

# CCP2015

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**XXVII IUPAP Conference on Computational Physics  
December 2-5, 2015 IIT Guwahati**

## Time Table

**Jointly organized by**

Indian Institute of Technology Guwahati

and

The Institute of Mathematical Sciences, Chennai  
India



## Programme

Time	02.12.15 Wednesday	03.12.15 Thursday	04.12.15 Friday	05.12.15 Saturday
09:00-09:45	REGISTRATION & TEA	PLENARY-04 HANS	PLENARY-07 BARRY	PARALLEL SESSION-VI
09:45- 10:30		PLENARY-05 TURAB	PLENARY-08 LUCA	
10:30-10:45	WELCOME	TEA BREAK	TEA BREAK	TEA BREAK
10:45-11:30	PLENARY-01 GABRIEL	PLENARY-06 WILLIAM	PLENARY-09 ANNETTE	PLENARY-12 CARLO
11:30-12:15	PLENARY-02 STEVE	AWARD CEREMONY-14	PLENARY-10 SHYAM	PLENARY-13 NORBERT
12:15-13:00	PLENARY-03 YUTAKA	AWARD CEREMONY-15	PLENARY-11 RICHARD	POSTER AWARD CLOSING
13:00-14:00	LUNCH	LUNCH	LUNCH	LUNCH
14:00-15:30	PARALLEL SESSION-I	PARALLEL SESSION-II	PARALLEL SESSION-IV	All Plenary, Award Ceremony and Industry Sessions will be held in Bhupen Hazarika Auditorium.
15:30-15:45	TEA BREAK	TEA BREAK	TEA BREAK	
15:45-17:15	POSTER SESSION-I	PARALLEL SESSION-III	PARALLEL SESSION-V	
17:15-17:30	TEA BREAK	TEA BREAK	TEA BREAK	
17:30-19:00	CULTURAL PROGRAMME	INDUSTRY SESSION: SHWD	POSTER SESSION-II	
19:00-20:30	DINNER	DINNER	CONFERENCE DINNER	

## December 02, 2015 • Wednesday

09:00 Registration and Tea

10:30 Welcome

### Plenary 01,02 & 03

Time	Speaker	Talk Title
10:45	Gabriel Kotliar	Understanding Strongly Correlated Materials thru Theory Algorithms and High Performance Computers
11:30	Steven Gottlieb	Lattice Field Theory Applications in High Energy and Nuclear Physics
12:15	Yutaka Ishikawa	An Overview of the Next Flagship Supercomputer in Japan

13:00 Lunch

### 14:00- 15:30 Parallel Session-I

H-1: Atomic, Molecular and Optical Physics		
Time	Speaker	Talk Title
14:00	E Krishnakumar (Invited)	Dynamics of Electron & Molecule Resonances: A Challenge to Computational Physics
14:30	Satrajit Adhikari (Invited)	Beyond Born-Oppenheimer Theories: Diabatic PESs for Spectroscopic & Scattering Processes
15:00	Ramesh Kumar (Oral)	Finite element modeling and analysis of the effect of frequency on the electromagnetic compression of tubes
15:15	Aditya Manuwal (Oral)	Optimization of a Dielectric Mirror Design for 532 nm Laser

L-3: Astrophysics, Plasma, Gravitation and Cosmology		
Time	Speaker	Talk Title
14:00	P Ajith (Invited)	Towards gravitational-wave astronomy
14:30	B Chaudhury (Oral)	Computational Modeling of Microwave Streamer Dynamics
14:45	Tanay Ghosh (Oral)	Rotation of Polarization Vector of Electromagnetic Wave due to Linearly Accelerated Frame

L-4: Computational Biological Physics		
Time	Speaker	Talk Title
14:00	Prabal K Maiti (Invited)	Effect of Dendrimer in HIV-1 inhibition
14:30	Sandip Sarkar (Oral)	A Possible Explanation of Oriented Bar Filling-in at the Blind-Spot in the light of Hierarchical Prediction Mechanism
14:45	Prabir Khatua (Oral)	Conformational Fluctuations of $A\beta_{42}$ Peptide Monomer and its Interaction with Surrounding Solvent
15:00	Sandip Mondal (Oral)	Interaction Between the $\lambda$ –repressor Protein and Its Operator DNA: A Molecular Dynamics Study

<b>MA: Fluid Dynamics, Oceanography, Geophysics and Climate modelling</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Gautam Biswas (Invited)	Simulation of Multi-Fluid System: Understanding Drop Impact
14:30	T K Sengupta (Invited)	Non-equilibrium thermodynamics of Rayleigh-Taylor instability
15:00	S Jayavel (Oral)	Computational study of fluid flow characteristics due to confining walls with local waviness
15:15	K S Santhosh (Oral)	DSMC simulations of flow over micro textured surfaces

<b>H-2: High Energy, Nuclear and Particle physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Y Kuramashi (Invited)	Tensor Network Scheme For Lattice Gauge Theories
14:30	Nilmani Mathur (Invited)	Heavy quark physics using large scale simulations
15:00	P Bhattacharya (Oral)	Detailed 3D Simulation of the GEM-based detector

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Stefano Sanvito (Invited)	The magnetic genome project
14:30	Sugata Mukherjee (Oral)	First-principles calculation of the transport properties of Graphene/hBN/Graphene heterostructured nanomaterials
14:45	A Chakrabarty (Oral)	Multiscale modelling of carburization of steel through Fe-110 surface
15:00	Vijay S Kumawat (Oral)	Optimization of SAE 1080 carbon steel strip for heat treatment process parameters using L9 orthogonal array

