

MSSC2025

TORINO 8-12 SEP 2025



VIEW ONLINE

MORNING SESSION

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

AFTERNOON SESSION

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

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

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