# **CCP2016**

# **Monday 11 July 2016**

#### Parallel Track B: Computational Biological Physics, Soft Matter, Polymer (11:00-13:00)

#### -Conveners: Shobhana Narasimhan; Irvy (Igle) Gledhill

time	[id] title	presenter
11:00	[22] Dynamic Modelling on the Crystallization of Mono-sized Cubical Particles under Mechanical Vibrations	Prof. AN, Xizhong
11:20	[39] Dynamical Properties of Granular Materials	Prof. PURI, Sanjay
11:40	[93] Electric field effects on the ionization cluster size distribution (ICSD) using the GEANT4 Monte Carlo toolkit.	Mr NGCEZU, Sonwabile
12:00	[94] Finding motifs in DNA and protein sequences using set match	Mr CHIRWA, Robert
12:20	[6] Protein dynamics as a function of ionic strength, calcium ion concentration and temperature: Calmodulin as a first step	Mr ANEJA, Sahil
12:40	[95] Understanding the role of the subtstrate in off-lattice simulations of graphene growth on copper	Mr ENSTONE, Gwilym

#### Parallel Track B: Computational Biological Physics, Soft Matter, Polymer (14:00-14:20)

#### -Conveners: Shobhana Narasimhan; Irvy (Igle) Gledhill

time [id] title	presenter
14:00 [109] Networks of Spiking Neurons for the Control of Movement	Prof. SOLLA, Sara A.

#### Parallel Track B: Computational Physics Education Session (14:20-16:15)

### -Conveners: Barry Klein; Spencer Wheaton

time	[id] title	presenter
14:20	[42] INVITED SPEAKER: Paradigms for Electronic Structure Codes	Dr SALAGARAM, Trisha
14:50	[40] Visualizing higher order Brillouin zones with applications	Dr ANDREW, Richard
15:10	[117] Learning problem-solving skills in a distance education physics course	Prof. RAMPHO, Gaotsiwe Joel
15:30	[41] GPUs in a Computational Physics course	Dr ADLER, Joan
	[5] Coding considerations for standalone molecular dynamics simulations of atomistic structures	OCAYA, Richard

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# Tuesday 12 July 2016

#### Parallel Track B: High Enegy, Nuclear and Particle Physics (09:30-10:40)

#### -Conveners: Marius Potgieter

time [id] title		presenter
09:30 [125] INVITED SPEAKER: Thomas Di ALICE Experiment at the LHC	ietel (University of Cape Town) for the	Dr DIETEL, Thomas
10:00 [64] Monte Carlo Computation of the E	Effective Sherman Function	Mr DRAGOWSKI, Michal
10:20 [11] 2-Secure and certify studies to wo	ork on production of Spiked plutonium.	Prof. MOHAMED SALEH, Ashraf Elsayed

#### Parallel Track B: High Enegy, Nuclear and Particle physics (11:00-13:00)

#### -Conveners: Thomas Dietel

time	[id] title	presenter
11:00	[118] Study of Effective atomic numbers of Bioactive Glasses for Photon Interaction	Dr MALIPATIL, Anil Shantappa
	[85] A fast - Monte Carlo toolkit on GPU for treatment plan dose recalculation in proton therapy	SENZACQUA, Martina
11:40	[71] On formation of bubble structure near the island of inversion	Prof. BHATTACHARYA, Rupayan
12:00	[90] Bound states and decays in Relativistic Quantum Mechanics.	GIACHETTI, Riccardo
12:20	[70] Finite element model of a calibration chamber	Dr ORJUBIN, Gérard
12:40	[58] A study on Quark-Gluon plasma equation of state using with finite quark mass	Dr KUMAR, Yogesh

#### Parallel Track B: Material and Nano Science, Quantum Many Body and Strongly Correlated Systems (14:00-16:20)

#### -Conveners: Happy Sithole

time	[id] title	presenter
	[24] Temperature specification in atomistic molecular dynamics and its impact on simulation efficacy	OCAYA, Richard
14:20	[101] Computational modelling of sulfides minerals	Dr LETSOALO, Thabo
	[15] ab initio studies of thermoelectric materials for energy conversion applications	Dr WAFULA, Henry
	[88] Computational Studies of Ru and Sr-doped anatase TiO <sub>2</sub> on three low index surfaces for application on DSSCs	Mr NEMUDZIVHADI, Hulisani
15:20	[106] Stability and magnetic interaction of embedded Fe clusters in diamond	Dr BENECHA, Evans
15:40	[86] Solar cell performance of AgInS <sub>2</sub> materials from DFT and GW/BSE calculations	Dr DONGHO NGUIMDO, G.M.
16:00	[98] Molecular dynamics studies of Schottky and Frenkel defects in cubic boron nitride	Dr MOSUANG, Thuto

