SAIP2022 / Programme Monday 04 July 2022

### **SAIP2022**

# Monday 04 July 2022

### Physics of Condensed Matter and Materials - Zoom Platform (11:30-13:00)

#### -Conveners: Rudolph Erasmus

| time  | [id] title  | presenter                     |
|-------|---|-------------------------------|
|       | [287] Lattice expansion studies of the crystal structure transformation in intermediate valent \$\rm{Ce_2Rh_2Ga}\$            | XHAKAZA, sindisiwe            |
|       | [311] Property and structural characterisation of Fe and Ni bonded NbC cermets for improved tribological applications         | PETERS, Gerrard               |
|       | [117] Thermal stability of diketopyrrolopyrrole-based terpolymers with tunable broad band absorption for polymer solar cells. | Mr NCHINDA, Leonato<br>Tambua |
|       | [106] Synthesis and modification of Boron Nitride nanotubes using ion implantation  | Mr LISEMA, Lehlohonolo        |
| 12:30 | [118] Highly methane responsive nanosensor layer based on mesoporous nanostructured belts-like Indium Oxide                   | KGOMO, Mosima                 |
|       | [278] Electrochemical Synthesis and Characterization of PANI/Graphene-foam<br>Composite Films                                 | Mr CHILUKUSHA, Daniel         |

### Physics of Condensed Matter and Materials - Zoom Platform (15:00-16:30)

#### -Conveners: Cliffton Masedi

| time  | [id] title   | presenter                |
|-------|--|--------------------------|
|       | [123] Phase Stability of Li2Mn1-xTMxO3 (TM= Ni, Co, Cr and Ru) Cathode<br>Material Using Cluster Expansion and Monte Carlo Simulations             | MPHAHLELE,<br>Mamonamane |
|       | [174] DEVELOPMENT OF MACHINE LEARNING MODELS FOR PREDICTING ENERGIES OF SODIUM-ION BATTERY MATERIALS   | Ms MONARENG, Keletso     |
|       | [220] The phase stability, mechanical and electronic properties of CsCl-type intermetallic: TiTM (TM = Ni, Ru and Pd), a first-principles approach | NGOBE, Bongani           |
| 15:45 | [262] Effect of Mn addition on the ductility of FeCo soft magnetic alloy   | LEDWABA, Tebogo          |
|       | [171] Ab initio and Cluster Expansion study on Magnesium Spinel (MgX2Z4: where X=Sc, Y and In; Z=S and Se)   | TIBANE, KHUMBULANI       |
|       | [252] The effects carbon and boron on the T-MnAl alloy properties employing the first principle approach.  | SEBE, ITUMELENG          |

SAIP2022 / Programme Tuesday 05 July 2022

# Tuesday 05 July 2022

#### Physics of Condensed Matter and Materials - Zoom Platform (11:30-13:00)

#### -Conveners: Daniel Wamwangi

| time  | [id] title   | presenter                     |
|-------|--|-------------------------------|
| 11:30 | [34] Characterization of defects in Ar+ implanted ZnO semiconductor using positron annihilation technique.                               | Mr KHULU, Musawenkosi         |
| 11:45 | [177] Magnetocaloric effect in Dy based chromium oxides  | SIBANDA, Eugene               |
| 12:00 | [185] Effect of solvents on the extraction and absorption study of natural dye from Bidens pilosa for dye sensitized solar cells         | Mrs RANDELA, Ronel<br>Ronella |
| 12:15 | [277] Synthesis of copper nanowires for application as flexible transparent conducting electrodes  | Mr HOY, Nicholas              |
| 12:30 | [190] Preparation and characterization of porous ZnFe2O4 hollow fibers with enhanced sensing response and selective detection of acetone | NEMUFULWI, Murendeni          |
| 12:45 | [165] Impact of rapid thermal annealing on the properties of different Ag layer thicknesses Ag/ITO bilayer films                         | Mr OLLOTU, Emmanuel<br>Rasiel |

### Physics of Condensed Matter and Materials - Zoom Platform (15:00-16:30)

#### -Conveners: Ramogohlo Diale

| time  | [id] title  | presenter                                 |
|-------|---|---|
| 15:00 | [9] First-principles study on interaction of O2 with (100) surfaces of sperrylite and platarsite minerals                               | NEMUTUDI, Bradley<br>Mr NEMUTUDI, BRADLEY |
| 15:15 | [306] Study of inorganic lead halide perovskites properties using density functional theory for photovoltaic and optoelectronic devices | MALEKA, Prettier<br>Morongoa              |
| 15:30 | [213] Ground state phase stability simulation of Fe-X-Al alloys (X= Pd and Ag)  | Ms MKHONTO, Chrestinah                    |
|       | [275] Ab-initio study of hydrofluoric acid and ethylene carbonate adsorption on<br>the Nb-doped on the LiMn2O4 surfaces                 | Mr RAMOGAYANA, Brian                      |
| 16:00 | [238] Machine Learned Buckingham Interatomic Potentials for Co-doped<br>Li-Mn-O spinel.   | HLUNGWANI, DONALD                         |
| 16:15 | [250] Evaluating the small Ti7 cluster in α-TiCl3 medium  | Ms MAZIBUKO, Andile                       |