<b>L-1: Quantum Many Body and Strongly Correlated Systems</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Mark Jarrell (Invited)	Typical Medium Dynamical Cluster Simulations of Interacting and Strongly Disordered Systems
14:30	Kedar S. Damle (Invited)	Sign-free Quantum Monte Carlo simulation of certain frustrated quantum magnets
15:00	S Pradhan (Oral)	Exciton Condensation in a Correlated Model with a Strong Orbital Magnetic Field
15:15	Sudeshna Sen (Oral)	Site-disorder induced distribution of Kondo scales in the Anderson-Hubbard model: A typical medium theory study using the local moment approach

<b>H-4: Soft Matters, Polymers Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	M Bachmann (Invited)	Statistical Analysis of Transitions in Finite Polymer Systems
14:30	R Chakrabarti (Invited)	Single polymer chain with internal friction
15:00	P H Lana Martins (Oral)	Interlocking Order Parameter Fluctuations in Structural Transitions Between Adsorbed Polymer Phases
15:15	A Ahmed A Jaleel (Oral)	Collapse transition of short polymers on simple cubic lattice

<b>H-3: Statistical Physics, Complex System and Nonlinear Dynamics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	J S Wang (Invited)	Computational methods for quantum thermal transport in nanostructures
14:30	Joseph Mathew (Oral)	Vortex Soliton Solutions in Poly-Acetylene
14:45	M Suneel Durve (Oral)	First Order Phase Transition in Modified Vicsek Model

15:30 Tea

**15:45 Poster Session-I: Lecture Hall Complex**

17:15 Tea

17:30 Cultural Programme

19:00 Dinner

## December 03, 2015 • Thursday

### Plenary 04,05 & 06

Time	Speaker	Talk Title
09:00	Hans Jurgen Herrmann	Packing of wires in cavities and growing surfaces
09:45	Turab Lookman	Information-driven approach to materials discovery and design

10:30 Tea

Time	Speaker	Talk Title
10:45	William A Goddard	In silico predictions of 3D structures and binding sites for GPCR-ligand complexes

Award Ceremony:	
11:30	IUPAP Young Scientist Award - 2014
12:15	IUPAP Young Scientist Award - 2015

13:00 Lunch

### 14:00-15:30 Parallel Session-II

L-1: Atomic, Molecular and Optical Physics		
Time	Speaker	Talk Title
14:00	H Ramachandran (Invited)	Modelling Dielectric Structures with Bends using the Beam Propagation Method
14:30	Md Abdul Khan (Oral)	Few-body model approach to the bound states of helium-like exotic three-body system.
14:45	Prashanth Jyothi (Oral)	Spectroscopic investigation of some bipyridines-A comparative study using DFT and GF-matrix method in overlay technique.

L-3: Astrophysics, Plasma, Gravitation and Cosmology		
Time	Speaker	Talk Title
14:00	Adam Amara (Invited)	Information from Cosmology Experiments
14:30	Pankaj Joshi (Invited)	Gravitational Collapse, Black Holes and Space-time Singularities in Einstein Gravity
15:00	Manash J Boruah (Oral)	Modeling and experimental light scattering studies of interstellar dust analogue samples using DDA.
15:15	Anuj K Dubey (Oral)	Frame Dragging from Charged Rotating Body

<b>L-4: Computational Biological Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Birgit Strodel (Invited)	Thermodynamics and kinetics of amyloid aggregation from atomistic simulations
14:30	S Bhattacharya (Oral)	Uncertainty in Markov state models with missing states & rates: application to a room temperature kinetic model obtained using high temperature molecular dynamics
14:45	Aditya G Rao (Oral)	Molecular dynamics simulations of Monomeric Chorismate mutase bound to a Transition state analogue
15:00	K Bhattacharjee (Oral)	A DFT Study Of Methylation Reactions Of CH <sub>3</sub> N <sub>2</sub> <sup>+</sup> With Guanylate And Deoxyguanylate

<b>H-2: Computational Physics Education</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Scott A Lathrop (Invited)	Expanding Access to Computational Science Education
14:30	A Dasgupta (Invited)	Open Source Computation in Physics Education
15:00	Prashant K Rathod (Oral)	Use of SCILAB to draw Lissajous Figures

<b>MA: Fluid Dynamics, Oceanography, Geophysics and Climate modelling</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	R. Adhikari (Invited)	Computation of many-body hydrodynamic interactions in active colloidal suspensions
14:30	K Natarajan (Oral)	Computational studies on Small Wind Turbine performance characteristics
14:45	Devavrat Kashyap (Oral)	Aspects of computation of incompressible viscous flows through a compressible flow solver
15:00	Harshit Dwivedi (Oral)	Dynamic Response of circular tunnel under Viscoelastic medium

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	A Marco Saitta (Invited)	Reaction networks and free-energy landscapes via a novel topological approach: ab initio Miller-like experiments and beyond
14:30	Ransell Dsouza (Oral)	Seebeck coefficient of Monolayer and Bilayer Graphene
14:45	Kotagiri G Prasad (Oral)	Structural, vibrational and ferroic properties of AgTaO <sub>3</sub> from first principle calculations
15:00	A D Rao (Oral)	Impact of Mo <sup>6+</sup> on Electrical Properties of Copper Ferrite
15:15	Sanchali Mitra (Oral)	Density Functional Theory optimization of Palladium Gold alloy for designing plasmonic waveguide based room temperature hydrogen sensor

