



PRE-CONFERENCE SEMINAR ON COMPUTATIONAL & DATA-DRIVEN MODELLING



Hosted by Council for Scientific and Industrial Research,
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REPUBLIC OF SOUTH AFRICA

PROGRAMME

Programme Director: Dr Rose Modiba

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8:30 – 9:00	Registration	
9:00 – 9:10	Welcoming Address	Dr Rose Modiba
9:10 – 9:40	Opening Address	Dr Werner Janse van Rensburg
9:40 – 10:00	Electronic stability study of tin dioxide as a catalyst for lithium-air batteries	<u>Khomotso Maenetja</u> and Phuti Ngoepe
10:00 – 10:20	Effect of chemical composition on structural and magnetic properties of binary Fe-Ni alloys – ab initio study	<u>Donald Mkhonto, Lebedike Mampuru and Maje Phasha</u>
10:20 – 10:40	First-principles study of binary austenitic ni-cu alloys	<u>Maje Phasha, Veronica Morudu and Caroline Mphela</u>
10:40 – 11:10	Tea	
11:10 – 11:30	Numerical methods in predicting residual stresses in laser powder bed fusion developed parts – a review	<u>Ayodeji Oyedeji, Natasha Sacks, Andrew Venter and Johannes Pötschke</u>
11:30 – 11:50	Effect of alloying on $\beta 2$ -ordered feal with Pd and Ir for high temperature application and ductility enhancement	<u>Christine Mkhonto, Phuti Ngoepe and Hasani Chauke</u>
11:50 – 12:10	Effect of platinum group elements (pges) on structural, stability and ductility of fe5ni4s8 (p4_2/nmc) pentlandite: cluster expansion method	<u>Barnard Molala, Mofuti Mehlaphe, Peace Mkhonto and Phuti Ngoepe</u>
12:10 – 12:30	Phase stability of B2 and L10 ptmn1-xfex alloys: a cluster expansion approach	<u>Ramogohlo Diale, Phuti Ngoepe, Maje Phasha, Joseph Moema and Hasani Chauke</u>
12:30	Lunch	
13:30 – 13:50	First principle studies on stabilities of reactive products of Li-O2 and Li-S batteries	Cliffton Masedi
13:50 – 14:10	Characterization of cubic Ti2AlNb (110) surface using density functional theory	<u>David Tshwane, Steve Dima, Prettier Maleka and Rapela Maphanga</u>
14:30	Closure	
14:30	Coffee	