Single Atom Doped Metal Catalysts
ACCMS-ICMG-023 <b>P-12</b>	UDAY KUMAR M	B. M. S. COLLEGE OF ENGINEERING, BENGALURU	Structural And Optical Properties Of Strontium Filled Cosb <sub>3</sub> Skutterudite
ACCMS-ICMG-027 <b>P-13</b>	MAHANTESHA B K	MANGALORE UNIVERSITY	Effect Of Electron Irradiation On Surface, Transport And Relaxation Properties Of Li Ion Conducting Polymer Composite
ACCMS-ICMG-028 <b>P-14</b>	MOHIT MITTAL	NIT WARANGAL	Photocatalytic Activity Of Cadmium Sulphide Nanoparticles Synthesized By Hydrothermal Method
ACCMS-ICMG-033 <b>P-15</b>	LAXMAN TATIKONDEWAR	SAVITRIBAI PHULE PUNE UNIVERSITY	Ultra Thin Excitonic Solar Cells From Transition Metal Dichalcogenides
ACCMS-ICMG-035 <b>P-16</b>	ERAKULAN E.S.	SRM UNIVERSITY	B <sub>2</sub> H <sub>6</sub> Splitting On Catalytic Surfaces And Role Of BH <sub>3</sub> Towards Hydrogen Spillover
ACCMS-ICMG-036 <b>P-17</b>	NIVEDITA KENGE	CSIR NATIONAL CHEMICAL LABORATORY, PUNE	Nature Of Ag-O Interactions And Prerequisites For Ethylene Epoxidation : Insights From Periodic Density Functional Theory
ACCMS-ICMG-037 <b>P-18</b>	SUTAPA CHATTOPADHYAY	SAVITRIBAI PHULE PUNE UNIVERSITY	Investigation Of Topological Properties In 2D Cadmium Chalcogenide (Cdx, X = S, Se, And Te) Buckled Honeycomb Monolayer On Substitution Of Two Cd Atoms By Sn Atoms.
ACCMS-ICMG-040 <b>P-19</b>	ANJANA TRIPATHI	SRM UNIVERSITY - AP AMRAWATI	Promoting Reactivity Of Graphene Based Catalysts With Doping Of Boron Atom: A Roadmap To Achieve LH Mechanism For CO Oxidation
ACCMS-ICMG-041 <b>P-20</b>	S B P ABIRAMI	THIAGARAJAR COLLEGE OF ENGINEERING, MADURAI	Stress Wave Propagation In Ferromagnetic Shape Memory Alloy Polymer Composite

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ACCMS-ICMG-042 <b>P-21</b>	PACHINEELA RAMBABU	IIT HYDERABAD	Spin Transport Properties Of Cofecral/Gaas/Cofecral Through First Principle Calculations
ACCMS-ICMG-044 <b>P-22</b>	SAMADHAN KAPSE	SRM UNIVERSITY, AMARAVATI	Electronic Descriptors And Design Principles Of Graphene Based Electrocatalyst For OER Using QM/ML Approach
ACCMS-ICMG-045 <b>P-23</b>	E. MEHER ABHINAV	SRMIST	Investigation Of Structural, Electronic, Magnetocaloric Properties Of A-Site Doped $\text{La}_2\text{NiMnO}_6$ For Environmental Friendly Refrigeration
ACCMS-ICMG-049 <b>P-24</b>	KUNCHANAPALLI RAMYA	SRM UNIVERSITY, AP-AMARAVATI	Effect Of Electronic Coupling On Charge Transport Across Molecular Junctions
ACCMS-ICMG-052 <b>P-25</b>	SHEENA AGARWAL	NATIONAL CHEMICAL LABORATORY	Understanding Catalytic Activity Of CoPt Alloys As Function Of Composition In Dfmcs : A First Principles Investigation.
