

MSSC2008 School Programme

REGISTRATION

Monday 15th	
8:30 - 8:50	Lecture Theatre C - Chemistry RCS
10:50 - 11:10	Room 232 (UG Common Room) - Chemistry Building

MORNING SESSIONS : Lecture Theatre C - Chemistry RCS

Coffee Break : Room 232 (UG Common Room) – Chemistry Building

	Monday 15th	Tuesday 16th	Wednesday 17th	Thursday 18th	Friday 19th
9:00 - 9:55	Translation symmetry, Space groups, Bloch functions, Fermi energy R. Orlando	Geometry optimisation of solids C. M. Zicovich	Vibrational frequencies calculation and tools for their analysis R. Dovesi	The effect of pressure: equations of state; bulk modulus M. Alfredsson	Local defects in crystalline materials G. Mallia
9:55 - 10:50	Hamiltonians and basis sets N. M. Harrison	One-electron properties F. Corà	Ab initio Thermodynamics L. M. Liborio	Elastic constants W. Perger	Localized crystalline orbitals and related quantities C. M. Zicovich
	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>
11:10 - 12:05	The structure of the CRYSTAL code C. Roetti	Spin polarized solutions. Spin densities and related quantities R. Orlando	From bulk to surface. Relaxation and reconstruction. Models and strategies A. Wander	Dielectric properties. CPHF/CPKS M. Ferrero	Post-HF techniques and the CRYSCOR project S. Casassa
12:05 - 12:55	CRYSTAL input/output. Basic features B. Civalleri	Total energy calculation and SCF convergence tools N. M. Harrison	Models and strategies for metallic systems: bulk and surface K. Doll	CRYSTAL in parallel: replicated and distributed (MPP) data I. J. Bush	Quantum transport in nanojunctions A. Ferretti

AFTERNOON SESSIONS

Basic tutorials : Room 135 – Chemistry Building

Coffee Break and Poster Session : Room 232 (UG Common Room) – Chemistry Building

	Monday 15th	Tuesday 16th	Wednesday 17th	Thursday 18th	Friday 19th
14:30 - 16:15	Geometry input & geometry editing	Total energy (Single-point calculation)	13:00 - 15:45 <i>Lunch & Poster Session</i>	Vibrational frequencies	Basic modelling of surfaces and defects
	<i>Coffee Break</i>	<i>Coffee Break</i>		<i>Coffee Break</i>	<i>Coffee Break</i>
16:45 - 18:30	Basis set input & basis set editing	Geometry optimisation	16:00 ... <u>Self-guided Tour</u>	One-electron properties	Basic modelling of defects

Advanced tutorials : Room 232 A – Chemistry Building

Coffee Break and Poster Session : Room 232 (UG Common Room) – Chemistry Building

	Monday 15th	Tuesday 16th	Wednesday 17th	Thursday 18th	Friday 19th
14:30 - 16:15	Magnetic properties	Advanced options in geometry optimisation and frequencies calculation	13:00 - 15:45 <i>Lunch & Poster Session</i>	Dielectric properties	CRYSCOR
	<i>Coffee Break</i>	<i>Coffee Break</i>		<i>Coffee Break</i>	<i>Coffee Break</i>
16:45 - 18:30	Magnetic properties	Advanced options in geometry optimisation and frequencies calculation	16:00 ... <u>Self-guided Tour</u>	Dielectric properties	CRYSCOR

EVENING

	Monday 15th	Tuesday 16th	Wednesday 17th	Thursday 18th	Friday 19th
			20:00 <u>Social Dinner</u>		