<b>H-1: Software and Hardware Development</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Scott Klasky (Invited)	SIRIUS: Science-driven Data Management for Multi-tiered Storage
14:30	Austin Cherian (Invited)	
15:00	Dheeraj K Sinha (Oral)	Two Dimensional Numerical Simulator for Modeling NDC Region in SNDC Devices

<b>H-4: Soft Matters, Polymers Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	T Hatano (Invited)	Critical slowing down at jamming transition
14:30	A Dasmahapatra (Oral)	Monte Carlo Simulation of Crystallization in Binary Polymer Blends
14:45	Bikramjit Sharma (Oral)	Computational Investigation of Hydration Structure and Dynamics of Iodate Ion
15:00	Kartik Sau (Oral)	Atomistic Modeling and Simulation of Fast Sodium Ion Conductors: Na <sub>2</sub> M <sub>2</sub> TeO <sub>6</sub> (M=Ni, Zn, Co, Mg)

<b>H-3: Statistical Physics, Complex System and Nonlinear Dynamics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Wolfhard Janke (Invited)	Finite-Size Scaling at the Droplet Condensation-Evaporation Transition
14:30	P Chaudhuri (Invited)	Onset of flow in soft glasses: linking percolation to flow heterogeneities
15:00	Shantanu Kadam (Oral)	Development of kinetic Monte Carlo Methods for the Stochastic Simulation of Chemical Systems
15:15	J T Kjellstadli (Oral)	Systematic Study of the Burst Size Distribution in the Local Load Sharing Fiber Bundle Model

15:30 Tea

15:45 – 17:15 **Parallel Session-III**

<b>H-2: Computational Physics Education</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	KPN Murthy (Invited)	Non-Boltzmann Ensembles and Monte Carlo Simulation
16:15	Somin Wadhwa (Oral)	Study of Random Numbers & their applications in computational physics using Monte-Carlo method
16:30	S Bukkuru (Oral)	Identifying Interstitials in MD simulations - Max Space Clustering Method



<b>MA: Fluid Dynamics, Oceanography, Geophysics and Climate modelling</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	Tapan Mukerji (Invited)	Computational Rock Physics: Imaging and Process Modeling at the Pore Scale
16:15	Kumari Trinavee (Oral)	Flow and heat transfer analysis in a circular microchannel with alumina based nanofluid
16:45	Gilson A R Lima (Oral)	Gap Filling of Precipitation Data by Singular Spectrum Analysis

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	P Mahadevan (Invited)	The dilute magnetic semiconductors: A playground for the Zaanen-Sawatzky-Allen phase diagram
16:15	Yamini Sharma (Oral)	Hydrogen storage in binary and ternary intermetallics
16:30	Anmol Kumar (Oral)	DAMQT-2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules
16:45	Yasunari Zempo (Oral)	Symmetric Smoothed Particle Hydrodynamics Method for Real-Space Electronic Structure Calculation

<b>L-1: Quantum Many Body and Strongly Correlated Systems</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	Honggang Luo (Invited)	Phase diagram of one-dimensional t-J model with long-range dipolar interactions
16:15	F Agostini (Invited)	Electron-Nuclear Correlation: A Time-Dependent Perspective
16:45	Saurabh Basu (Oral)	Three body interaction effects on the phase diagram of spinor bosons
17:00	Swagata Acharya (Oral)	Novelties in the Extended Periodic Anderson Model: A View from Low-Temperature DMFT (CTQMC) Studies

<b>H-1: Software and Hardware Development</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	Prabhu Ramachandran (Invited)	Extensible, reusable, and reproducible computing: a case study of PySPH
16:15	A G Chatterjee (Oral)	Scaling of a fast Fourier transform and a pseudo-spectral fluid solver up to 65536 processors
16:30	Gaurav Kumar (Oral)	A Framework to Simulate Semiconductor Devices Using Parallel Computer Architecture

<b>H-3: Statistical Physics, Complex System and Nonlinear Dynamics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	60 Years of Alex Hansen	
16:15	S Karmakar (Invited)	Short-time $\beta$ -relaxation in glass-forming liquids is cooperative in nature
16:45	Santanu Sinha (Oral)	Dynamic wettability alteration in immiscible two-phase flow in porous media

17:15 Tea

## Industry Session

<b>Software and Hardware Development:</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
17:30	Rama Kishan V Malladi	Unleash Application Performance with Intel Software on Next-Gen Hardware
18:00	Gaurav Mishra	NVIDIA
18:30		FUJITSU

19:00 Dinner

## December 04, 2015 • Friday

### Plenary 07,08

Time	Speaker	Talk Title
09:00	Barry I. Schneider	How Novel Algorithms and Access to High Performance Computing Platforms are Enabling Scientific Progress in Atomic and Molecular Physics
09:45	Luca Baiotti	Numerical relativity for binary neutron stars

10:30 Tea

### Plenary 09,10 & 11

Time	Speaker	Talk Title
10:45	Annette Zippelius	Dense Granular Flow of Frictional Particles
11:30	Shyam S Rai	Imaging Earth's Interior through Noise Interferometry
12:15	Richard Martin	Undergraduate Computational Physics Education: Uneven History and Promising Future