ACCMS-ICMG-053 <b>P-26</b>	VANSHREE PAREY	SRM UNIVERSITY AP	Enhanced Phosgene Sensing On Highly Active Boron Centered Carbon Allotropes : First Principles Study
ACCMS-ICMG-055 <b>P-27</b>	ASHISH KORE	VNIT NAGPUR	Coexisting Topologically Insulating And Thermoelectric Phases Via Strain Engineering In $\text{MgBi}_3$ Topological Insulator ( $\text{MA} = \text{CH}_3\text{NH}_3$ ): A First Principle Study
ACCMS-ICMG-056 <b>P-28</b>	SURESH R	CENTRAL UNIVERSITY OF TAMILNADU	Ab-Initio Study Of Novel Intermediate Band Solar Cell Materials: $\text{ZnSi}_{(1-x)}\text{M}_{(x)}\text{P}_2$ ( $\text{M}=\text{Ti, V}$ )
ACCMS-ICMG-057 <b>P-29</b>	VIJAYALAXMI THITE	VNIT	An Inside Into Photoluminescence Property Of Colloids Of Zn-Fe Layered Double Hydroxide.
ACCMS-ICMG-058 <b>P-30</b>	GITANJALI TABHANE	VISVESVARAYA NATIONAL INSTITUTE AND TECHNOLOGY NAGPUR	Excellent Energy Density And Dielectric Properties Of Zno Reinforced PVDF/ $\text{BaTiO}_3$ Nanocomposite
ACCMS-ICMG-	ANOOP KUMAR	INDIAN INSTITUTE OF	Electrolytic Solvation Effects In Fluoroethylene Carbonates And Trifluoropropylene Carbonate: A

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060 <b>P-31</b>	KUSHWAHA	TECHNOLOGY BHUBANESWAR	Comparative Study Based On First Principles Calculation
ACCMS-ICMG-061 <b>P-32</b>	SUSHRI SOUMYA JENA	INDIAN INSTITUTE OF TECHNOLOGY BHUBANESWAR	First Principles Investigation Of Silaboranes ( $\text{Si}_n\text{H}_{n+1}$ ; $N=4-13$ ) As Potential Electrolyte In Lithium-Ion Batteries.
ACCMS-ICMG-063 <b>P-33</b>	ALOKA RANJAN SAHOO	INDIRA GANDHI CENTRE FOR ATOMIC RESEARCH	A DFT Study On Electronic Structure Of Cr Doped Pristine And Doped $\text{MoS}_2$ Multilayers
ACCMS-ICMG-064 <b>P-34</b>	POOJA ANAND MITHARI	VNIT, NAGPUR	Dip And Dry Coated MWCNT Thinfilm As Counter Electrode In Dye Sensitized Solar Cell.
ACCMS-ICMG-069 <b>P-35</b>	AMRITA GOGOI	INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH KOLKATA	Developing Guiding Principles For Designing Improved Catalysts For Ammonia Borane Dehydrogenation Using Density Functional Theory
ACCMS-ICMG-070 <b>P-36</b>	DR. RADHAKRISHNAN SIVAPRAKASAM	CENTRAL ELECTROCHEMICAL RESEARCH INSTITUTE	Simple And Template-Free Fabrication Of One-Dimensional Nickel Phenylphosphonate Nanorods And Their Calcined Derivatives As An Advanced Electrode Materials For Energy Storage Application
ACCMS-ICMG-071 <b>P-37</b>	SATYA PRAKASH DASH	IIT KHARAGPUR	A Survey On Continuous Control With Deep Reinforcement Learning
ACCMS-ICMG-072 <b>P-38</b>	CHAVAN KASHINATH TUKARAM	INDIRA GANDHI CENTRE FOR ATOMIC RESEARCH, KALPAKKAM	Electronic Structure Studies Of Bare And Passivated Cadmium Telluride Cages With Fe/Co Doping
ACCMS-ICMG-075 <b>P-39</b>	THOMAS MATHEW	ST. STEPHENS COLLEGE UZHAVOOR	Structural, Electronic And Optical Properties Of $\text{Sn}_9\text{O}_5\text{Cl}_4(\text{CN}_2)_2$ Using Density Functional Theory
ACCMS-ICMG-076 <b>P-40</b>	SUJITH C P	CENTRAL UNIVERSITY OF KERALA	Density Functional Study Of Structural And Electronic Properties Of Ternary Transition Metal Sulphides $\text{MA}_3(\text{M} \equiv \text{Hf, Zr}; \text{A} \equiv \text{Pb, Sn})$

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ACCMS-ICMG-077 <b>P-41</b>	MEGHNA C.H	CENTRAL UNIVERSITY OF KERALA	Tamm States In Topological Insulator – Photonic Crystal Structure
ACCMS-ICMG-078 <b>P-42</b>	DR. PRASHANT VIJAY GAIKWAD	DEPARTMENT OF PHYSICS, SAVITRIBAI PHULE PUNE UNIVERSITY	Family Of Two-Dimensional Octagonal Monolayers.
