

ASESMA 2016 - PRELIMINARY Schedule of lectures and hands-on computer labs - as of 7th June

<u>WEEK 1</u>	13-Jun Monday	14-Jun Tuesday	15-Jun Wednesday	16-Jun Thursday	17-Jun Friday	18-Jun Saturday
Morning: 8:30 - 13:00						
8:30 - 10:30	<u>Registration</u> Welcome Introduction	Theory of DFT Kohn-Sham approach xc functionals. Nicola Marzari	Metals k-points, smearing Magnetism. Omololu Akin-Ojo	Moving atoms at $T \neq 0$ Molecular Dynamics. Sandro Scandolo	Beyond Kohn-Sham DFT+U, etc. Nicola Marzari	<i>Excursion</i>
Break						
11:00 - 13:00	Crystals, Bloch Th. Bands, questions. Shobhana Narasimhan	Practice of DFT Through KS Eqs. Shobhana Narasimhan	Moving atoms at $T=0$ Forces, relaxation. Sandro Scandolo	Atomic vibrations Phonons. Ryo Maezono	Beyond DFT - excitations Optical properties. Matteo Gatti	
		Adv. Participants: Tu discussion of their work; W-Th GW/BSE M. Gatti			Spin-orbit interactions. Richard Martín	
Lunch Break: 13:00 - 14:00						
Afternoon: 14:00 - 18:30						
14:00 - 16:00	Computer Lab Linux, Xmgrace, Xcrysden, etc. Florian Thöle and Mentors/Tutors	Computer Lab Intro to QE - Total energy, k-pts, cutoff. Nisha Mammen and Mentors/Tutors	Computer Lab Band structure metals/insulators. Sinead Griffin and Mentors/Tutors	Computer Lab Phonons in quantum Espresso. Tomohiro Ichiba and Mentors/Tutors	TBA	Discussion of projects Presentation by participants
Break						
16:30 - 18:30	Computer Lab Continued	Computer Lab Continued	Computer Lab Continued	Computer Lab Continued	continued	
Evening						
Time TBA TBA	TBA Discussion	TBA Discussion	TBA Discussion	TBA Discussion	TBA Discussion	

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Week 2 - VERY TENTATIVE

<u>WEEK 2</u>	20-Jun Monday	21-Jun Tuesday	22-Jun Wednesday	23-Jun Thursday	24-Jun Friday
<u>Morning: 8:30 - 13:00</u>					
8:30 - 10:30	TDDFT Mark Casida	Tutorial on MD Ali Hassanali	Lecture Short - related to a project	Lecture Short - related to a project	Projects
<i>Break</i>					
11:00 - 13:00	TDDFT continued	MD Continued	Projects	Projects	Projects
<i>Lunch Break: 13:00 - 14:00</i>					
<u>Afternoon: 14:00 - 18:30</u>					
14:00 - 16:00	Start Projects	Projects	Projects	Short project reports	Short project reports
<i>Break</i>					
16:30 - 18:30	Projects	Projects	Projects	Projects	Projects
<u>Evening</u>					
TBA	TBA	TBA	TBA	TBA	Future!
TBA	Discussion	Discussion	Discussion	Discussion	Discussion