SAIP2023 / Programme Tuesday 04 July 2023

## **SAIP2023**

## Tuesday 04 July 2023

Poster Session 1 (15:40-17:40)

[id] title	presenter	
[2] Graphene/TiO2 as electron transport layer to enhance energy efficiency of perovskite solar cells	Dr MALEVU, Thembinkosi	
[4] A mechanistic non-process dependent study of the prediction and optimization of mineral beneficiation and metal extraction.	Mr MVITA, META	
[9] A comparison study of some structural, vibrational, elastic and electron spin resonance properties of bulk- and nano-sized particles for ZnxCo1-xFe2-xAlxO4 ferrite samples	Mr MASUKU, Sizwe Jackson	
[13] Ball Milling synthesis and characterization of highly crystalline TiO2-ZnO hybrids for photovoltaic applications	MALEVUTD, Thembinkosi	
[26] Effect of Co on structural, stability and ductility of Fe5Ni4S8 (P4_2/nmc): Cluster expansion method	Dr MKHONTO, Peace Prince Prof. NGOEPE, Phuti E.	
[27] Effect of temperature on β-TiCl3 medium	Ms MAZIBUKO, Andile	
[36] THE CATALYTIC ACTIVITY OF MO <sub>2</sub> (M= Ti, V, Mn) ON (110) SURFACE OF Na-AIR BATTERY	NGOBENI, PERCY	
[38] Probing the Stability of Nickel Titanium Surfaces for Oxygen Adsorption: A DFT Study	CHAUKE, vukosi	
[40] The Minimal load potential of elastic membranes	MOHAMMADI, Seyyed Abbas	
[56] Binding nature of fibrin molecules on to Au92 and Ag92 nanoparticles	MAKGOBA, Malesela Walter	
[64] Computer simulation of Silver (Ag) and Nickel (Ni) Nanomaterials	MATSHABA, Malili	
[70] Effect of Gd3+ moles on the structure, morphology and luminescence properties of BaAl2O4:x% Gd3+ (0 $\le$ x $\le$ 1) nanomaterial prepared using a sol-gel method.	Dr MHLONGO, Rebecca	
[72] Reactive molecular dynamics simulations of the atomic oxygen impact on Poly(2,5-benzimidazole)	ELLIS, Ernst	
[76] Electronic, elastic and thermoelectric properties of hexagonal CuSe phase	MS RAMOSHABA, MOSHIBUDI	
[81] Structural Changes of LiXCo2O4 (1 $\leq$ x $\leq$ 2) Nanoporous Cathode Materials upon Lithiation	BEAUTY, Shibiri	
[92] Computational and Experimental Studies on Mn-rich LiMn1.5Ni0.5O2 Cathode Material	Mr KGOEDI, Moloko	
[100] Synthesis and CO gas sensing applications of two-dimensional hexagonal boron nitride nanosheets at different temperatures	Mr KEKANA, MAGOPA TSHEPHO MCDONALD	
[102] Development of \$TiO_{2}\$ nanotube arrays with a modified energy band gap for hydrogen evolution	MUTUBUKI, Arnold	

