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Chemistry and Materials Science Special Interest Group (SIG) Seminar

09:00–17:00   Thursday 5 December in *King Shaka* room (*Domestic Centre*)

	Chair: Hasani Chauke	
09:00–09:10	**Welcome**	Cornie van Sittert
09:10–09:40	Biosensing of DNA damage in Alzheimer's disease by Computational and Experimental methods	Krishna Bissety
09:40–10:00	DFTB study of Li_xTiO_2 with trigonal bipyramid structures: an insight into lithium-ion battery anode materials	Mulatedzi Gandamipfa
10:00–10:20	Chemical Reactivity Properties of Bioactive Pentacyclic Triterpenoic Acids by Conceptual DFT	Thishana Singh
10:20–10:40	High performance computing of super heavy elements of the periodic table	Jeanet Conradie
10:40–11:00	*Morning Tea*	
	Chair: Thishana Singh	
11:00–11:30	Molecular Finite Element Density Functional Calculations employing a Cusp Factor to enable convergence at the nuclei	Moritz Braun
11:30–11:50	Using Site Occupation Disorder and Surface Energies to Determine Pt_3Pd_2 and Pt_2Pd_3 Electrocatalyst Models	Kyle Meerholz
11:50–12:10	Molecular dynamics study of the influence of temperature on $Ti_7/LiCl$ structure	Andile Mazibuko
12:10–12:30	POSTER SESSION	
12:30–13:30	*Lunch*	
	Chair: Marile Landman	
13:30–13:50	First Principles study of Zn/Cu doped hematite surfaces for Photoelectrochemical water splitting.	Joseph Simfukwe
13:50–14:10	Tuning the electronic properties and interfacial interactions of $WS_2/ZrO_2(001)$ heterostructures by an external electric field, interlayer coupling and monolayer to few–layer of WS_2 sheets	Francis Opoku
14:10–14:30	Solving the Schrodinger equation in one and two Dimensions using Sinc functions and employing Python and Numpy.	Obiageli Ezenwachukwu
14:30–14:50	Reactivity of H_2O and SO_x (x = 0 – 3) on a Pt (111) surface – A DFT Study	Marietjie Ungerer
14:50–15:20	*Afternoon Tea Break*	
	Chair: Jeanet Conradie	
15:20–15:40	Anion receptor design for the development of $[PtCl_6]^{2-}$ selective reagents	Cyprian Moyo
15:40–16:00	Density functional modelling of doping strategies to control vacancies in silicon.	Abdulgaffar Abdurrazaq
16:00–16:20	Computational investigation of the binding characteristics of β-amyloid fibrils	Ephraim Marondedze
16:20–17:00	**SIG Meeting**	Cornie van Sittert
	End of Day	