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# 5th African School on Electronic Structure Methods and Applications (ASESMA-2018) | (smr 3234)

## Monday 22 October 2018

- (08:30-20:00)

time	title	presenter
08:30	Registration	
09:00	Welcome	H.E. DR. ENG. GETAHUN MEKURIA; ANSHEBO, TEKETEL YOHANNES; SERIANI, NICOLA
09:30	Introduction	ANSHEBO, TEKETEL YOHANNES
10:15	Break	
10:45	Crystals, Bloch Th.	NARASIMHAN, SHOBHANA
11:35	Bands, questions	SHaidu, YUSUF
12:30	Lunch	
14:00	Computer Lab Linux, Xmgrace, Xcrysden, etc.	THOELE, FLORIAN & MENTORS/TUTORS
19:00	Evening session (time TBA): Materials science research in Africa	AMOLO, GEORGE O.

## Tuesday 23 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Theory of DFT	MARTIN, RICHARD
09:20	Kohn-Sham approach xc functionals	AMOLO, GEORGE O.
10:15	Break	
10:45	Band structure	NARASIMHAN, SHOBHANA
11:35	Through KS Eqs	SHaidu, YUSUF
12:30	Lunch	
14:00	Computer Lab Intro to QE - Total energy, k-pts, cutoff	MAMMEN, NISHA & MENTORS/TUTORS
19:00	Evening session (time TBA): How to give a scientific talk	GRIFFIN, SINEAD

## Wednesday 24 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	DFT in practice k-points, smearing	AKIN-OJO, OMOLOLU
10:15	Break	
10:45	Pseudopotentials, forces, relaxation	TBA
12:30	Lunch	
14:00	Computer Lab Band structure metals/insulators	GRIFFIN, SINEAD & MENTORS/TUTORS
19:00	Evening session (time TBA): How to write a scientific paper	NARASIMHAN, SHOBHANA

# Thursday 25 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Advanced Functionals, DFT + U, etc.	SERIANI, NICOLA
10:15	Break	
10:45	Atomic vibrations, Phonons	TBA
12:30	Lunch	
14:00	Computer Lab Phonons in quantum Espresso	TBA
19:00	Evening session (time TBA): Women in Science	

## Friday 26 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Excitations, Start TDDFT	CASIDA, MARK E.
10:15	Break	
10:45	Excitations, Many-body theory	GATTI, MATTEO
12:30	Lunch	
14:00	Computer Lab Metals	
16:00	Discussion of projects	
19:00	Evening session (time TBA)	

# Monday 29 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Molecular dynamics	LUIJTEN, ERIK
10:15	Break	
10:45	MD Continued	LUIJTEN, ERIK
12:30	Lunch	
14:00	MD Tutorial	LUIJTEN, ERIK
19:00	Evening session (time TBA): Introduction to biological physics	MAMMINO, LILIANA

## Tuesday 30 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Short talk TBA & Projects	
10:15	Break	
10:45	Projects	
12:30	Lunch	
14:00	Short talk TBA & Projects	
19:00	Evening session (time TBA): Establishing a research programme in Africa: the EAFR	AKIN-OJO, OMOLOLU

## Wednesday 31 October 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Short talk TBA & Projects	
10:15	Break	
10:45	Projects	
12:30	Lunch	
14:00	Short talk TBA & Projects	
19:00	Evening session (time TBA): Discussion	

# Thursday 01 November 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Short talk TBA & Projects	
10:15	Break	
10:45	Projects	
12:30	Lunch	
14:00	Short talk TBA & Projects	
19:00	Evening session (time TBA): Awards	

## Friday 02 November 2018

**- (08:30-20:00)**

time	title	presenter
08:30	Short talk TBA & Projects	
10:15	Break	
10:45	Projects	
12:30	Lunch	
14:00	Project reports - Closing session	
19:00	Evening session (time TBA): Discussion	