ACCMS-ICMG-080 <b>P-43</b>	SHASHI BHUSAN MISHRA	IIT MADRAS	First Principle Study Of Photocatalytic Reduction Of Carbon Dioxide Using TiO <sub>2</sub> /Graphene Oxide Hetero-Junction.
ACCMS-ICMG-083 <b>P-44</b>	DR. SRIHARI DODLA	SRM IST	Numerical Studies Of The Deformation Behavior For Fe-Cu On Different Length Scales
ACCMS-ICMG-084 <b>P-45</b>	KEDAR YADAV	IIT KANPUR	Novel Low Dense Carbon Allotropes With Tunable Band Gaps
ACCMS-ICMG-085 <b>P-46</b>	SURENDER SINGH	INDIAN INSTITUTE OF TECHNOLOGY KANPUR	Electronic Structure, Lattice-Dynamics And Superconductivity In Ag-Au Alloys
ACCMS-ICMG-087 <b>P-47</b>	SURYAKANTI DEBATA	INDIAN INSTITUTE OF TECHNOLOGY (ISM) DHANBAD	Theoretical Investigation Of Charge Transport Properties In Bowl-Shaped Perylene-Derivatives
ACCMS-ICMG-088 <b>P-48</b>	PADMAKUMARI R	MANGALORE UNIVERSITY	Effect Of Curcumin Doping On Optical, Structural And Luminescent Properties Of PVA Polymer Films
ACCMS-ICMG-091 <b>P-49</b>	AJITKUMAR ANKUSH CHAVAN	IIITDM	Feasibility And Assessment Of PCM Based Heat Sink For Self-Powered Devices
ACCMS-ICMG-092 <b>P-50</b>	DR. G. KRUTHIKA	CENTRAL UNIVERSITY OF TAMIL NADU	Theoretical Investigations On Two Dimensional Cs <sub>2</sub> TiBr <sub>6</sub> /TiO <sub>2</sub> Heterostructure For Solar Cell Applications

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ACCMS-ICMG-096 <b>P-51</b>	SAHANAKUMARI. R	MANGALORE UNIVERSITY	Microstructural, Optical And Electrical Properties Of Mos <sub>2</sub> Doped Sodium Alginate
ACCMS-ICMG-104 <b>P-52</b>	VIVEKANANDA MAHANTA	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	A Polymer Of Natural Product For Energy Storage In Hybrid Vanadium Flow Battery
ACCMS-ICMG-105 <b>P-53</b>	CHINMAYA MIRLE	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	Anthraquinone Derivative For Organic Redox Flow Battery In Basic Medium
ACCMS-ICMG-106 <b>P-54</b>	M RAJA	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	Binder Free Thin Carbon Fiber Electrode For Vanadium Redox Flow Battery Applications
ACCMS-ICMG-107 <b>P-55</b>	HARUN KHAN	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	Thin Bilayer Micro-Mesoporous Membrane For High Energy Efficient Vanadium Redox Flow Battery
ACCMS-ICMG-108 <b>P-56</b>	GANAPATHI RAO KANDREGULA	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	Molecular Engineering Of Donors And Acceptors For Tuning The Absorption Behavior And Electron Injection For BODIPY Based Dyes In DSSCs: A Computational Study
ACCMS-ICMG-109 <b>P-57</b>	L.K NIVEDHA	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	Impact Of Various Binders And Non-Precious Metal Catalyst Decorated Ketjen Black Carbon As Cathode In Alkaline Zinc-Air Battery
ACCMS-ICMG-102 <b>P-58</b>	XIAOHE SONG	NATIONAL UNIVERSITY OF SINGAPORE	Magnetism Of Two-Dimensional Metallic Vte <sub>2</sub>
ACCMS-ICMG-103 <b>P-59</b>	YANFANG ZHANG	INSTITUTE OF PHYSICS AND UNIVERSITY OF CHINESE ACADEMY OF SCIENCES	Recovery Of The Dirac States Of Graphene By Intercalating Two-Dimensional Traditional Semiconductors
ACCMS-ICMG-117 <b>P-60</b>	LAKSHAY DHEER	JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH	Van der Waals hetero-structures of 1H-MoS <sub>2</sub> and N-substituted Graphene for catalysis of Hydrogen Evolution Reaction

