

XXVII IUPAP Conference on Computational Physics (CCP 2015)

Journal of Physics: Conference Series Volume 759

Guwahati, India
2 – 5 December 2015

Editors:

**Sitangshu Bikas Santra
Purusattam Ray**

ISBN: 978-1-5108-3226-8
ISSN: 1742-6588

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2015) by the Institute of Physics
All rights reserved. The material featured in this book is subject to
IOP copyright protection, unless otherwise indicated.

Printed by Curran Associates, Inc. (2016)

For permission requests, please contact the Institute of Physics
at the address below.

Institute of Physics
Dirac House, Temple Back
Bristol BS1 6BE UK

Phone: 44 1 17 929 7481
Fax: 44 1 17 920 0979

techtracking@iop.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

Table of contents

Volume 759

**XXVII IUPAP Conference on Computational Physics (CCP2015)
2–5 December 2015, Guwahati, India**

**Accepted papers received: 22 September 2016
Published online: 11 November 2016**

Preface

011001

OPEN ACCESS

[XXVII IUPAP Conference on Computational Physics \(CCP2015\)](#)

Sitangshu Bikas Santra and Purusattam Ray

011002

OPEN ACCESS

[Peer review statement](#)

Papers

Plenary Talks

012001

OPEN ACCESS

[Liquid Fluidized Beds of Granular Particles](#)

Andrea Fiege and Annette Zippelius.....1

012002

OPEN ACCESS

[How Novel Algorithms and Access to High Performance Computing Platforms are Enabling Scientific Progress in Atomic and Molecular Physics](#)

Barry I. Schneider.....10

012003

OPEN ACCESS

[Energy fluxes in turbulent separated flows](#)

J.-P. Mollicone, F. Battista, P. Gualtieri and C.M. Casciola.....21

012004

OPEN ACCESS

[Modeling of neutron-star mergers: a review while awaiting gravitational-wave detection](#)

Luca Baiotti.....29

012005

OPEN ACCESS

[Undergraduate computational physics education: uneven history and promising future](#)

Richard F Martin.....37

012006

OPEN ACCESS

[Seismic interferometry and ambient noise tomography: theoretical background and application in south India](#)

Ritima Das and S S Rai.....47

012007

OPEN ACCESS

[Lattice field theory applications in high energy physics](#)

Steven Gottlieb.....54

Statistical Physics, Complex system and Non-linear Dynamics

012008

OPEN ACCESS

[An Overview on Short and Long Time Relaxations in Glass-forming Supercooled Liquids](#)

Smarajit Karmakar.....62

012009

OPEN ACCESS

[Numerical test of finite-size scaling predictions for the droplet condensation-evaporation transition](#)

Andreas Nußbaumer, Johannes Zierenberg, Elmar Bittner and Wolfhard Janke.....70

012010

OPEN ACCESS

[Kinetics of Order-Disorder Transitions in Binary Mixtures: A Monte Carlo Study](#)

Prasenjit Das, Tanusri Saha-Dasgupta and Sanjay Puri.....78

012011

OPEN ACCESS

[Disorder induced hysteresis in diluted kinetic Ising model](#)

Sourav Chattopadhyay and S B Santra.....84

012012

OPEN ACCESS

[Search for the Heisenberg spin glass on rewired cubic lattices with antiferromagnetic interaction](#)

Tasrief Surungan.....90

Soft materials and Polymer Physics

012013

OPEN ACCESS

[The impact of bonded interactions on the ground-state geometries of a small flexible polymer](#)

Tomas Koci, Kai Qi and Michael Bachmann.....96

012014

OPEN ACCESS

[How does the tail length and the separation between the tagged monomers influence the reconfiguration of a chain with internal friction for different solvent-quality?](#)

Nairhita Samanta and Rajarshi Chakrabarti.....103

012015

OPEN ACCESS

[Collapse transition of short polymers on simple cubic lattice](#)

Asweel Ahmed A Jaleel and S. V. M. Satyanarayana.....110

012016

OPEN ACCESS

[Birefringence and temperature-gradient refractive index study of a laterally Fluorinated Terphenyl LC compound.](#)

M. Lyndem, D. Bhattacharjee, R. Dabrowski and A. Bhattacharjee.....115

012017

OPEN ACCESS

[Miscibility studies of Polyethylene Glycol with Polystyrene in Toluene by Various Physical and Advanced Techniques](#)

