

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	Introduction to McStas Peter	McStas - samples Erik	Simulation pipe-lines Emmanuel
9:45-10:30	DFT lattice dynamics and MD Sanghamitra		McStas Instrument classes John	Advanced samples Erik	Tools for automation Peter
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: Erik McStas Diffract. Laue	Practicals: Erik McStas/Structure	Practicals: John
11:30-12:15	Gaussian approximation Emmanuel	Oriented towards dynamics	Practicals: Peter McStas/TAS	Liquid, Powder and SX	VE: Lattice dynamics – TAS/ToF
12:00-14:00	lunch	lunch	lunch	lunch	lunch
14:00-14:45	Practicals: Miguel MD: liquids and powders	Excursion to Teide	Practicals: John McStas/ToF	Practicals: Emmanuel	Practicals: Sanghamitra VE: Molecular Spec.
14:45-15:30			Practicals: Miguel McStas/QENS	McStas: Liquids, powders dynamics	- ToF/TOSCA/Lagrange
15:30-15:45	coffee break		coffee break	coffee break	coffee break
15:45-16:30	Practicals: Sanghamitra Lattice dynamics		Practicals: Sanghamitra McStas Instr:	Practicals: Peter McStas: SX dynamics	Practicals: Emmanuel VE: Gaussian approx - ToF
16:30-17:15	phonons in crystals		Molecular Spectroscopy		
	Sunday 23 rd	Registration at the Hotel		Saturday 29 th	Bye Bye
~ 20:00	lunch	lunch	lunch	lunch	lunch