13:00 Lunch

### 14:00 – 15:30 Parallel Session-IV

<b>H-1: Atomic, Molecular and Optical Physics</b>		
Time	Speaker	Talk Title
14:00	G Vemuri (Invited)	Realization of a PT-symmetric dimer in coupled semiconductor lasers
14:30	H Wanare (Invited)	Interplay between light and magnetic field in inducing anisotropy in atomic systems
15:00	A Mihailescu (Oral)	Towards Improved Theoretical Investigations of Ultrashort and Intense Laser Pulses Interaction with Plasmas. Updating Traditional Particle-in-Cell with Kalman Filtering.
15:15	Rahul Saha (Oral)	Interaction of atoms with Intense Laser field: A Numerical study in the Single-active Electron Approach

<b>L-3: Astrophysics, Plasma, Gravitation and Cosmology</b>		
Time	Speaker	Talk Title
14:00	T Souradeep (Invited)	Bayesian Cosmological inference beyond statistical isotropy
14:30	G Rajaraman (Invited)	Strongly correlated classical plasmas under external forcing and dissipation - examples using molecular dynamics approach
15:00	Azad A Mansoori (Oral)	Evaluation of long term solar activity effects on GPS derived TEC
15:15	Debraj Mandal (Oral)	Study of trapped particle nonlinearity in Ion Acoustic solitary wave using Vlasov simulation

<b>L-4: Computational Biological Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	S Bandyopadhyay (Invited)	Correlated conformational features and hydration dynamics of protein-DNA complexes
14:30	Sunita Negi (Oral)	Temperature dependent conformation studies of Calmodulin protein using Molecular Dynamics simulations
14:45	Pradeep K Shukla (Oral)	Theoretical Study of DNA Damage at Molecular Level
15:00	Shalini Awasthi (Oral)	Sampling Free Energy Surfaces as Slices by Combining Umbrella Sampling and Metadynamics

<b>MA: Fluid Dynamics, Oceanography, Geophysics and Climate modelling</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	P Perlekar (Invited)	Two and three dimensional binary-fluid turbulence
14:30	Sarede Yadav (Oral)	Numerical simulation of dense suspension flow in a symmetric T-shape 3D bifurcation channel
14:45	Dattaraj B Dhuri (Oral)	Lattice Boltzmann Method for Wave Propagation in Complex Media

<b>H-2: High Energy, Nuclear and Particle physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	A Juettner (Invited)	Flavour physics and lattice QCD
14:30	S Mukhopadhyay (Oral)	Exact solutions to model surface and volume charge distributions
14:45	Manish Kumar (Oral)	Prediction of mass of $Z'$ boson from the study of $B_s^0 \rightarrow \mu^+ \mu^-$ and $B_d^0 \rightarrow \mu^+ \mu^-$ decays

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Rajeev Ahuja (Invited)	Materials for Li and Na Batteries : A Computational Materials Science Point of View
14:30	Shishir K Pandey (Oral)	Doping an antiferromagnetic insulator : A route to an antiferromagnetic metallic phase
14:45	Abhijit Chatterjee (Oral)	Capturing local atomic environment dependence of activation barriers in 3D nanostructured metal alloys using cluster expansion
15:00	Ravi Kashikar (Oral)	Defect States and Magnetism in Graphene

<b>L-1: Quantum Many Body and Strongly Correlated Systems</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Wei Ku (Invited)	Spin/Orbital Correlation and Itinerancy-Enhanced Quantum Fluctuation in Iron-Based Superconductors
14:30	Jugal P Bordalai (Oral)	Computing Mobility in Quantum Well Device
14:45	Ajit Kumar Jena (Oral)	Polyanion driven insulating behaviour in antiferromagnetic LiFePO <sub>4</sub>

<b>H-4: Soft Matters, Polymers Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	T Schilling (Invited)	Percolation in colloidal model systems
14:30	Sourav Kundu	Single stranded DNA sequencing using graphene nanopore device
14:45	Anna Varughese (Oral)	Microscopic studies in Binary Lennard-Jones system
15:00	A V Anil Kumar (Oral)	Structure and dynamics of binary colloidal mixtures in an external potential barrier: Effect of depletion interaction

<b>H-3: Statistical Physics, Complex System and Nonlinear Dynamics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
14:00	Mathis Plapp (Invited)	Phase-field models for the growth and evolution of complex structures
14:30	S Sinha (Invited)	Chaos, Complexity and Computation: Patterns in oscillatory media
15:00	Tasrief Surungan (Oral)	Search for Heisenberg spin glass on rewired cubic lattices with antiferromagnetic interaction
15:15	Prasenjit Das (Oral)	Order Disorder Transitions in Critical and Off-Critical Binary Mixtures

15:30 Tea

15:45 – 17:15 **Parallel Session-V**

<b>H-1: Atomic, Molecular and Optical Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	D Roy Chowdhury (Invited)	Near field coupled Metamaterials for Terahertz Wavelengths
16:15	Rudraditya Sarkar (Oral)	Theoretical study of photoelectron spectrum of CH <sub>2</sub> F <sub>2</sub>
16:30	Mitsuki Togoshi (Oral)	Maximum Entropy Method for Optical Spectral Analysis using Real-Time Time-Dependent Density Functional Theory

<b>H-2: High Energy, Nuclear and Particle physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	P Majumdar (Invited)	Lattice QCD simulations using the OpenACC platform
16:15	Ajay Kumar Rai (Oral)	Mass spectra, di-gamma and di-leptonic decay rates of the quarkonia
16:30	Ashim Roy (Oral)	Simulation of $\pi^0 - \gamma$ Separation Study for Proposed CMS Forward Electromagnetic Calorimeter