R Padmanaban and K Venkatramanan.....121

012018

OPEN ACCESS

[Heterogeneous dynamics in linear polymer melts near glass transition temperature](#)

Jalim Singh and Prasanth P. Jose.....127

012019

OPEN ACCESS

[Microscopic structure and dynamics of glass like domains in a low density binary mixture](#)

Anna Varughese and Prasanth P. Jose.....133

Computational Biological Physics

012020

OPEN ACCESS

[Energetics of dendrimer binding to HIV-1 gp120-CD4 complex and mechanistic aspects of its role as an entry-inhibitor](#)

Suman Saurabh, Anil Kumar Sahoo and Prabal K. Maiti.....139

012021

OPEN ACCESS

[When the clock strikes: Modeling the relation between circadian rhythms and cardiac arrhythmias](#)

Pavithraa Seenivasan, Shakti N. Menon, S. Sridhar and Sitabhra Sinha.....150

012022

OPEN ACCESS

[Temperature dependent conformation studies of Calmodulin Protein using Molecular Dynamics](#)

Sahil Aneja, Vivek Kumar Bhartiya and Sunita Negi.....158

012023

OPEN ACCESS

[A Two-Layer Mathematical Modelling of Drug Delivery to Biological Tissues](#)

Koyel Chakravarty and D C Dalal.....166

012024

OPEN ACCESS

[Probing the energy landscape of alanine dipeptide and decalanine using temperature as a tunable parameter in molecular dynamics](#)

A Chatterjee and S Bhattacharya.....172

012025

OPEN ACCESS

[On the Origin of Photodynamic activity of Perylene Quinone Framework](#)

Dibyajyoti Parida, Pattath D. Pancharatna and Musiri M Balakrishnarajan.....178

012026

OPEN ACCESS

[Allosteric dynamics of SAMHD1 studied by molecular dynamics simulations](#)

K K Patra, A Bhattacharya and S Bhattacharya.....184

012027

OPEN ACCESS

[A Possible Explanation of Oriented Bar Filling-in at the Blind- Spot in the light of Hierarchical Prediction Mechanism](#)

R Raman and S Sarkar.....190

Quantum many body and strongly correlated systems

012028

OPEN ACCESS

[Spin dependent disorder in a junction device with spin orbit couplings](#)

Sudin Ganguly and Saurabh Basu.....196

012029

OPEN ACCESS

[First principles study on structural, phase transition and electronic structure of Zinc Sulfide \(ZnS\) within LDA, GGA and mBJ potential](#)

Kh. Kabita and B. Indrajit Sharma.....202

012030

OPEN ACCESS

[Thermally assisted tunneling of charge carriers between trapping sites in calcite \(CaCO₃\) mineral](#)

J.M. Kalita and G. Wary.....208

012031

OPEN ACCESS

[Tunneling conductance through normal metal - superconductor junctions: effects of Rashba spin orbit coupling and magnetic field](#)

Priyadarshini Kapri, Sudin Ganguly and Saurabh Basu.....214

012032

OPEN ACCESS

[Effect of Strong Orbital Magnetic Field on the Exciton Condensation in an Extended Falicov Kimball Model](#)

S Pradhan and A Taraphder.....220

012033

OPEN ACCESS

[Study of 4f electron based compound \$\text{Sm}_{1-x}\text{Gd}_x\text{AlO}_3\$, a thermoelectric \(TE\) material: FP-LAPW method](#)

Sandeep, D P Rai, A Shankar, M P Ghimire and R K Thapa.....225

012034

OPEN ACCESS

[Three body interaction effects on the phase diagram of spinor bosons](#)

Sk Noor Nabi and Saurabh Basu.....229

012035

OPEN ACCESS

[Disorder, three body interaction and Bose glass phase in a spinor atomic gas in an optical lattice](#)

Sk Noor Nabi and Saurabh Basu.....235

012036

OPEN ACCESS

[Condensate characteristics of bosons in a tilted optical lattice](#)

Sunayana Dutta and Saurabh Basu.....241

012037

OPEN ACCESS

[A DMFT+CTQMC Investigation of Strange Metallicity in Local Quantum Critical Scenario](#)

Swagata Acharya, M. S. Laad and A. Taraphder.....247

Material and Nano Sciences

012038

OPEN ACCESS

[Electronic properties of aluminium and silicon doped \(2, 2\) graphyne nanotube](#)

Jyotirmoy Deb, Barnali Bhattacharya and Utpal Sarkar.....253

012039

OPEN ACCESS

[Modeling of absorption and scattering properties of core-shell nanoparticles for application as nanoantenna in optical domain](#)