#### Parallel Track B: Atomic Molecular and Optical Physics (15:40-16:20)

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## -Conveners: Martin Weigel

time [id] title	presenter
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[73] Computational study of nonlinear spectroscopy including saturated absorption and four wave mixing in two and multi-level atoms	Dr GOVENDER, Kessie Ms PATEL, Meena
[75] Improved Maximum Entropy Method applied to Real-time Time-Dependent Density Functional Theory	Mr TOOGOSHI, Mitsuki

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# Wednesday 13 July 2016

#### Parallel Track B: Material and Nano Science, Quantum Many Body and Strongly Correlated Systems (10:15-13:00)

#### -Conveners: Thomas Vojta

time	[id] title	presenter
10:15	[47] INVITED SPEAKER: From 2D to 3D and 1D: Manipulating charge and spin at oxide heterointerfaces	Dr COOPER, Valentino
10:45	[38] INVITED SPEAKER: Why and how to calculate momentum dependent self-energy for strongly correlated materials	Dr DAS, Tanmoy
11:15	[54] Device Simulation using Symmetric Smoothed Particle Hydrodynamics	Prof. ZEMPO, Yasunari
11:35	[13] Progress toward the discovery of a room-temperature superconductor: theoretical studies of the observed superconductivity above 200K in the sulfur hydride system at high pressure	Prof. KLEIN, Barry
11:55	[96] Structural determination and electronic properties of one-dimensional Te crystals encapsulated inside carbon nanotubes	Dr MEDEIROS, Paulo V C
12:15	[128] Computational study of dye adsorption in nano TIO <sub>2</sub> film for the applications in dye sensitized solar cells using different computational techniques	Dr MALUTA, Nnditshedzeni Eric
12:35	[74] Effect of Mo alloying elements on Ni silicides formation	Dr DERAFA, Achour

#### Parallel Track B: Material and Nano Science, Quantum Many Body and Strongly Correlated Systems (14:00-16:00)

## -Conveners: Valentino Cooper

time	[id] title	presenter
14:00	[122] INVITED SPEAKER: Impacts of interlayer and substrate interactions on low dimensional crystals	Prof. SON, Young-Woo
14:30	[131] INVITED SPEAKER: Quantum critical behavior of a superfluid-insulator transition	Prof. VOJTA, Thomas
15:00	[105] Investigation of Two-dimensional lattice thermal transport in graphene using phonon scattering mechanism	Prof. CHOUDHARY, Kamal Kumar
15:20	[56] Confining Boundary Conditions For Simulation of Electron-Ion Plasma by Antisymmetrized Wave Packet Molecular Dynamics	Dr VALUEV, Ilya
15:40	[52] First principles study of layered xLi <sub>2</sub> MnO <sub>3</sub> •(1-x)LiMO <sub>2</sub> (M = Mn, Ni, Co, etc.) cathode materials	Dr KEBEDE, Mesfin Abayneh Mr GELETO, Seid Mohammed

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# **Thursday 14 July 2016**

#### Parallel Track B: Software and Hardware Development (09:00-10:10)

-Conveners: Mitsuhisa Sato

time [id] title	presenter
09:00 [51] MORTICIA, A software package for determining optical surveillance system effectiveness.	Mr RAMKILOWAN, Ari
09:20 [72] High Performance Memory Efficient Finite Difference Time Domain Algorithms for Large Meshes	Dr VALUEV, Ilya
09:40 [97] Particle simulations on the GPU using the Blaze-DEM code	Dr GOVENDER, Nicolin

## Parallel Track B: Software and Hardware Development (10:30-11:30)

-Conveners: Ilya Valuev

time	[id] title	presenter
10:30	[130] INVITED SPEAKER: Challenges for Parallel Programming Models and Languages of post-petascale and exascale computing	Prof. SATO, Mitsuhisa
11:00	[132] INVITED SPEAKER: High Performance Computing Developments in South Africa and the Continent in support of increasing demands of Research	Dr SITHOLE, Happy