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
15:45	G P Das (Invited)	Substrate induced modulation of physical and chemical properties of quasi two-dimensional nanostructures
16:15	Santosh Dubey (Oral)	Molecular Dynamics Simulations of Deformations Behavior of Metallic Nanowires
16:30	Suchitra (Oral)	Pressure induced structural phase transition and tunable work function of ReO <sub>3</sub>
16:45	Ram Sevak Singh (Oral)	Electronic properties evolution in Sc-doped anatase TiO <sub>2</sub> : A computational study

17:15 Tea

17:30 **Poster Session-II: Lecture Hall Complex**

19:00 Conference Dinner

## December 05, 2015 • Saturday

### 09:00 – 10:30 Parallel Session-VI

<b>H-1: Atomic, Molecular and Optical Physics</b>		
Time	Speaker	Talk Title
09:00	Gagan Kumar (Invited)	Terahertz guided wave devices using plasmonic metamaterials
09:30	V R Byru (Oral)	Experimental and theoretical study of 3-methyl-4-nitrobenzoic acid using DFT and GF-matrix method
09:45	A R Rao (Oral)	Optimization of RF excitation frequency for maximum optical power output of ring cavity

<b>L-4: Computational Biological Physics</b>		
Time	Speaker	Talk Title
09:00	D Sengupta (Invited)	Association at the membrane: Do lipophobic effects mediate membrane protein assembly
09:30	R Swaminathan (Oral)	Modeling the influence of Macromolecular Crowding on an Enzymatic Reaction: Role of Crowder Density and Crowder Stickiness
09:45	Rajany Kv (Oral)	The Statistical Properties of Spiral- and Scroll-wave Turbulence in Two Mathematical Models of Cardiac Tissue
10:00	Dibyajyoti Parida (Oral)	On the Origin of Photodynamic activity of Perylene Quinone Framework

<b>MA: Fluid Dynamics, Oceanography, Geophysics and Climate modelling</b>		
Time	Speaker	Talk Title
09:00	L. S. Luo (Invited)	Multiscale Modeling and Simulation of Gaseous Microflows
09:30	B Kumbhakar (Oral)	Unsteady MHD Free Convection Flow with Hall Effects of a Radiating and Heat Absorbing Fluid Past a Moving Vertical Plate with Variable Ramped Temperature
09:45	Srinivas Jangili (Oral)	Effect of Buoyancy Force on Entropy Generation in a Vertical Parallel Plate Channel
10:00	Bidyut B Gogoi (Oral)	An accurate predictor-corrector HOC solver for the two-dimensional shock tube problem

<b>H-2: High Energy, Nuclear and Particle physics</b>		
Time	Speaker	Talk Title
09:00	Satyaki Bhattacharya (Invited)	Multivariate techniques in analysis of the LHC data
09:30	Manoj K Warriar (Oral)	Multi-scale Modeling of Radiation Damage: Large Scale Data Analysis
09:45	Yogesh Kumar (Oral)	Droplet formation of quark-gluon plasma with the effect of curvature term at finite chemical potential

<b>L-2: Material and Nano Sciences</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
09:00	Yuan P Feng (Invited)	2D Materials and Devices for Spintronics: First-principles Studies
09:30	K A Iskakova (Oral)	The Break of the uniform position of the transition layers
09:45	Murari M Sinha (Oral)	Study of lattice dynamics of Fe <sub>2</sub> SiO <sub>4</sub> - and Mg <sub>2</sub> SiO <sub>4</sub> -spinels
10:00	Ranjit Thapa (Oral)	Metal-Free Catalyst with Efficient ORR activity: First Principles Analysis
10:15	Amit Anand (Oral)	High Pressure Phase Transition Properties of Lutetium Monopnictide : A Density Functional Theory Study

<b>L-1: Quantum Many Body and Strongly Correlated Systems</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
09:00	S. Biermann (Invited)	Screened exchange dynamical mean field theory
09:30	Apurba Barman (Oral)	Phase diagram of Bosons on a tripartite optical lattice: Effects of long range and three-body interaction potentials
09:45	S Samanta (Oral)	Electronic Structure at the Interface of Two Double Perovskites: Sr <sub>2</sub> FeMoO <sub>6</sub> /La <sub>2</sub> CoMnO <sub>6</sub>
10:00	Ilyas Noor Bhatti (Oral)	Quantum lattice models: Ground state and low lying excitation

<b>H-4: Soft Matters, Polymers Physics</b>		
<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
09:00	S P Thampi (Invited)	Intrinsic free energy in active nematics
09:30	S Palchowdhury (Oral)	Self-Assembly of Cations in Aqueous Solutions of Hydroxyl-Functionalized ionic liquids: molecular dynamics studies
09:45	Navin Singh (Oral)	DNA under random force
10:00	Pankaj Mishra (Oral)	Freezing transitions in binary mixtures of two-dimensional colloidal suspensions

10:30 Tea

### **Plenary 12, 13**

<b>Time</b>	<b>Speaker</b>	<b>Talk Title</b>
10:45	Carlo Massimo Casciola	Energy fluxes, scale energy and turbulent separation
11:30	Norbert Attig	Impacts of Current Hardware and Software Developments on Simulation Sciences

