2017 CHPC National Conference

Monday 04 December 2017

Material Science: I (11:00-12:30)

-Conveners: Cornie van Sittert

time	[id] title	presenter
11:00	[218] MODELLING ADVANCED MATERIALS WITH HIGH PERFORMANCE COMPUTING	Prof. CATLOW, Richard
11:30	[127] Tuning the electronic, magnetic and optical properties of 2D materials: Ab initio insights	Dr OUMA, Cecil
11:50	[124] Computational study of anatase TiO2 as an anode material energy storage devices	Mr GANDAMIPFA, Mulatedzi
12:10	[143] Effect of pressure on structural, mechanical, dynamical and electronic properties of ReSe2 :A theoretical investigation	Mr MAHMOUD, Mahmoud

Material Science: II (13:30-15:00)

-Conveners: Eric van Steen

time	[id] title	presenter
13:30	[135] DENSITY FUNCTIONAL STUDY OF ELECTRONIC, OPTICAL AND ADSORPTION PROPERTIES DYE ON ANATASE AND BROOKITE TIO2 SURFACES FOR APPLICATION IN DYE SENSITIZED SOLAR CELLS	Dr MALUTA, Eric
14:00	[26] Charge transport, interfacial interactions and synergistic mechanism in BiNbO4/MWO4 (M = Zn and Cd) heterostructures for hydrogen production: insights from a DFT+U study	Mr OPOKU, Francis
14:20	[64] STRUCTURE PROPERTY RELATIONSHIPS IN ORGANIC SOLAR CELLS MATERIALS	Mr MAMBA, Sandile
14:40	[110] Beyond Li-ion: Computational Modelling Studies on Stability of Li-S-Se System	Mr MASEDI, Cliffton

Tuesday 05 December 2017

Material Science: III (11:00-12:30)

   -Conveners: George Amolo

time	[id] title	presenter
11:00	[184] Computational modeling as a complementary and predictive tool in materials science research	Dr AMOLO, George
11:20	[29] Spin-transfer torque field switching of magnetization in vertically-stacked multilayers	Dr UKPONG, Aniekan
11:40	[73] Phase diagram for the adsorption of oxygen and water on Pt(100) and Pt(111)	Mr CILLIERS, Pierre
12:00	[52] DMol3/COSMO-RS Prediction of Aqueous Solubility and Reactivity of Selected Azo Dyes: Effect of Global Orbital Cut-off and COSMO Segment Variation	Mr WAHAB, Olaide

Wednesday 06 December 2017

Material Science: Material Science (11:00-12:30)

    -Conveners: Eric Maluta

time	[id] title	presenter
11:00	[191] Limits of Langmuir	Prof. VAN STEEN, Eric
11:30	[79] Validation of the OSCAR-5 Code System against Experimental Data on Fuel Burnup and Material Activation in Research Reactors	Dr VAN HEERDEN, Francois
11:50	[94] ELSI: A unified software interface for Kohn-Sham electronic structure solvers	YU, Victor
12:10	[133] Computational and experimental study on heats of adsorption of MBT, MBO and MBI onto pyrite mineral surfaces	Dr MKHONTO, Peace