Jutika Devi, Rashmi Saikia and Pranayee Datta.....259

012040

OPEN ACCESS

[First principles calculation of thermoelectric parameters of Monolayer- and Bilayer- Graphene and Heterostructures of Graphene and *h*-BN](#)

Ransell D'Souza and Sugata Mukherjee.....265

012041

OPEN ACCESS

[Capturing local atomic environment dependence of activation barriers in metals using cluster expansion models](#)

Nimish Kulkarni and Abhijit Chatterjee.....273

012042

OPEN ACCESS

[A hybrid density functional study of silicon and phosphorus doped hexagonal boron nitride monolayer](#)

R E Mapasha, E Igumbor and N Chetty.....279

012043

OPEN ACCESS

[Modelling of Palladium Gold alloy- dielectric stratified loaded plasmonic waveguide for hydrogen detection at room temperature](#)

Sanchali Mitra, Rik Chattopadhyay and Shyamal Kumar Bhadra.....285

012044

OPEN ACCESS

[Magnetic Metamaterials: A comparative study of resonator geometry and metal conductivity](#)

Shashank Rangu, Kamireddy Sreekar, Ravinithesh Reddy Annapureddy, Kausik Basak, Murtaza Bohra and Dibakar Roy Chowdhury.....291

012045

OPEN ACCESS

[Computational Study of Au_mSi_n \(m+n=2-6\) Nanoalloy Clusters Invoking Density Functional Based Descriptors](#)

P. Ranjan, A. Kumar and T. Chakraborty.....297

012046

OPEN ACCESS

[Study of lattice dynamics of Fe₂SiO₄- and Mg₂SiO₄-spinel](#)

M M Sinha and Harleen Kaur.....303

012047

OPEN ACCESS

[A three-dimensional fully coupled thermo-mechanical model for Self-reacting Friction Stir Welding of Aluminium AA6061 sheets](#)

Piyush Singh, Pankaj Biswas and Sachin D. Kore.....307

012048

OPEN ACCESS

[Young's modulus of defective graphene sheet from intrinsic thermal vibrations](#)

Siby Thomas, M S Mrudul, K M Ajith and M C Valsakumar.....313

Atomic, Molecular and Optical Physics

012049

OPEN ACCESS

[Numerical analysis of terahertz surface plasmon polaritons propagating in a parallel plate configuration](#)

Sukhdeep Kaur, Sarabjeet Kaur, Manpreet Kaur and Gagan Kumar.....318

012050

OPEN ACCESS

[Ab - initio non-adiabatic couplings among three lowest singlet states of \$H_3^+\$: Construction of multisheeted diabatic potential energy surfaces](#)

Bijit Mukherjee, Saikat Mukherjee and Satrajit Adhikari.....325

012051

OPEN ACCESS

[Effect of oxide barrier height in spin dependent tunneling in MTJ of FeO-MgO multilayer structure](#)

M Bhattacharjee, H Nemade and D Bandyopadhyay.....333

012052

OPEN ACCESS

[Enhanced terahertz transmission through a periodic array of tapered rectangular apertures](#)

Koijam Monika Devi, Amarendra K. Sarma and Gagan Kumar.....338

012053

OPEN ACCESS

[Terahertz surface plasmon polaritons propagation in slanted pillar geometries](#)

Maidul Islam and Gagan Kumar.....344

012054

OPEN ACCESS

[Few-body model approach to the bound states of helium-like exotic three-body systems](#)

Md A Khan.....350

012055

OPEN ACCESS

[Finite element modelling and analysis of the effect of frequency on the electromagnetic compression of tubes](#)

Ramesh Kumar and Sachin D Kore.....358

012056

OPEN ACCESS

[Efficient shortcut techniques in evanescently coupled waveguides](#)

Koushik Paul and Amarendra K. Sarma.....364

012057

OPEN ACCESS

[Experimental and theoretical study of 3-methyl-4- nitrobenzoic acid using DFT and IVP methods](#)

J Prashanth, Jai Kishan Ojha, B Venkatram Reddy and G Ramana Rao.....370

012058

OPEN ACCESS

[Non-adiabatic effects in the \$\tilde{A}^2B_2\$ and B2A1 states of \$CH_2F_2^+\$ through coupling vibrational modes](#)

Rudraditya Sarkar.....378

012059

OPEN ACCESS

[Atom assisted cavity cooling of a micromechanical oscillator in the unresolved sideband regime](#)