12:15 Poster Award & Closing

13:00 Lunch



**Poster Session-I: Lecture Hall Complex**  
15:45-17:15 December 02, 2015 • Wednesday

<b>Atomic, Molecular and Optical Physics:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Bijita Sarma	AMOP-P-156	Hybrid cavity optomechanical cooling of a micromechanical resonator by two-level atomic system
Rupam Konwar	AMOP-P-188	Bilinearization of nonautonomous nonlinear schrodinger equation and its soliton solution
David Pegu	AMOP-P-223	Theoretical investigations on Spectroscopic [IR and Raman], NLO, Frontier molecular orbitals and electronic structure of 4-fluro-4-hydroxy Benzophenone using Gaussian Hybrid computational calculations
Maidul Islam	AMOP-P-225	Terahertz surface plasmon polaritons propagation in slanted pillar geometries.
K Monika Devi	AMOP-P-244	Enhanced terahertz transmission through a periodic array of tapered rectangular apertures
Ashish K Rajak	AMOP-P-309	Electromagnetic Hemming of Aluminium sheets

<b>Astrophysics, Plasma, Gravitation and Cosmology:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Jakub Hromadka	APGC-P-163	Hybrid computer modelling in plasma physics
Sarani Chakraborty	APGC-P-174	Effect of non-zero cosmological constant on the motion of light ray.
Parizath Deb Roy	APGC-P-243	Imaging polarimetry of comets to explore the dust grain evolution at low phase angle
Saswati Roy	APGC-P-485	Photon Surfaces due to different space-time geometry

<b>Computational Biological Physics:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Koyel Chakravarty	CBIO-P-274	A Two-Layer Mathematical Modelling of Drug Delivery to Biological Tissues
Sarvesh K Pandey	CBIO-P-322	Quantification of Aromaticity Based on Interaction Coordinates: A New Approach
Debashish Acharya	CBIO-P-226	Synthesis of Silver Nanoparticle and the Study of Their Antibacterial Effect

<b>Fluid Dynamics, Oceanography, Geophysics and Climate modelling:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Dinesh Ramesh	FDCM-P-108	Comparative study on heat transfer and flow properties of engine oil based nanofluids
Sougata Biswas	FDCM-P-121	Moffatt vortices in the lid-driven cavity flow
Abida Choudhury	FDCM-P-219	A Study of Lightning Flash from MCSs over Northeast India
Raushan Kumar	FDCM-P-292	A Kinetic Theory Based Boltzmann Level Flux-Limited Numerical Scheme for 1-D Euler Equations of Gas Dynamics

Swarup Barik	FDCM-P-348	Influences of non-linear chemical reactions on transport coefficients in an oscillatory Couette flow
Sakshi Devi	FDCM-P-373	Transient Dynamic Response of Cylindrical Shell subjected to an Internal Loading in Elastic Medium

### High Energy, Nuclear and Particle physics:

Presenter	Abstract	Poster Title
Zalak Urjit Shah	HENP-P-95	Excited state mass spectra of $\Omega_c$ baryon
D S Bhattacharya	HENP-P-195	Track Distortion in the Large Prototype of a Time Projection Chamber for the International Linear Collider
Debika Banerjee	HENP-P-434	Study of rare baryonic decays $\lambda_b \rightarrow \lambda \ell^+ \ell^-$ in $Z'$ model

### Material and Nano Sciences:

Presenter	Abstract	Poster Title
Naidu V Atchiah	MNSC-P-203	Effect of Substrate Index of Refraction on the Optical and Structural Properties of MgF <sub>2</sub> Single layer Antireflection thin films
Debashish Das	MNSC-P-213	First principles electronic structure investigations on the effects of composition and sub-lattice occupancy in Co(Cr <sub>1-x</sub> Fe <sub>x</sub> ) <sub>2</sub> O <sub>4</sub>
Jeetu Donderiya	MNSC-P-216	High Pressure Structural Phase Transition and Electronic Properties of NdX (X = P, As, Sb) Compounds : A First Principles Study
Siby Thomas	MNSC-P-221	Young's modulus of graphene using intrinsic thermal vibrations
Jyotirmoy Deb	MNSC-P-229	Electronic Properties of Aluminium and Silicon Doped (2, 2) Graphyne Nanotube
Edwin Mapasha	MNSC-P-235	A hybrid density functional study of silicon and phosphorus doped hexagonal boron nitride monolayer
Ashis Kundu	MNSC-P-252	Ab initio study of vibrational and elastic properties of Mn <sub>2</sub> NiGa inverse Heusler alloy
Prabhat Ranjan	MNSC-P-272	Computational Study of Au <sub>m</sub> Si <sub>n</sub> (m+n=2-6) Nanoalloy Clusters Invoking DFT Based Descriptors
Piyush Singh	MNSC-P-294	A three-dimensional fully coupled thermo-mechanical model for Self-reacting Friction Stir Welding in Aluminium alloy AA6061
Sushant K Behera	MNSC-P-302	Linear scaling density functional approach for realizing pressure effect on anisotropic Co <sub>3</sub> O <sub>4</sub> nanostructures
A M Gopakumar	MNSC-P-316	Modification of Thermoelectric Behaviour of PbTe-SrTe Superlattice Through Bulk Doping
Shashank Rangu	MNSC-P-483	Magnetic Metamaterials: A comparative study of resonator geometry and metal conductivity