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ACCMS-ICMG-119 <b>P-61</b>	MANOJ KUMAR SINGH	IIT KANPUR	Effect of impact energy on damage evolution in laminated composite
ACCMS-ICMG-120 <b>P-62</b>	DEEPAK GOYAL	SRMIST	Mechanochemical bulk synthesis of CZTSe photovoltaic absorber
ACCMS-ICMG-121 <b>P-63</b>	MAYANK GUPTA	IIT MADRAS	Tight Binding Model Study of Centrosymmetric and Non-centrosymmetric Halide Perovskites
ACCMS-ICMG-123 <b>P-64</b>	KEVIN AMITH MATHIAS	MANIPAL INSTITUTE OF TECHNOLOGY,MANIPAL	Experimental studies on mechanical and dielectric properties of liquid-filled dielectric silicone rubber composites
ACCMS-ICMG-073 <b>P-65</b>	SUHASINI SATHIYAMOORTHY	SRMIST	Design Optimization On Fabrication Method Of Thermoelectric Generator Module
ACCMS-ICMG-125 <b>P-66</b>	P.MALLIGA	SATHYABAMA INSTITUTE OF SCIENCE AND TECHNOLOGY	Investigation on growth and optical characterization of L-Alanine Potassium Hydrogen Orthophosphate Single crystal for laser application
ACCMS-ICMG-008 <b>P-67</b>	NEHA KAUSHAL	CSIR-CSIO	Near Infrared Spectroscopy As An Efficient Tool For The Qualitative And Quantitative Determination Of Detergent Adulteraton In Milk
ACCMS-ICMG-025 <b>P-68</b>	SREEDEVI GOGULA	ANU	Structural, Optical And Luminescence Properties Of Core Shell Heterostructure Cdszn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> Nanocomposite For LED Application
ACCMS-ICMG-029 <b>P-69</b>	NIRMAL RAJEEV YERRAMALLA	ACHARYA NAGARJUNA UNIVERSITY	Investigations On Highly Photocatalytic CTAB Templated Titania Nanoparticles Doped With Europium
ACCMS-ICMG-034 <b>P-70</b>	DR. SANDHYA COLE	ACHARYA NAGARJUNA UNIVERSITY	Structural,Optical And Luminescence Properties Of Core Shell Heterostructure Cdszn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> Nanocomposite For LED Application
ACCMS-ICMG-062	PANDURANGARAO KANKANALA	ANDHRA LOYOLA INSTITUTE OF	Nanocrystalline Electrochromic Tungsten Oxide Thin

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<b>P-71</b>		ENGINEERING AND TECHNOLOGY,	Films- Effect Of Titanium Dopant
ACCMS-ICMG-065 <b>P-72</b>	DEEPU KUMAR	IIT MANDI	Anisotropic Electron-Photon-Phonon Coupling In Layered $MoS_2$
ACCMS-ICMG-082 <b>P-73</b>	RANJETH	SRMIST	Extracellular Matrix From Marine Invertebrates For Faster Biomineralization And Tailored Mechanical Properties Of Scaffolds With Tunable Interconnected Porous Architecture For Bone Regeneration
ACCMS-ICMG-093 <b>P-74</b>	DR. S KIRUTHIKA	CENTRAL UNIVERSITY OF TAMIL NADU	First Principle Studies On $Na_2LiAlH_6$ For Battery Application
ACCMS-ICMG-012 <b>P-75</b>	DR.SUDIPTA KANUNGO	INDIAN INSTITUTE OF TECHNOLOGY GOA	Prediction Of Novel Electronic Phase Due To Breakdown Of Strong Spin-Orbit Coupling In Iridates
ACCMS-ICMG-015 <b>P-76</b>	DR.MADHVENDRA NATH TRIPATHI	GURU GHASIDAS VISHWAVIDYALAYA (CENTRAL UNIVERSITY)	DFT Study Of The Lead-Free Halide Double Perovskite And Nitride Materials For Photovoltaics
ACCMS-ICMG-030 <b>P-77</b>	DR.THILLAI GOVINDARAJA	CHUNGBUK NATIONAL UNIVERSITY	First Principles Study On The Dehydrogenation Of Ethylene Diamine Monoborane Adducts And Its Cyclic Products
ACCMS-ICMG-043 <b>P-78</b>	PROF.MANICKAM MAHENDRAN	THIAGARAJAR COLLEGE OF ENGINEERING, MADURAI 625015	Hydrogen Storage In Ti-Decorated Porous Graphene.
