

(21) Simulation and Modeling

Co-chairs R. S. Swathi
Indian Institute of Science Education and
Research
Thiruvananthapuram 695016
Email: swathi@iisertvm.ac.in

Cristina Sissa
Parma University, Dip. Chimica
Parco Area delle Scienze 17/A
43124, Parma -Italy
Email: cristina.sissa@unipr.it

(21) Simulation and Modeling

DETAILED PROGRAMME

Monday : 12-12-2016

Session I : 12.00-13.15

12.00-12.30 Invited Talk (1)	<u>S.N. Sahu</u>	ABS-Email-ICYRAM
12.30-12.45 Oral (1)	<u>Rasmita K. Nayak</u> Sudhakar Das Trinath Sahu Ajit K. Panda	ABS-453-ICYRAM Structural Asymmetry Induced Nonmonotonous Electron Mobility in Coupled Double Quantum Well Structure
12.45-13.00 Oral (2)	<u>S. Illa-Tuset</u> S K Pati, J Faraudo	ABS-650-ICYRAM Quatsomes (Qs) loaded with Dyes: Molecular Dynamic Simulations and Quantum Mechanics calculations

Monday : 12-12-2016

Session II : 14.15-15.45

14.15-14.45 Invited Talk (2)	<u>Biswarup Pathak</u> Arup Mahata	ABS-Email-ICYRAM Atomistic Modeling of Nanocluster Based Electrodes for Fuel Cell Applications
14.45-15.00 Oral (3)	<u>Bharath Raghavan</u> Tribikram Gupta	ABS-135-ICYRAM Gas Flow through Different Pore Geometries of Nanoporous Graphene
15.00-15.15 Oral (4)	<u>Anupam Purwar</u> Debiprosad Roy Mahapatra	ABS-740-ICYRAM Modelling of Thermal Barrier coating with Vertical Cracks using Finite Element Analysis
15.15-15.30 Oral (5)	<u>Simantini Majumdar</u> Sujata Tarafdar Tapati Dutta, Shantanu Das	ABS-39-ICYRAM A Fractional Viscoelastic Model for the Bacterial Biofilms

Tuesday : 13-12-2016

Session III : 14.15-15.45

14.15-14.45 Invited Talk (3)	<u>Mukul Kabir</u>	ABS-Email-ICYRAM Phosphorene Spintronics: Role of Defect-Transition Metal Complexes
14.45-15.15 Invited Talk (4)	<u>R. S. Swathi</u> Owais C. H Mahroof Kalathingal	ABS-Email-ICYRAM Energetics of Adsorption of Monocyclic Carbon Rings on Graphene: Distance and Orientation Dependence from Analytical Approaches
15.15-15.30 Oral (6)	<u>Mohammed Azeezulla</u> <u>Nazrulla</u> Sailaja Krishnamurthy	ABS-613-ICYRAM Stretching the Threshold of Reversible Dynamics in Silicon Clusters: A case of Carbon Alloyed Si ₆
15.30-15.45 Oral (7)	<u>Renjith S Pillai</u> G Maurin	ABS-111-ICYRAM Spectacular Adsorption Behaviors of Metal-Organic Frameworks

Poster Session :

Tuesday : 13-12-2016 : 10.15-13.15 hrs

21-Poster-01	Ganesh R Chate G C Manjunath Patel A S Deshpande Amit G Shanbhag	ABS-10-ICYRAM Modelling of acid cured phenol formaldehyde based sand mould system using design of experiments
21-Poster-02	Yogendra Kumar Rajesh Kumar	ABS-42-ICYRAM Quantum Cryptography : A Revolutionary Security Technology
21-Poster-03	Siddharth Suman Mohd. Kaleem Khan Manabendra Pathak R.N. Singh	ABS-112-ICYRAM Understanding Influence of Hydride Precipitated at a Crack Tip on Crack Propagation in Zircaloy-4 Fuel Cladding using XFEM
21-Poster-04	J Mohanty A. Talapatra	ABS-190-ICYRAM Anisotropy Induced Switching Field Distribution in Patterned Media
21-Poster-05	R. P. Yadav A.K. Mittal S.N. Pandey	ABS-194-ICYRAM Ripple formation on Silicon surfaces produced by ion bombardment at oblique incidence
21-Poster-06	Sumit Sharma Raj Chawla	ABS-241-ICYRAM Variation in Young's Modulus of Defective Single-Walled Carbon Nanotubes

21-Poster-07	Sumit Sharma Raj Chawla	ABS-245-ICYRAM Mechanical properties of Single-Walled Carbon Nanotubes Containing Vacancy defects: A molecular dynamics study
21-Poster-08	Aniruddha Ghosh Anshul Yadav Arvind Kumar	ABS-339-ICYRAM Numerical and Experimental Investigation of Transient Temperature Distribution and HAZ Characteristics of Welded Plate
21-Poster-09	Hirak Chatterjee	ABS-379-ICYRAM Light Scattering by Gold Nanospikes
21-Poster-10	Sanjay kumar Ravindra Mukhiya Sanju Tanwar Rishi Sharma V K Khanna	ABS-401-ICYRAM Simulation Study of Different Capacitive Micromachined Ultrasonic Transducer (CMUT) Structures
21-Poster-11	Narayan Sahoo Ajit K Panda Trinath Sahu	ABS-455-ICYRAM External Electric Field induced Multisubband Electron Mobility in Asymmetrically Barrier Delta Doped Double Quantum Well Structure
21-Poster-12	Sai Siddarth Inderchand Manjubala	ABS-599-ICYRAM Metamaterial lens in microwave frequency range for medical applications
21-Poster-13	M Juliyana R Santhana Krishnan	ABS-666-ICYRAM On the effect of shear response in foam core by introducing semicircular tapered shear keys
21-Poster-14	Raheela Rasool Najeeb-ud-Din Shah G.M Rathder	ABS-707-ICYRAM Modelling and simulation of Ferroelectric Metal Oxide Semiconductor(MOS) capacitors
21-Poster-15	S Shruthi S Aishwarya	ABS-726-ICYRAM Effect of Cell Shape on the Flexural strength of Honeycomb Sandwich Panel
21-Poster-16	Regula Sri Nidhi Hrushi Kesav Y Shivraj Narayan	ABS-736-ICYRAM Modeling and Simulation of a Gear Housing Pattern made of ABS Material for FDM Based 3D Printing
21-Poster-17	T. Narayana Murty R. N. Singh D. Srivastava	ABS-756-ICYRAM Modelling the stress field in and around the semi constrained inclusion using Elastic plastic FEM

21-Poster-18	Shivanshu Dixit Ragvendra Kumar Mishra	ABS-759-ICYRAM Impact Damage and ballistic Response of Carbon/Epoxy Composites Laminates with stacking [45/0/-45/90]ns & [0/90]ns cross stacking sequence using Abaqus CAE
21-Poster-19	Laxman Naik G. Ramesh B. Venkatram Reddy	ABS-Email-ICYRAM Investigation of Torosional Potential, Molecular Dynamics and Vibrational Pproperties of Pyrrole-2-carboxaldehyde Using Experimental and Theoretical Methods
21-Poster-20	Madhu Sarwan Sadhna Singh	ABS-Email-ICYRAM Pressure Induced Phase Transition of Semiconducting Alloy $Tl_xGa_{1-x}As$