**Quantum Many Body and Strongly Correlated Systems:**

Presenter	Abstract	Poster Title
Khoirom Kabita	QMBS-P-61	First principles study on structural, phase transition and electronic structure of Zinc Sulfide (ZnS) within LDA, GGA and mBJ potential.
Jitumani Kalita	QMBS-P-129	Thermally assist tunneling of charge carriers between trapping sites in calcite (CaCO <sub>3</sub> ) mineral
Sk Noor Nabi	QMBS-P-324	Disorder, three body interaction and Bose glass phase in a spinor atomic gas on an optical lattice
Shashi B Mishra	QMBS-P-379	Ab initio Molecular Dynamics as a Tool to Synthesize Crystalline Materials: Case Study on LiFePO <sub>4</sub>
Sunayana Dutta	QMBS-P-512	Condensate Characteristics of bosons in a tilted optical lattice

**Software and Hardware Development:**

Presenter	Abstract	Poster Title
A Perepelkina	SHWD-P-256	Acoustic wave simulation with DiamondTorre algorithm
Prithish Halder	SHWD-P-317	JaSTA: The java application to study the electromagnetic scattering of aggregates from micron to nano scale

**Soft Matters, Polymers Physics:**

Presenter	Abstract	Poster Title
Sangkha Borah	SMPB-P-143	Ab initio Molecular Dynamics Study of Selenate in Aqueous Environment
Debarati Sarkar	SMPB-P-161	Dynamics of loop closure in a chemically active polymer
Jalim Singh	SMPB-P-166	Heterogeneous dynamics of linear polymer melts by calculating four point correlation functions
Manoj Dhiman	SMPB-P-184	3D thermohaline double-diffusive salt fingers
Mohit Hemath	SMPB-P-228	Studies on Chicken Fiber Reinforcement in Isophthalic Polymer Metal Matrix Nanocomposite
Chitrita Kundu	SMPB-P-230	Crystallization of Diblock Copolymer from Microphase Separated Melt
Anvy Moly Tom	SMPB-P-515	Aggregation Dynamics of Rigid Polyelectrolytes

**Statistical Physics, Complex System and Nonlinear Dynamics:**

Presenter	Abstract	Poster Title
Morten Vassvik	SPCS-P-214	Modelling Interface Dynamics in Two-Phase Flow in Porous Media
Bappaditya Roy	SPCS-P-295	Explosive percolation in growing cluster model from randomly added growth centers
Sul Ah Ahn	SPCS-P-336	Research Activity in Computational Physics utilizing High Performance Computers: Co-authorship Network Analysis
S Venkatesan	SPCS-P-352	Nucleation versus percolation scenario in fracture: a molecular dynamics simulation study
Biplab Bhattacharjee	SPCS-P-509	Topological Distance Dependent Transition in Flocks with Binary Interactions

## Poster Session-II: Lecture Hall Complex

17:30-19:00 December 04, 2015 • Friday

<b>Atomic, Molecular and Optical Physics:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
M Bhattacharjee	AMOP-P-56	Effect of Oxide Barrier Height in Spin Dependent Tunneling in MTJ of FeO-MgO Multilayer Structure
Koushik Paul	AMOP-P-321	Efficient shortcut techniques in evanescently coupled waveguides
Laxman N Jarupula	AMOP-P-414	Spectroscopic investigation of some pyridine-dicarboxylic acids using experimental and theoretical methods
Rajitha Kv	AMOP-P-423	Efficient cloning and dragging of arbitrary microwave pulse into optical frequency pulse in a Doppler-broadened atomic medium
Sandeep Sharma	AMOP-P-425	Diffractionless beam propagation in optically written waveguide
Pradeep Upadhyaya	AMOP-P-482	Raman study of C=O, C-N and C-H stretching vibration of NN-dibutyl formamide: A comparison with quantum chemical calculation

<b>Astrophysics, Plasma, Gravitation and Cosmology:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Kalpajyoti Borah	APGC-P-343	Optimally-dissipative wave-particle splitting scheme for ideal magnetohydrodynamics
K S Singh	APGC-P-363	Effect of magnetic field on laser ablation during plasma formation: Experimental and finite element model study
Roshni Atulkar	APGC-P-450	Variability of sporadic E-layer at mid latitude station during high solar activity year 2012
Shivangi Bhardwaj	APGC-P-451	Solar Transients disturbing the mid latitude Ionosphere during the High Solar Activity
Bhupendra Malvi	APGC-P-470	Morphological Investigation of Disturbed Ionosphere During Intense Geomagnetic Storm
Arup Das	APGC-P-349	Distance Estimations to some selected Dark clouds

<b>Computational Biological Physics:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Kajwal Kumar Patra	CBIO-P-137	Allosite Dynamics of SAMHD1 probed by molecular dynamics simulations.
Susmita Ghosh	CBIO-P-139	Dynamics of Deca-alanine under extension.
Suresh Babu Vepuri	CBIO-P-490	Quantum Mechanics and Molecular Dynamics study to comprehend the Hydrogen bond Structure - Activity Relationship in Dipyridamole Supramolecule

<b>Computational Physics Education:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Youngim Jung	CPHE-P-337	Research Impact and Trend of Computational Physics in

		South Korea
Mandeep Singh	CPHE-P-430	A study on modeling and simulation of Multiple-Gate MOSFETs

### Fluid Dynamics, Oceanography, Geophysics and Climate modelling:

Presenter	Abstract	Poster Title
Chitrarth Prasad	FDCM-P-58	Comparative Study of a Higher Order Compact Scheme for Hyperbolic Equations
Amit Soni	FDCM-P-461	Numerical investigations on flow past flapping wings
Arpan Das	FDCM-P-466	Three-dimensional numerical investigations on dynamic stall of a pitching wing
Chandan Bose	FDCM-P-472	Parametric study of limit-cycle oscillations in a nonlinear fluid structure interaction system
Neeraj Paul M	FDCM-P-479	Three-dimensional computations on wake and dynamic characteristics of flow past sphere rotating about transverse axis

