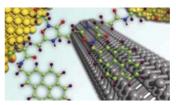
## **PhD Programme in Chemical and Materials Sciences**

## **PhD Days 2023**

February 7<sup>th</sup> & 23<sup>th</sup>, 2023 - Department of Chemistry - Aula Magna









The students of the XXXVI Cycle of the PhD Programme in Chemistry and Materials Sciences present their research activities.

## **Programme**

7 February 2023			
Time		Name	Title
9:00	9:30	Sodupe Mariona	The role of computational chemistry in today's chemical research
9:30	10:00	Bravetti Federica	Computational and experimental method for crystal structure determination: CSP, SSNMR and powder XRD
10:00	10:30	Asteggiano Alberto	Extraction and analytical techniques for the characterization, quantification, and valorization of plant metabolites by mass spectrometry
		Coffee break	
11:00	11:30	Naveed Ahmed	Abatement of pollutants from water via photodegradation/adsorption processes
11:30	12:00	Centrella Barbara	Design and synthesis of copper complexes and possible application for redox chemistry in MOFs
12:00	12:30	Ricchebuono Alberto	Surface phenomena at supported metal nanoparticles: an integrated experimental and theoretical approach
		Lunch Break	
14:00	14:30	Ferri Davide	Watching catalysts at work in a liquid environment
14:30	15:00	Deplano Gabriele	Cu-based catalysts for C-H bond activation
15:00	15:30	Rosso Francesca	Ti-zeolite catalysts for partial oxidation reactions
		Coffee break	
16:00	16:30	Perrero Jessica	Phenomena at Interstellar Core and Mantle Grains: A Quantum Mechanical Approach
16:30	17:00	Mecarelli Enrica	Characterization and quantification of biomarkers via chromatography-mass spectrometry
17:00	17:30	Nannuzzi Chiara	Surface properties and characterization of VOx/TiO2 based catalysts for NH3-SCR reaction
17:30	18:00	Deninno Gianluca	Characterization of materials and surfaces through ISO-25178 morphological parameters

23 February 2023			
Time		Name	Title
9:00	9:30	Gebert Annett	New Ti alloys for biomedical applications: advanced processing, microstructure and surface property design
9:30	10:00	Alessio Andrea	High-brilliance X-ray techniques for oxide functionalization and characterization
10:00	10:30	Castiglione Davide	Building-up Molecular Complexity with Homologation Chemistry: New Concepts and Applications
		Coffee break	
11:00	11:30	Tiwari Kirti	Design of antimicrobial mechanism of metallic patterned hydrophobic surfaces produced by dealloying and plastic flow deformation of metallic glasses
11:30	12:00	Zarate Ana	Innovative materials for emerging photovoltaics
12:00	12:30	Zollo Alessia	New approaches for in-door air purification based on visible-light photocatalysis
		Lunch break	
14:00	14:30	Langer Thierry	3D Pharmacophores: Versatile Tools for Computer-Assisted Molecular Design
14:30	15:00	Lanfranco Alberto	Synthesis and Applications of Functionalised Carboranes for the Treatment of Mesothelioma and Diffused Thoracic Tumours
15:00	15:30	Ribaldone Chiara	Study and Implementation of Molecular Dynamic based algorithm in the quantum mechanical ab initio CRYSTAL code
		Coffee break	
16:00	16:30	Dereje Degnet	Synthesis and characterization of NIR fluorescent nanocarriers for photodynamic therapy
16:30	17:00	Difalco Alessandro	Synthesis and characterization of Heusler alloys for thermoelectric and spintronic applications
17:00	17:30	Molokova Anastasia	Elucidating the deactivation pathways of Cu-zeolite-based industrial DeNOx catalysts
17:30	18:00	Rocca Riccardo	Computational study of chemical-physical properties of materials for Li-ion batteries