Erice 2018
QUANTUM CRYSTALLOGRAPHY
Course schedule

	Saturday 2 June	Sunday 3 June	Monday 4 June	Tuesday 5 June	Wednesday 6 June	Thursday 7 June	Friday 8 June	Saturday 9 June
8:30-9:00	Introduction to both courses (Annalisa, Paola, Erin, Joke, Lukas, Andy, Piero, Dylan)							
9:00-9:45	Joke Hadermann Introduction to Electron Diffraction	Concomitant Workshops: Regine Irmer and Jacob Overgaard Data Treatment; Nancy team: multipolar refinement of charge and spin density; Macchi: multipolar refinement of charge density	Peter Müller: Crystal structure refinement by least squares I	Concomitant Workshops: Regine Irmer and Jacob Overgaard Data Treatment; Nancy team: multipolar refinement of charge and spin density; Macchi: multipolar refinement of charge density	Concomitant Workshops: Torino team: Crystal Orbitals Calculations; Jayatilaka Grabowsky Genoni: X-ray constrained wave functions; Nancy team: multipolar refinement of charge and spin density;	Concomitant Workshops: Torino team: Crystal Orbitals Calculations; Jayatilaka Grabowsky Genoni: X-ray constrained wave functions; Nancy team: multipolar refinement of charge and spin density;	Concomitant Workshops: Macchi Krawchuk Atomic polarizabilities; Grabowsky Hirshfeld Atom refinement; Giannozzi periodic DFT calculations con Quantum Espresso	Jayatilaka: X-ray constrained wave functions part 2
9:45-10:30	Lou Massa: Quantum Crystallography, an historical introduction		Philip Nakashima: Quantitative convergent beam electron diffraction QCEB I					Scherer: Organometallic bonding (concepts) under pressure
10:30-11:00	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:00-11::45	Jan Pieter Abrahams: General theory of diffraction	Concomitant Workshops: Regine Irmer and Jacob Overgaard Data Treatment; Nancy team: multipolar refinement of charge and spin density; Macchi: multipolar refinement of charge density	Poster Presentations: Rising stars in Quantum Crystallography (9 talks)	Concomitant Workshops: Regine Irmer and Jacob Overgaard Data Treatment; Nancy team: multipolar refinement of charge and spin density; Macchi: multipolar refinement of charge density	Concomitant Workshops: Torino team: Crystal Orbitals Calculations; Jayatilaka Grabowsky Genoni: X-ray constrained wave functions; Nancy team: multipolar refinement of charge and spin density;	Concomitant Workshops: Torino team: Crystal Orbitals Calculations; Jayatilaka Grabowsky Genoni: X-ray constrained wave functions; Nancy team: multipolar refinement of charge and spin density;	Concomitant Workshops: Macchi Krawchuk Atomic polarizabilities; Grabowsky Hirshfeld Atom refinement; Giannozzi periodic DFT calculations con Quantum Espresso	Giessibl: atomic force microscopy
11:45-12:30	Jan Pieter Abrahams: General theory of diffraction							Elsässer: femto-seconds X-ray diffraction
12:30-14:30	Lunch	Lunch	Excursion	Lunch	Lunch	Excursion	Lunch	Lunch
14:30-15:15	Overgaard: Accurate X-ray diffraction Measurements	Claiser: Neutron diffraction and sipn density multipolar model		Civalleri: Periodic Systems: models and strategies	Genoni: Extremely Localized Molecular Orbitals in Quantum Crystallography		Ryde: Quantum refinement for biological applications	Spackman: Quantum Crystallography and Crystal Engineering: Experimental lattice energies from X-ray diffraction data?
15:15-16:00	Madsen: Dynamics in crystals in the context of quantum crystallography	Deutsche Neutron diffraction and sipn density multipolar model		Giannozzi Introduction to DFT and the plane-wave pseudopotential method	Macchi: Atomic polarizabilities and dielectric properties		Merz: Quantum refinement for drug design applications	Round Table, The Future of Quantum Crystallography introduction by Bo Iversen.
16:00-16:30	Coffee Break	Coffee Break		Coffee Break	Coffee Break		Coffee Break	Coffee Break
16:30-17:15	Macchi Atom centered Multipolar expansion of the charge density	Rahm: experimental quantum chemistry		Erba:From Energy and Wavefunction to Advanced Properties of Solids	Contreras: Quntum Topology		Guillot:Experimental charge densitystudies in biomolecules	Round Table: The Future of Quantum Crystallography (few short talks)
17:15-18:00	Grabowsky: Hirshfeld Atom Refinements	Jayatilaka: X-ray constrained wave functions part 1		Neumann: dispersion corrected DFT methods and crystal strructure predictions	Poster Presentations: Rising stars in Quantum Crystallography (5 talks)		Dittrich: Transferable Electron Densities (please confirm)	Joint Closing Remarks
18:00-18:30	Introduction to Erice (Martin Schmidt)	Poster Session 1		Poster Presentations: Rising stars in Quantum Crystallography (3 talks)	Poster Session 2		Poster Presentations: Rising stars in Quantum Crystallography (3 talks)	
20:00	Sicilian Dinner							Farewell Party