### High Energy, Nuclear and Particle physics:

Presenter	Abstract	Poster Title
Abhik Jash	HENP-P-54	Effect of surface roughness on the electrostatic field of an RPC
Madan Singh	HENP-P-445	Implication of $\theta_{13}$ on Majorana Neutrino mass matrices with One Texture Zero and One Vanishing Eigenvalue

### Material and Nano Sciences:

Presenter	Abstract	Poster Title
Sandip P Choudhury	MNSC-P-313	Humidity Sensing By Pure And Ni-Doped SnO <sub>2</sub> Thin Film Using Impedance Analysis
Jutika Devi	MNSC-P-344	Modeling of absorption and scattering properties of core-shell nanoparticles for application as nanoantenna in optical domain
S S Chabungbam	MNSC-P-382	Effect of disorders in the martensitic transformation temperature and exchange parameters in Ni-Fe-Ga alloy
Ujjal Saikia	MNSC-P-383	To study the structural stability and effect of Spin Orbit Coupling on Cu-Nb layered nanocomposite
Shikha Awasthi	MNSC-P-386	Synthesis, Characterization, and Mechanical Properties of Pulsed Electrodeposited Nickel Nanocomposite Reinforced with Diamond, Carbon Nanotubes, and Graphene
Parijat Borgohain	MNSC-P-387	First Principles investigation of electronic and magnetic properties in Ni-Co-Mn-In Heusler alloy
Omkar Tripathy	MNSC-P-419	Molecular Dynamics Investigation of Sr doped LaMnO <sub>3</sub>
Rit Pratik Mishra	MNSC-P-422	Adsorption and separation of CO <sub>2</sub> , CO, CH <sub>4</sub> , N <sub>2</sub> and their mixtures in zeolitic imidazolate frameworks: A molecular

		simulation study
Sushanta Bordoloi	MNSC-P-429	A Review on Issues in Device Modeling at Liquid Nitrogen Temperature
Ashok Kumar Ray	MNSC-P-436	Silicon Carbide: An emerging material for High Power Device Applications
Paresh Chandra Rout	MNSC-P-469	Origin of lowered magnetic moments in epitaxially strained thin films of multiferroic Bi <sub>2</sub> FeCrO <sub>6</sub>
Manash K Sharma	MNSC-P-242	Modelling in magnetron sputtering by particle in cell method

### **Quantum Many Body and Strongly Correlated Systems:**

<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Sudin Ganguly	QMBS-P-33	Spin dependent disorder in a junction device with spin orbit couplings
Priyadarshini Kapri	QMBS-P-424	Tunneling conductance through normal metal-superconductor junctions : effects of Rashba spin orbit coupling and magnetic field
Sandeep Chettri	QMBS-P-452	Doping effects on thermoelectric properties of Sm <sub>1-x</sub> Gd <sub>x</sub> AlO <sub>3</sub> , a first principles study

### **Software and Hardware Development:**

<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Gunajit Kalita	SHWD-P-67	Designing reversible arithmetic, logic circuits to implement micro-operations in quantum computation
S Bhattacharyya	SHWD-P-484	Design and Simulation of a Digital Lock-in Amplifier

### **Soft Matters, Polymers Physics:**

<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
Faria Rehman	SMPB-P-42	Effect of eigenvalue solution on characteristics of double diffusive salt fingers
Gurmeet Singh	SMPB-P-279	Electrostatics Insights for Aggregation of Small Linear Molecules: An ab initio study
Sudipta Kumar Bera	SMPB-P-327	Theoretical and experimental studies of time domain analysis of free and confined Brownian motion
D Bhattacharjee	SMPB-P-338	Optical, electrical and conductivity study of 7.05O.7 Dimeric Liquid Crystal Compound
P Radhakrishnan	SMPB-P-342	An Analysis Of Miscibility Studies Of Polyethylene Glycol with Polystyrene In Toluene
Dipak Kumar Sahoo	SMPB-P-418	Green Ionic Liquids for Toxic SO <sub>2</sub> Capture: in silico Screening of Cholinium-based Ionic Liquids with Pharmaceutically Active Anions
Marpliephar Lyndem	SMPB-P-481	Birefringence and temperature-gradient refractive index study of a laterally Fluorinated Terphenyl LC compound

<b>Statistical Physics, Complex System and Nonlinear Dynamics:</b>		
<b>Presenter</b>	<b>Abstract</b>	<b>Poster Title</b>
S Chattopadhyay	SPCS-P-13	Study of Dynamic Phase Transition in Diluted Magnetic System: Hysteresis Loop Analysis
Himangsu Bhaumik	SPCS-P-366	Study of stochastic dissipative sandpile on small world networks
Subhadeep Roy	SPCS-P-369	Numerical Modeling for Nucleation vs Percolation Criterion in Disordered Materials
Chandra Jeet Yadav	SPCS-P-371	Springback Analysis of I - sectioned bar of Linear Work-Hardening Materials under Torsional Loading
Sumanta Kundu	SPCS-P-510	Network topology of the desert rose
Chandreyee Roy	SPCS-P-511	Fiber bundle model with highly disordered breaking thresholds

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