Bijita Sarma and Amarendra K Sarma.....384

Astrophysics, Plasma, Gravitation and Cosmology

012060

OPEN ACCESS

[Black Hole Paradoxes](#)

Pankaj S. Joshi and Ramesh Narayan.....389

012061

OPEN ACCESS

[Strongly correlated classical plasmas under external forcing and dissipation - an example using Molecular Dynamics](#)

Harish Charan and Rajaraman Ganesh.....397

012062

OPEN ACCESS

[Bayesian Cosmological inference beyond statistical isotropy](#)

Tarun Souradeep, Santanu Das and Benjamin Wandelt.....403

012063

OPEN ACCESS

[Solar Transients Disturbing the Mid Latitude Ionosphere during the High Solar Activity](#)

Shivangi Bhardwaj, Parvaiz A Khan, Roshni Atulkar, Bhupendra Malvi, Azad Ahmad Mansoori and P K Purohit.....411

012064

OPEN ACCESS

[Effect of non zero cosmological constant on the motion of light ray](#)

Sarani Chakraborty and A. K. Sen.....417

012065

OPEN ACCESS

[Frame-dragging from charged rotating body](#)

Anuj Kumar Dubey and A. K. Sen.....421

012066

OPEN ACCESS

[Hybrid computer modelling in plasma physics](#)

J Hromadka, T Ibehej and R Hrach.....427

012067

OPEN ACCESS

[Morphological Investigation of Disturbed Ionosphere during Intense Geomagnetic Storms](#)

Bhupendra Malvi, Prateek S. Srivastav, Azad A. Mansoori, Roshni Atulkar, Shivangi Bhardwaj and P. K. Purohit.....432

012068

OPEN ACCESS

[Study of trapped particle nonlinearity in Ion Acoustic solitary wave using Vlasov simulation](#)

Debraj Mandal and Devendra Sharma.....438

012069

OPEN ACCESS

[Evaluation of long term solar activity effects on GPS derived TEC](#)

Azad A Mansoori, Parvaiz A Khan, Rafi Ahmad, Roshni Atulkar, Aslam A M, Shivangi Bhardwaj, Bhupendra Malvi, P K Purohit and A K Gwal.....445

High energy, Nuclear and Particle Physics

012070

OPEN ACCESS

[Lattice QCD simulations using the OpenACC platform](#)

Pushan Majumdar.....451

012071

OPEN ACCESS

[Detailed 3D Simulation of the GEM-based detector](#)

P Bhattacharya, S Biswas, B Mohanty, N Majumdar and S Mukhopadhyay.....459

012072

OPEN ACCESS

[Effect of surface roughness on the electrostatic field of an RPC](#)

A Jash, N Majumdar, S Mukhopadhyay and S Chattopadhyay.....465

012073

OPEN ACCESS

[Exact solutions to model surface and volume charge distributions](#)

S Mukhopadhyay, N Majumdar, P Bhattacharya, A. Jash and D.S. Bhattacharya.....472

012074

OPEN ACCESS

[Simulation of \$\pi^0\$ - \$\gamma\$ Separation Study for Proposed CMS Forward Electromagnetic Calorimeter](#)

Ashim Roy, Shilpi Jain, Sunanda Banerjee, Satyaki Bhattacharya and Gobinda Majumder.....478

012075

OPEN ACCESS

[Track distortion in the Large prototype of a Time Projection Chamber for the International Linear Collider](#)

Deb Sankar Bhattacharya, Purba Bhattacharya, Supratik Mukhopadhyay, Nayana Majumdar, Sudeb Bhattacharya, Sandip Sarkar, Paul Colas, David Attie, Serguei Ganjour and Aparajita Bhattacharya.....485

012076

OPEN ACCESS

[Excited State Mass Spectra of \$\Omega_c^0\$ Baryon](#)

Z Shah, K Thakkar, A K Rai and P C Vinodkumar.....491

012077

OPEN ACCESS

[Implication of \$\theta_{13}\$ on Majorana Neutrino mass matrices with One Texture Zero and One Vanishing Eigenvalue](#)

Madan Singh, Radha Raman Gautam and Manmohan Gupta.....497

012078

OPEN ACCESS

[Multi-scale Modeling of Radiation Damage: Large Scale Data Analysis](#)

