



PRE-CONFERENCE SEMINAR ON COMPUTATIONAL & DATA-DRIVEN MODELLING



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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: Computational modelling techniques: energy, minerals and metal alloy groups at Materials Modelling Centre, UL	<u>Prof Khomotso Maenetja</u>
9:40 – 10:00	A comparative analysis between isotropic and full optimization binary diagram influenced by Ni-doping on the LiMn ₂ O ₄ spinel type.	<u>Kemeridge Malatji</u> , Regina Rapela Maphanga and Phuti Esrom Ngoepe
10:00 – 10:20	Investigating titanium doping effect on lithium-rich electrode stability and performance	<u>Moloko Emmanuel Kgoedi</u> , Raesibe Ledwaba, Phuti Ngoepe, Noko Ngoepe and Mallang Masedi
10:20 – 10:40	Structural, thermodynamic, magnetic, and mechanical properties of Mn-Ir bimetallic alloys: an ab initio study	<u>Sikho Maxhayi</u> , Ndanduleni Lethole, Maje Phasha and Ramogohlo Diale
10:40 – 11:10 Tea		
11:10 – 11:30	Electronic and equilibrium properties of molybdenum disulphide: DFT study	<u>Magopa Kekana</u> , Thuto Mosuang, Abram Mahladiisa, Malili Matshaba, Luckey Silhivhilu and Bulelwa Ntsendwana
11:30 – 11:50	Computational study of water adsorption on the TiNi (110) surface.	<u>Vukosi Chauke</u> , David Tshwane and Hasani Chauke
11:50 – 12:10	Theoretical study on corrosion behaviour of titanium metal alloyed with precious metals	<u>Zanele Helen Phasha</u> , Mamookho Elizabeth Makhatha, Donald Mkhonto and Maje Jacob Phasha
12:10 – 12:30	First-principle study of TiNi-Nb shape memory alloys for biomedical applications	<u>Abel Mathews</u> , <u>Mandy Madigoe</u> , Rosinah Modiba and Mpho Sithole
12:30 Lunch		
13:30 – 13:50	Investigating the magnetic and mechanical properties of NdCeFe ₁₄ B permanent magnets: ab initio study	<u>Mphamela Enos Baloyi</u> , Ramogohlo Diale, Phuti Ngoepe and Hasani Chauke
13:50 – 14:10	Ground-state structures and properties of L10 Mn ₁ -XAIPtX and MnAl ₁₁ -XPtX alloys: a cluster expansion approach	<u>Thabang Mokwena</u> , Ramogohlo Diale, Phuti Ngoepe and Hasani Chauke

14:30 – 15:00	Fatigue life prediction of cylindrical roller bearings subjected to different operating conditions	<u>Themba Mashiyane</u> , Lagouge Tartibu, Dawood Desai and Smith Salifu
15:00-15:30	Effect of V and Ni addition on the Ti-Pt shape memory alloys for high temperature applications	<u>Rosinah Modiba</u>
15:30	Closure	
15:30	Coffee	