SAIP2023 / Programme Tuesday 04 July 2023

7.11.2020 / 1.108141111111	Tuesday 04 July 2
[110] Optimization of multi-walled carbon nanotubes for improved heat transfer	MASOLO, hlabane Beauty
[113] Confocal Raman and AFM Characterization of Mesoporous Titania Electrode Substrates for Perovskite Solar Cell Applications	Dr AHIA, Chinedu Christian
[114] Intrinsic defect interactions in a monolayer silicene: An ab-initio DFT study	MABOE, Paul
[122] Investigation of the fundamental interactions of the PtSb2 Surface with the MBTK molecule	Mr NDHLOVU, ivyn
[123] Thermal conductivity enhancement in gold decorated graphene nanosheets in ethylene glycol based nanofluid	Dr MBAMBO, Makhangele
[126] V2O5 nanostructures for gas sensing: doping, and low temperature detection of Methanol, Ethanol and NO2 with superior response of H2S	MOKWENA, Mick Molukie
[127] Cluster expansion calculations on the discharge product of magnesium-ion batteries	TIBANE, KHUMBULANI
[131] Investigation of the structural, elastic and vibrational stability of PtTe, PtTe2, Pt2Te3 and Pt3Te4 tellurides structures	MAAKA, TSHEPO
[156] First principle study of structural and thermodynamic stability of ternary NaVSe2	Dr TSHWANE, DAVID
[134] Phase stability of calcium manganese oxide (CaMn2O4) polymorphs cathode materials in calcium ion batteries.	Mr ROBERTS, OSWALD
[142] Incorporation of copper nanorods in organic solar cells	SEIMELA, Thapelo
[148] Effects of defects on gas sensor performance of β-Ga2O3	GATSI, Nyepudzai Charsline
[163] Structural, Electronic, Mechanical and Thermodynamic Properties of Ternary NaVS2: DFT Study	MOGAKANE, LETHABO
[165] First principles study of structural, elastic, electronic and optical properties of triclinic CsAlS2 chalcogenide.	Mr PHALE, Boitemogelo
[168] Optimization of deposition voltage for growth of CdZrS thin films for window layer of CdTe-based solar cell device application.	MOHAPI, TSHEPO KARABO WILLIAM
[186] Self-Consistent Charge Density-Functional Tight-Binding Parameterization for the Mg–Si system	Dr PHOSHOKO, Katlego
[226] 2D/3D heterojunction of MAPbI3/OA2PbI4 thin films for Photovoltaic Hydrogen Evolution	THUBANE, Sandile
[228] The structural, electronic and dynamical properties of pyrite-type minerals: DFT and Atomistic Simulations.	MEHLAPE, Mofuti
[232] High selective and sensitive acetone gas sensor: Effects of Cerium metal ion on pyramid-like In2O3 products	KGOMO, Mosima
[235] Electronic Stability and Surface Study of Tin Dioxide	MAENETJA, khomotso
[241] Investigating the effect of sodium partial substitution on nanostructured Li2MnO3 cathodes during the simulated charge process	Mrs MOGASHOA, Tshidi
[242] Improve physical properties of rare earth metal doped strontium sulphide for optoelectronic purpose	Mr SHAKA, Samuel
[252] Computational studies of optoelectronic properties of CH3NH3PbI3 as a photolayer in perovskite solar cell	RUGUT, Elkana
[276] Microstructure and strain dependence on growth time of hydrothermally synthesized nanocrystalline porous sodalite	KITEME, KYALO Ngesu
[279] STUDY OF THE IMMOBOLISATION OF PALLADIUM BY SILICON AND ZIRCONIUM IN GRAPHITE.	Mr MTWAZANA, GCOBANI

SAIP2023 / Programme Tuesday 04 July 2023

[297] Overview of Ion Beam Analysis (IBA) actitivities at iThemba LABS-NRF	NKOSI, Mlungisi
[309] Structural, elastic, electronic, bonding, and optical properties of PtBiTe and PtBi <sub>2</sub> structures.	MULAUDZI, Masilu Godfrey
[310] Synthesis and Characterization of Ti3C2 MXene electrode via In-situ HF and direct HF etching methods for application in battery-supercapacitor hybrid devices.	TALANE, Tsholo
[312] Characterization of neutron-induced defects in SnO2 using positron annihilation technique	Ms MOTJOPE, Dineo
[319] Li adsorption on a self-healed graphane for the next generation ion batteries.	Dr MAPASHA, Edwin
[321] Analysis of green emitting Tb3+ activated BaAl2O4/CaAl2O4/AlHO2/ Tb2O3/TbAlO3 mixed phases nanophosphors prepared via citrate sol-gel method	BELE, ABONGILE
[326] A study of thermal response of chromium-tin (Cr-Sn) bimetal films using in-situ RBS by Artificial Neural Networks	SEGOLA, Ingrid
[327] Magnesium-Silicon Alloy Phase Stability Predictions: A cluster expansion study.	Dr PHOSHOKO, Katlego
[329] Optimization of electron transport layer in polymer solar cell	NTOBENG, Modisa
[338] Investigation of reduced graphene oxide as an alternative carbonaceous material for lithium ion batteries: A density functional theory study	Mr MLOTSHWA, Thokozane Mxolisi
[343] Chemical Trends in defect stability and electronic properties of 3d transition metal doped WS2	NYANDORO, Brian
[346] Microstructural characterization of low elastic modulus $\beta$ -Ti alloy fabricated by arc melting process	MADIGOE, Mandy
[347] Gas sensing properties of rare-earth substituted MgFe2O4 ferrite nanoparticles	MKWAE, Prince
[35] Influence of rare-earth elements (RE = Ce, Nd, Gd) on Structural, ESR and Mössbauer spectroscopy studies of Ni0.5Co0.5RE0.03Fe0.197O4 synthesized by glycol-thermal method	Dr NHLAPO, T. A
[174] Proton beam and femtosecond laser writing lithography method for semiconductor microstructures	Mr GUGA, Aluwani
[198] Understanding the origin of Bunny-Hop light curves of periodic methanol masers	NEL, Andrea
[116] Combining large radio and optical astronomical surveys: exploring the MeerKAT Galaxy Cluster Legacy Survey	Mr NEL, S.J.J.