



Computation aided characterization

Online Workshop March 26th, 2025

26/03/2025

09:00– 9:15	Admission
09:15 – 9:30	A. La Magna , CNR-IMM Catania Introduction
9:30 – 10:00	I. Deretzis , CNR-IMM Catania Atomistic approaches for the interpretation of structural, spectroscopic and electrical properties of materials
10:00 – 10:30	G. Nicotra , CNR-IMM Catania Advanced electron microscopy
10:30 – 11:00	Coffee break
11:00 – 11:30	S. D'Agostino , CNR-NANOTEC Lecce Computational Approaches for the study of light-matter interaction processes
11:30 – 12:00	R. Cardia , CNR-SPIN Napoli Computational Approaches for the characterization of 2D materials for spintronics
12:00 – 12:30	E. Scalise , Università degli Studi di Milano-Bicocca Atomistic modelling and simulations of crystal phase transitions and extended defects
12:30– 14:00	Lunch break
14:00 – 14:30	D. Sangalli , CNR-ISM Montelibretti Modelling electronic excitations in material science
14:30 – 15:00	G. Fratesi , Università degli Studi di Milano Ab initio simulations of surfaces and adsorbed systems
15:00 – 15:30	Coffee break
15:30 – 16:00	L. Martin Samos , CNR-IOM Trieste Theory vs experiments: understanding, reproducing and/or predicting
16:00 – 16:30	G. Herrero Saboya , CNR-IOM Trieste How to link defect atomic structures with their corresponding spectroscopic signature
16:30 – 17:00	Round table

Organizing & Scientific Committee

A. La Magna, Ioannis Deretzis, A.M. Mio, CNR-IMM Catania
 F. Genuzio, L. Martin Samos, N. Salles, CNR-IOM Trieste
 D. Simeone, CNR-NANOTEC Lecce
 R. Cardia, G. Cantele, CNR-SPIN Napoli
 E. Molteni, S. Achilli, Università degli Studi di Milano
 F. Bazzocchi, M. De Luca, T. Rodani, Area Science Park Trieste

REGISTRATION FORM

(deadline March 25th, 2025)

<https://link.cnr.it/nffa-di-registration>

