SASESMA 2019 Winter School

10 – 20 June 2019

Preliminary programme (subject to change without notice.)

Venues:

Lectures: Natural Sciences 1, Hall 5-42 (all welcome)

Hands-on: Natural Sciences 1, Lab 5-55 (registered participants only)

Note: Visitors from both UP and other institutions are welcome to attend the lectures, but due to limited space, we request that only registered participants attend the hands-on sessions.

	10 June Monday	**11 June Tuesday**	**12 June Wednesday**	**13 June Thursday**	**14 June Friday**
Tea Coffee 8:00 – 8:30					
Morning Session I: 8:30 - 10:30	Registration, Welcome, Introduction to groups / interests	The electronic structure Hamiltonian *[Prof Chetty]*	Pseudopotentials [Prof Delugas]	Implementation of DFT *[Prof Martin-Samos]*	CHPC and Computational aspects *[Dr Govender]*
Break 10:30 – 11:00					
Morning Session II 11:00 - 13:00	Introduction: Solid state physics, Symmetry, Bloch's theorem, etc. *[Prof Theron]*	DFT basics: Kohn-Sham & Hohenberg-Kohn theorems,etc. *[Prof Chetty]*	Exchange-correlation and hybrid functionals [Prof Martin-Samos]	Implementation of DFT (continues) *[Prof Martin-Samos]*	Achieving optimal performance of DFT codes on HPC systems *[Prof Lombardi]*
Lunch 13:00 - 14:00					
Afternoon Session 14:00 - 16:00	Computer Lab: Linux, Xmgrace, SciDaVis, Xcrysden,etc. [Mr Odendaal]	Computer lab: Installation & Intro to QE - Total energy, k-points, cutoff.	Computer lab: Band structure / DOS / charge densities. Metals / semiconductors / insulators	Computer lab: Structure relaxation	Discussion