MORNING SESSION

LECTURES

Time	MONDAY 8th	TUESDAY 9th	WEDNESDAY 10th	THURSDAY 11th	FRIDAY 12th
8:15 - 8:40	**Registration**				
8:40 - 9:20	**Opening Remarks** *Alessandro Erba*	**One-Electron Properties of Solids** *Furio Corà*	**Density Functional Perturbation Theory and its Time-Dependent Extension** *Jacques Desmarais* **Calculating Excitons from CRYSTAL** *Manuel Antonio García Blázquez*	**van der Waals Interactions in the DFT Framework** *Jan Gerit Brandenburg*	**Spin-Orbit Coupled Calculations** *Jacques Desmarais*
9:20 - 10:00	**Tackling the Many-Body Problem: the DFT Approach** *Stefano Pittalis*	**Chemical Bonding in Materials** *Jacques Desmarais* **Fock-Exchange in Solids with a Local Basis Set: Hybrid DFAs Made Efficient** *Giacomo Ambrogio*	**Modelling IR and Raman Spectra and Non-Linear Optical Properties** *Lorenzo Maschio*	**Molecular Dynamics with CRYSTAL** *Chiara Ribaldone* **Cost-effective Composite HF/DFT Methods for High Throughput Screening and Machine Learning Applications** *Mattia Raimondo*	**Strongly Anharmonic Systems with CRYSTAL** *Matteo Calandra*
10:00 - 10:25	Cofee Break	Cofee Break	Cofee Break	Cofee Break	Cofee Break
10:25 - 11:05	**Local Gaussian-Type Basis Functions for Solids** *Bartolomeo Civalleri*	**How to Model Defects and Surfaces** *Giuseppe Mallia*	**Density Functional Approach to Magnetism** *Stefano Pittalis*	**Exploiting Parallel Computing with CRYSTAL** *Ian Bush*	**Electron Transport Properties** *Eleonora Ascrizzi* **Modelling Diffusion Coefficients and Ionic Transport** *Laura Bonometti*
11:05 - 11:45	**The Periodic LCAO Approach** *Silvia Casassa*	**Mechanical Response of Materials: Pressure and Elasticity** *Maria Alfredsson*	**Harmonic Lattice Dynamics** *Anna Ferrari*	**Large Scale DFT Simulations on CPU/GPU Architectures** *Giacomo Ambrogio* **How to Model Metal-Organic Frameworks with CRYSTAL** *Lorenzo Donà*	**Phonon Transport Properties** *Antti Karttunen*
11:45 - 12:25	**Treatment of the Coulomb Interaction in Solids** *Jacques Desmarais*	**Predicting Physical Properties of Materials: A Crystallographer Perspective** *Anna Krawczuk*	**Thermodynamics and Thermoelasticity Beyond the Harmonic Approximation** *Alessandro Erba* **Anharmonic Vibrational States and Spectra** *Davide Mitoli*	**Tackling Size and Structural Complexity with CRYSTAL** *Marta Corno*	**Beyond Linear Response: Exploring Nonlinear Optical Phenomena with CRYSTAL** *Panaghiotis Karamanis*
12:25 - 14:30	Lunch	Lunch	Lunch	Lunch	Lunch

AFTERNOON SESSION

BEGINNERS

Time	MONDAY 8th	TUESDAY 9th	WEDNESDAY 10th	THURSDAY 11th	FRIDAY 12th
14.30 - 16:00	**Hands-On Kickoff** *Davide Mitoli* **Geometry Input** *Andreha Gelli*	**Geometry Optimization and Equation-of-State** *Giuseppe Mallia* **Modelling of 2D Systems** *Giuseppe Mallia*	**Poster Session**	**One-Electron Properties** *Giuseppe Mallia and Silvia Casassa*	**How to Deal with Spin** **Response Properties CPHF/KS** *Chiara Ribaldone*
16:00 - 16:30	Cofee Break	Ice Cream Break	*Free Time*	Ice Cream Break	Cofee Break
16:30 - 18:00	**Basis Set, SCF and Single-Point Energy** *Andreha Gelli*	**Harmonic Frequencies and Spectra** *Davide Mitoli*		**QTAIM** *Marcos Rivera*	**How to Simulate Defects** *Giuseppe Mallia*

EXPERIENCED USERS

Time	MONDAY 8th	TUESDAY 9th	WEDNESDAY 10th	THURSDAY 11th	FRIDAY 12th
14.30 - 16:00	**Hands-On Kickoff** **How to Run CRYSTAL in Parallel** *Giacomo Ambrogio*	**Equation-of-State and Pressure** **Elastic Properties** *Filippo Bodo*	**Poster Session**	**Harmonic and Anharmonic Vibrational Spectroscopies** *Davide Mitoli*	**Spin-Orbit Coupling and Non-Collinear DFT** *Jacques Desmarais*
16:00 - 16:30	Cofee Break	Ice Cream Break	*Free Time*	Ice Cream Break	Cofee Break
16:30 - 18:00	**One-Electron Properties** *Laura Bonometti* **QTAIM** *Marcos Rivera*	**Electron Transport Properties** *Eleonora Ascrizzi*		**Phonons and Thermodynamics** *Giacomo Ambrogio*	**Dispersion Corrections and Composite Methods** *Lorenzo Donà*

Time	MONDAY 8th	TUESDAY 9th	WEDNESDAY 10th	THURSDAY 11th	FRIDAY 12th
19:30 - 23:30			**Social Dinner**		

IMPERIAL

THOMAS YOUNG CENTRE
THE LONDON CENTRE FOR THE THEORY AND SIMULATION OF MATERIALS

UNIVERSITÀ DI TORINO

chimica 2023 - 2027 DIPARTIMENTO DI ECCELLENZA
Ministero dell'Università e della Ricerca