ACCMS-ICMG-127 <b>P-79</b>	SRIDEVI MEENACHISUNDARAM	SHIZUOKA UNIVERSITY, HAMAMATSU ,JAPAN	Magnetoelectric properties of self-assembled close-packed free-standing $CoFe_2O_3$ - $Pb(Zr,Ti)O_3$ thin films.
ACCMS-ICMG-013 <b>O-01</b>	AMRISH KUMAR	IIT DELHI	Rational Design Of Single Atom Catalysts Based On Cu, Ag And Au Alloys Using Machine Learning Approaches
ACCMS-ICMG-038 <b>O-02</b>	DR. V. ARAVINDAN	THIAGARAJAR COLLEGE OF ENGINEERING	First Principles Study Of Structural, Electronic, Magnetic And Elastic Properties Of The $Mn_2$ -X-Sb (X= Co, Fe) Inverse Heusler Alloys



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ACCMS-ICMG-048 <b>O-03</b>	DR. KAVITA JOSHI	CSIR-NCL	Combining DFT With ML To Study Size Specific Interactions Between Metal Clusters And Adsorbates
ACCMS-ICMG-101 <b>O-04</b>	TONG YANG	NATIONAL UNIVERSITY OF SINGAPORE	High-Throughput Screening Of Single Transition Metal Atoms Anchored On Mos <sub>2</sub> Monolayer For Nitrogen Fixation
ACCMS-ICMG-118 <b>O-05</b>	SUJITH KALLURI	SRM UNIVERSITY -AP	Thermal analysis of Myristic - Layric acid -Fe <sub>2</sub> O <sub>3</sub> composite as nano-enhanced organic phase change material
FRACMEET-094 <b>P-0F1</b>	RUHUL AMIN IBNE HAQUE	ST. XAVIERS COLLEGE	Modeling Fracture in Porous Rock
FRACMEET-097 <b>P-0F2</b>	SAMIUL HAQUE	ST. XAVIERS COLLEGE AUTONOMOUS	Variation from frosted to glassy texture and change in fractal character of desiccation cracks on acidifying a clay suspension
FRACMEET-115 <b>P-0F3</b>	VINAY VAIBHAV	THE INSTITUTE OF MATHEMATICAL SCIENCES	Response of Glassy Liquids to Thermal Gradients
FRACMEET-124 <b>P-0F4</b>	UMANG DATTANI	THE INSTITUTE OF MATHEMATICAL SCIENCES	Cavitation transition in pinned glass-forming liquids
FRACMEET-128 <b>P-0F5</b>	PURUSATTAM RAY	THE INSTITUTE OF MATHEMATICAL SCIENCES	Crack growth in heterogeneous environment
ACCMS-ICMG-110	SURYA PRATAP SINGH	SRMIST	
ACCMS-ICMG-111	SUMEDHA ROY	SRMIST	
ACCMS-ICMG-112	NIKHIL DWIVEDI	SRMIST	

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ACCMS-ICMG-113	M. PRIYADHARSHINI	LADY DOAK COLLEGE	
ACCMS-ICMG-114	R. SHREEAISHWARYA	LADY DOAK COLLEGE	
ACCMS-ICMG-116	MS. AATHIRA	CSIR-NCL	
ACCMS-ICMG-122	ABHIJITH V G	IIT MADRAS	
ACCMS-ICMG-095	MR.SHAIK MOHAMMEDABZAL	SRM UNIVERSITY	
FRACMEET-126	ARJUN H	THE INSTITUTE OF MATHEMATICAL SCIENCES	