MSSC2009 School Programme

REGISTRATION

Monday 14th	
8:30 - 8:50	**Lecture Theatre C - Chemistry RCS**
10:50 - 11:10	**PG Common Room - Chemistry Building**

MORNING SESSIONS : Lecture Theatre C - Chemistry RCS

Coffee Break : **PG Common Room – Chemistry Building**

	Monday 14th	Tuesday 15th	Wednesday 16th	Thursday 17th	Friday 18th
9:00 - 9:55	Translation symmetry, Space groups, Bloch functions, Fermi energy ***R. Orlando***	Total energy calculation and SCF convergence tools ***N. M. Harrison***	Local defects in crystalline materials ***G. Mallia***	CRYSTAL in parallel: replicated and distributed (MPP) data ***I. J. Bush***	Localized crystalline orbitals and related quantities ***C. M. Zicovich***
9:55 - 10:50	Hamiltonians and basis sets ***N. M. Harrison***	Geometry optimisation of solids ***C. M. Zicovich***	From bulk to surface. Relaxation and reconstruction. ***B. Montanari***	Parallel Optimisation - DL-FIND ***J. Carr***	Post-HF techniques and the CRYSCOR project ***L. Maschio***
	Coffee Break	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
11:10 - 12:05	The structure of the CRYSTAL code ***R. Orlando***	One-electron properties ***F. Corà***	Vibrational frequencies calculation and tools for their analysis ***R. Dovesi***	The effect of pressure: equations of state; bulk modulus; elastic constants ***M. Alfredsson***	TD-DFT ***L. Bernasconi***
12:05 - 12:55	CRYSTAL input/output. Basic features. Scripts ***G. Mallia***	Spin polarized solutions. Spin densities and related quantities ***R. Orlando***	Ab initio Thermodynamics ***L. M. Liborio***	Dielectric properties. CPHF/CPKS ***L. Bernasconi***	Quantum transport in nanojunctions ***A. Ferretti***

AFTERNOON SESSIONS

Basic tutorials : Room 135 – Chemistry Building

Coffee Break and Poster Session : **PG Common Room - Chemistry Building**

	Monday 14th	Tuesday 15th	Wednesday 16th	Thursday 17th	Friday 18th
14:30 - 16:15	Geometry input & geometry editing	Total energy (Single-point calculation)	13:00 - 15:45 *Lunch* & *Poster Session*	Vibrational frequencies	Basic modelling of surfaces and defects
	Coffee Break	*Coffee Break*		*Coffee Break*	*Coffee Break*
16:45 - 18:30	Basis set input & basis set editing	Geometry optimisation	16:00 ... *Self-guided Tour*	One-electron properties	Basic modelling of defects

Advanced tutorials : Room 232A – Chemistry Building

Coffee Break and Poster Session : **PG Common Room - Chemistry Building**

	Monday 14th	Tuesday 15th	Wednesday 16th	Thursday 17th	Friday 18th
14:30 - 16:15	Magnetic properties	Advanced options in geometry optimisation and frequencies calculation	13:00 - 15:45 *Lunch* & *Poster Session*	Dielectric properties	CRYSCOR
	Coffee Break	*Coffee Break*		*Coffee Break*	*Coffee Break*
16:45 - 18:30	Magnetic properties	Advanced options in geometry optimisation and frequencies calculation	16:00 ... *Self-guided Tour*	Dielectric properties	CRYSCOR

EVENING

	Monday 14th	Tuesday 15th	Wednesday 16th	Thursday 17th	Friday 18th
			20:00 *Social Dinner*		