

## Selected List of Participants for Oral Presentation in ACCMS 2016

S.I	ID	Name	Organization	Title
1	O-1003	Prof. Kombiah Iyakutti	SRM University	Non-regular hexagonal 2D-Dirac carbon: an allotrope of graphene - A First principle study
2	O-1027	Prof.Manickam Mahendran	Thiagarajar College of Engineering, Madurai	A DFT Study on the Hydrogen Storage in Ti-Decorated Porous Graphene
3	O-1044	Dr. T Vijaya krishna	Vasireddy Venkatadri Institute of Technology,A.P	Thermo-acoustical and computational investigations on green solvent 1-ethyl-3-methylimidazolium tetrafluoroborate with N-methylaniline
4	O-1047	Dr. Sergey Seriy	R.E.Alekseev Nizhny Novgorod State Technical University, Nizhny Novgorod, Russia	Modern Ab-Initio Calculations Based on Thomas-Fermi-Dirac Theory in High-Temperatures and High-Pressures Environment
5	O-1049	Dr. Chinnappan Ravi	IGCAR	Ab Initio Modelling of Phase Equilibria in Ti-V, Ti-Nb and Ti-Ta Alloys
6	O-1050	Dr.Yogeshkumar Sonvane	S. V. National Institute of Technology, Surat	Temperature, Size and Edge Roughness Dependence of Thermal Conductivity for Vacancy-Defective Monolayer MoS <sub>2</sub>
7	O-1053	Dr. Mohit Kumar	Weizmann Institute of Science	Field-induced doping-mediated tunability in work function of Al-doped ZnO: Kelvin probe force microscopy and first-principle theory
8	O-1057	Dr. Talgat M. Inerbaev	L.N. Gumilyov Eurasian National University	Spin Unrestricted Excited State Relaxation Study of Doped Anatase
9	O-1090	Dr. T. J. Dhilip Kumar	IIT Ropar	Metal Decorated BN Linker in MOF as Potential Hydrogen Storage Material
10	O-1094	Dr. S Harinipriya	SRM University, Kattankulathur.	Electrodeposited Ni/SiC composite solar selective coating on graphite - Geometry effect on the coatings
11	O-1119	Prof. Penchalaiah Palla	VIT University, Vellore	Perovskite solar cell with nontoxic cuprous oxide as hole transporting layer and graphene as transparent electrode: Theoretical study
12	O-1144	Dr. Pooja Srivastava	Indian Institute of Science, Bangalore	Isolation of pristine Nb <sub>4</sub> C <sub>3</sub> MXene from the Nb <sub>4</sub> AlC <sub>3</sub> MAX phase
13	O-1152	Dr. Bhalchandra Kakade	SRM University, Kattankulathur.	Why Pt skin@PdPt makes stable ORR Electrocatalyst?
14	O-1155	Dr. Dang Dinh Long	VNU-University of Engineering and Technology, Vietnam	An improvement of energy harvesting in organic solar cell using ZnO nanoparticles and nanorods

15	O-1159	Dr. P Murugan	CSIR-Centralelectrochemical Research Institute, Karaikudi	Comparative Studies on Structural, Electronic, and Magnetic properties of $RT_5$ Nano-slabs (R = Y, Ce, Sm and T = Fe, Co, Ni)
16	O-1176	Dr. Darwin Barayang Putungan	University of the Philippines Los Banos, Philippines	Descriptor-based analysis of CO methanation activity on reconstructed $1T'$ - $MoS_2$ monolayer through strain-induced tuning of C and O adsorption: A DFT study
17	O-1178	Dr. Madhvendra Nath Tripathi	Guru Ghasidas Vishwavidyalaya (Central University), C.G	Lead-free halide double perovskite $Cs_2AgBiX_6$ (X=Cl, Br, and I): A first-principles investigation
18	O-1193	Dr. Venkataramanan N S	SASTRA University, Thanjavur	Experimental and Theoretical Studies of Bifunctional RGO-CoFe alloy catalyst for OER and ORR reaction
19	O-1214	Ms. Deya Das	Indian Institute of Science, Bangalore	Monolayer $BC_2$ : a high capacity anode material for Li-ion batteries
20	O-1220	Dr. Satyananda Singh Chabungbam	Harish-Chandra Research Institute, Allahabad.	Phase stability, magnetism and transition temperatures in Ni-Fe-Ga alloys
21	O-1267	Dr. Kapil Gupta	Indo-Korea Science and Technology Center, Bangalore.	<u>C</u> omprehensively <u>I</u> ntegrated <u>E</u> nvironment for advanced <u>M</u> Aterials <u>S</u> imulations (CINEMAS)