



**PRE-CONFERENCE SEMINAR ON  
COMPUTATIONAL & DATA-DRIVEN MODELLING**

**Tuesday 8 November 2022**  
**Lord Charles Hotel, Somerset West**



Hosted by Council for Scientific and Industrial Research,  
Supported by the Department of Science and Innovation



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Science and Innovation  
REPUBLIC OF SOUTH AFRICA

**PROGRAMME**

**Programme Director: Dr Rose Modiba**

8:30 – 9:00 Registration		
9:00 – 9:10	Welcoming Address	Dr Rose Modiba
9:10 – 9:40	Opening Address	Dr Happy Sithole
9:40 – 10:00	Elucidating the Adsorption and Co-adsorption of Potassium and Oxygen on (110) MnO <sub>2</sub> , TiO <sub>2</sub> and VO <sub>2</sub> Surfaces	<u>Khomotso Maenetja</u> and Phuti Ngoepe
10:00 – 10:20	Effect of alloying on the phase stability and elastic properties of L12 Cu <sub>3</sub> Pt crystal structure	<u>Tiny Mathibeng</u> , Maje Phasha, Heinrich Moller and Alain Mwamba
10:20 – 10:40	Computational study of bulk and surface properties on ruthenium oxide (RuO <sub>2</sub> )	<u>Mmeshi Hiine</u> , Brian Ramogayana, Phuti Ngoepe and Khomotso Maenetja
10:40 – 11:10 Tea		
11:10 – 11:30	SIMULATION OF THE EFFECT OF EVAPORATION AND GAS COMPOSITION DURING PLASMA SPHEROIDIZATION OF TITANIUM PARTICLES	<u>Watano Alex Seya</u> , Andrei Kolesnikov, Jaco Van Der Walt and Hertzog Bissett
11:30 – 11:50	Phase stability of TiPtZr shape memory alloys using cluster expansion techniques	<u>Mordecai Mashamaite</u> , Phuti Ngoepe and Hasani Chauke
11:50 – 12:10	AB INITIO TECHNIQUES, VASP AND CASTEP, ARE USED TO INVESTIGATE THE ELECTRONIC PROPERTIES OF B <sub>2</sub> COMPOUNDS FORMED BETWEEN Ti AND GROUP VIII ELEMENTS – A COMPARATIVE STUDY	<u>Bongani Ngobe</u> , Ramogohlo Diale, Maje Phasha, Mahlaga Molepo and Hasani Chauke
12:10 – 12:30	COMPARISON OF DYNAMIC MODELLING TECHNIQUES OF A 6-EFFECT FALLING FILM EVAPORATOR	<u>Tendai Matiza</u> and Corné Van Daalen
12:30 Lunch		
13:30 – 13:50	Thermodynamic and magnetic properties of Pt <sub>50</sub> Mn <sub>50</sub> -XMX (M= Cr, Fe) alloys: A first-principles study	<u>Ramogohlo Diale</u> , Phuti Ngoepe, Maje Phasha, Joseph Moema and Hasani Chauke

13:50 – 14:10	Multi-scale simulations and phase stability prediction of mixed $\text{Li}_2\text{S}_1\text{-x Sex}$ system	Dr. Cliffton Masedi
14:30 – 15:00	Development of metal alloys using computational approach	Prof Hasani Chauke
15:00-15:30	Modelling and Simulation Landscape in South Africa	Prof Regina Maphanga
15:30	Closure	
15:30	Coffee	