M Warriar, U Bhardwaj and S Bukkuru.....503

Fluid Dynamics, Oceanography, Geophysics and Climate modeling

012079

OPEN ACCESS

[Non-equilibrium Thermodynamics of Rayleigh-Taylor instability](#)

Tapan K Sengupta, Aditi Sengupta, K S Shruti, Soumyo Sengupta and Ashish Bhole.....509

012080

OPEN ACCESS

[Influence of nonlinear chemical reactions on the transport coefficients in oscillatory Couette flow](#)

Swarup Barik and D. C. Dalal.....518

012081

OPEN ACCESS

[Moffatt vortices in the lid-driven cavity flow](#)

Sougata Biswas and Jiten C. Kalita.....524

012082

OPEN ACCESS

[Flexible flapping wings can exhibit quasi-periodic motion!](#)

Chandan Bose and Sunetra Sarkar.....531

012083

OPEN ACCESS

[Computational Study of Fluid Flow Characteristics past Circular Cylinder due to Confining Walls with Local Waviness](#)

R Deepakkumar, S Jayavel and Shaligram Tiwari.....538

012084

OPEN ACCESS

[Effect of Rayleigh Number and Density Stability Ratio on characteristics of Double-Diffusive Salt Fingers](#)

Manoj Dhiman, Faria Rehman and O.P Singh.....544

012085

OPEN ACCESS

[Gap Filling of Precipitation Data by SSA - Singular Spectrum Analysis](#)

A S F Filho and G A R Lima.....550

012086

OPEN ACCESS

[An accurate predictor-corrector HOC solver for the two dimensional Riemann problem of gas dynamics](#)

Bidyut B. Gogoi.....556

012087

OPEN ACCESS

[Computational studies on small wind turbine performance characteristics](#)

N Karthikeyan and T Suthakar.....562

012088

OPEN ACCESS

[Laminar convective heat transfer characteristic of Al₂O₃/water nanofluid in a circular microchannel](#)

K Trinavee, T K Gogoi and M Pandey.....568

Computational Physics Education

012089

OPEN ACCESS

[Open Source Computing in Physics Education](#)

Ananda Dasgupta.....576

012090

OPEN ACCESS

[Non-Boltzmann Ensembles and Monte Carlo Simulations](#)

K. P. N. Murthy.....580

012091

OPEN ACCESS

[Research Activity in Computational Physics utilizing High Performance Computing: Co-authorship Network Analysis](#)

Sul-Ah Ahn and Youngim Jung.....588

012092

OPEN ACCESS

[Identifying Interstitials in MD Simulations — Max Space Clustering Method](#)

S Bukkuru, U Bhardwaj, ADP Rao and M Warriar.....594

012093

OPEN ACCESS

[A study on modeling and simulation of Multiple- Gate MOSFETs](#)

Mandeep Singh, Gaurav Kumar, Sushanta Bordoloi and Gaurav Trivedi.....600

Software and Hardware development

012094

OPEN ACCESS

[Extensible, Reusable, and Reproducible Computing: A Case Study of PySPH](#)

Prabhu Ramachandran.....606

012095

OPEN ACCESS

[Exascale Storage Systems the SIRIUS Way](#)

S A Klasky, H Abbasi, M Ainsworth, J Choi, M Curry, T Kurc, Q Liu, J Lofstead, C Maltzahn, M Parashar, N Podhorszki, E Suchyta, F Wang, M Wolf, C S Chang, M Churchill and S Ethier.....613

012096

OPEN ACCESS

[Implementation of Digital Lock-in Amplifier](#)

Sabyasachi Bhattacharyya, Ragib Nasir Ahmed, Basab Bijoy Purkayastha and Kaustubh Bhattacharyya.....621

012097

OPEN ACCESS

[Designing reversible arithmetic, logic circuit to implement micro-operation in quantum computation](#)

Gunajit Kalita and Navajit Saikia.....629

012098

OPEN ACCESS

[A Framework to Simulate Semiconductor Devices Using Parallel Computer Architecture](#)

Gaurav Kumar, Mandeep Singh, Anand Bulusu and Gaurav Trivedi.....634

012099

OPEN ACCESS

[Two Dimensional Numerical Simulator for Modeling NDC Region in SNDC Devices](#)

Dheeraj Kumar Sinha, Amitabh Chatterjee and Gaurav Trivedi.....640

012100

OPEN ACCESS

[High performance FDTD algorithm for GPGPU supercomputers](#)

Andrey Zakirov, Vadim Levchenko, Anastasia Perepelkina and Yasunari Zempo.....646