SAIP2022 / Programme Thursday 07 July 2022

# Thursday 07 July 2022

#### Physics of Condensed Matter and Materials - Zoom Platform (11:30-13:00)

#### -Conveners: BHARATI BAMANA

| time  | [id] title  | presenter  |
|-------|---|--|
|       | [168] Structural and magnetic properties of $ \label{eq:cos_x} Cos_{x}$Nis_{(1-x)}$Crs_{2}$Os_{4}$ (x = 0.75, 0.80, 0.85) nanoparticles $ | JACOB, Mariam  |
|       | [183] Structural and magnetic properties of Co\$_{(1-x)}\$ Cu\$_{x}\$ Cr\$_{2}<br>\$O\$_{4}\$ nanoparticles                               | Ms NAGARAJ, Shobana                                      |
|       | [196] Synthesis, Structural, and Magnetic Properties of CoCr\$_{2}\$O\$_{4}\$/Cu\$_{2}\$O nanocomposites.                                 | NKOSI, Thabang Johannes<br>Mr NKOSI, Thabang<br>Johannes |
| 12:15 | [46] TRANSITION METAL CARBONATE PRECURSORS AS CATHODE MATERIALS FOR LI-ION BATTERIES: COMPUTATIONAL AND EXPERIMENTAL STUDY                | Ms MORUKULADI,<br>Mogahabo                               |
| 12:30 | [259] Investigating sodium incorporated Li2MnO3 nanostructured cathodes for lithium-ion batteries   | Mrs MOGASHOA, Tshidi                                     |
| 12:45 | [302] SIMULATIONS SYNTHESIS OF Na0.23TiO2 NANOSPHERE AT VARIED TEMPERATURES: BEYOND LI-ION BATTERIES.                                     | Ms RIKHOTSO, Blessing                                    |

### Physics of Condensed Matter and Materials - Zoom Platform (15:00-16:30)

#### -Conveners: Rudolph Erasmus

| time  | [id] title  | presenter                              |
|-------|---|--|
|       | [130] Structural and optical properties of TiO2 photoelectrodes fabricated for photoelectrochemical water splitting | Dr SULIALI, Nyasha                     |
| 15:15 | [198] Structural and Magnetic Study of NdCrTiO\$_{5}\$ Nanoparticles  | BAMANA, BHARATI                        |
| 15:30 | [206] FIRST-PRINCIPLE STUDIES OF CUBIC TI2AIV AND TETRAGONAL<br>TIAI2V STRUCTURAL STABILITY                         | MODIBA, Rosinah                        |
|       | [229] Magnetic Phase Transitions in Ce\$^{3+}\$ Substituted CoCr\$_2\$O\$_4\$ Nanoparticles                         | MOHANTY, PANKAJ                        |
|       | [231] Impact of Cr substitution on magnetic properties of cobalt-doped ZnO nanoparticles                            | Dr HANDALAGERE<br>SHANKARAPPA, Lokesha |
| 16:15 | [135] Phase stability prediction of mixed Li2S1-xSex system   | MASEDI, Cliffton                       |

SAIP2022 / Programme Friday 08 July 2022

# **Friday 08 July 2022**

### <u>Physics of Condensed Matter and Materials</u> - Zoom Platform (11:30-13:00)

-Conveners: Thulani Jili

| time  | [id] title   | presenter                |
|-------|--|--------------------------|
| 11:30 | [55] Non-Specialist Lecture: Neutron scattering prospects at the new<br>Multi-Purpose Reactor  | KESHAW, Jeetesh          |
| 12:00 | [181] Thermal conductivity of Chalcogenides Alloys: Energy and information storage applications                                      | WAMWANGI, Daniel         |
| 12:15 | [79] Media Structured for Nonlinear Optics   | TAVARES BUONO,<br>Wagner |
| 12:30 | [317] TEM OBSERVATION of ROOM TEMPERATURE STABILITY AND PHASE TRANSFORMATION OF SHI INDUCED TETRAGONAL TRACKS IN MONOCLINIC ZIRCONIA | Prof. LEE, Michael       |
| 12:45 | [337] Machine Learning Structure-Property Model for Carbon Steels  | Dr WESTRAADT, Johan      |