

MDANSE 2018

Materials and Neutron Scattering Instrument Modelling.

	<u>Monday 24th</u>	<u>Tuesday 25th</u>	<u>Wednesday 26th</u>	<u>Thursday 27th</u>	<u>Friday 28th</u>
08:45-9:00	Welcome				
9:00-9:45	Molecular Dynamics Miguel	Practicals: Sylvain Spin waves	Practicals: Peter McStas/ToF	McStas - samples Erik	Tools and simulation pipelines
9:45-10:30	DFT lattice dynamics and MD			Advanced samples Erik	Emmanuel
10:30-10:45	coffee break	coffee break	coffee break	coffee break	coffee break
10:45-11:30	SpinWaves for dummies Sylvain	Practicals: Thomas ASE	Practicals: Miguel MDANSE	Practicals: Erik McStas/Structure	Practicals: Emmanuel
11:30-12:15	Gaussian approximation Emmanuel	Oriented towards dynamics			VE: Lattice dynamics – TAS/ToF
12:00-14:00	lunch	lunch	lunch	lunch	lunch
14:00-14:45	Practicals: Miguel MD: liquids and powders	Introduction to McStas Peter	Excursion to Teide	Practicals: Emmanuel	Practicals: Sanghamitra
14:45-15:30		McStas Instr. classes Erik		McStas: Liquids, powders dynamics	VE's: Molecular Spec: ToF/OSIRIS
15:30-15:45	coffee break	coffee break		coffee break	coffee break
15:45-16:30	Practicals: Sanghamitra Lattice dynamics	Practicals: Erik McStas Diffract. Laue		Practicals: Peter McStas: SX dynamics	Practicals: Emmanuel VE: Gaussian approx - ToF
16:30-17:15	phonons in crystals	Practicals: Peter McStas/TAS			
	Sunday 23 rd	Registration at the Hotel		Saturday 29 th	Bye Bye
~ 20:00	lunch	lunch	lunch	lunch	lunch