

# Chemistry at the Surface

## Key Aspects in Materials Design and Catalysis

An International Workshop in Honor of  
Gaetano Granozzi and Elio Giamello

25<sup>th</sup>-27<sup>th</sup> November 2021, Baveno, Italy



### Plenary Speakers

Prof. Gianfranco Pacchioni (IT)  
Prof. Hans-Joachim Freund (DE)  
Prof. Catherine Louis (FR)  
Prof. Zbigniew Sojka (PL)  
Prof. Damien Murphy (UK)  
Prof. Jürg Osterwalder (CH)  
Prof. Jürgen Behm (DE)

### Topics

- **Surface chemistry**
- **Surface science**
- **Low dimensional systems**
- **Oxides chemistry**
- **(Photo)Catalysis**
- **Open-shell species**

The Workshop is embedded within the 6th PARACAT Network Symposium and features plenary lectures, key note and oral communications.

The Workshop commences on Thursday November 25<sup>th</sup> in the afternoon and is preceded by a morning session dedicated to the research activities of the PARACAT project.

### Location and Venue

The conference will take place at the [Grand Hotel Dino](http://www.bavenoturismo.it/en/storia-di-baveno) in Baveno a charming village along the Lake Maggiore shores, facing the Borromean Islands <http://www.bavenoturismo.it/en/storia-di-baveno>

### Registration Fees

	Before 1 <sup>st</sup> October 2021	After 1 <sup>st</sup> October 2021	One day conference
<b>Academics</b>	400 €	450 €	100
<b>Students</b>	350 €	400 €	100

The quote includes: welcome party, (Thursday 25<sup>th</sup> November evening), coffee breaks, lunches and accommodation for two nights at the Grand Hotel Dino.

Conference dinner: 60 €

### Organising and Scientific Committee

#### University of Turin

Mario Chiesa

Maria Cristina Paganini

Stefano Livraghi

Enrico Salvadori

#### University of Padua

Stefano Agnoli

Laura Calvillo

Antonella Glisenti

Gian Andrea Rizzi



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## Scientific Programme

Thursday 25/11/2021		Friday 26/11/2021		Saturday 27/12/2021	
09:00	Opening of the PARACAT Session	09:00	Catherine Louis <i>From Gold to non-Noble Catalysts for Selective Hydrogenation</i>	09:00	Hajo Freund <i>Model Systems for Heterogeneous Catalysis at the Atomic Scale</i>
09:15	Ilenia Serra <i>Pitfalls in Sample Preparation of Metalloproteins for Low Temperature EPR: the Example of Alkaline Myoglobin</i>	09:40	Francesco Carraro <i>Post Synthetic Metalation of MOFs: Pores as Nanoreactors</i>	09:40	Francesco Sedona <i>Oxygen Dissociation on Iron Phthalocyanine: Tuning the Catalytic Activity by the Supramolecular Order on Ag(110) and Ag(100).</i>
09:35	Maruan Bracci <i>Trap and study of the peroxidase intermediate Compound I using the combination of Rapid Freeze Quench – EPR</i>	10:00	Svetlozar Surnev <i>Interaction of Na with a two-dimensional WO3 layer on Pd(100): From doping to 2D sodium bronzes formation</i>	10:00	Plinio Innocenzi <i>Defects Controlled Optical Properties of h-BN Nanostructures</i>
09:55	David Fioco <i>Photoreactivity Studies of Cr(I) Complexes by EPR Spectroscopy</i>			10:20	Oliver Diwald <i>Rubbing Powders and Other Approaches to Activate Intergranular Charge Transfer in Metal Oxides</i>
10:15	Kavyprya Thangavel <i>EPR Investigations on Metal Organic Frameworks to Elucidate the Gas and Liquid Adsorption Properties</i>	10:30	Coffee-Break	10:50	Coffee-Break
10:35	Andrea Guidetti <i>Development of a Combined Methodology Towards Mechanistic Investigation of Rare Metal-Free, Light Activated Catalysts</i>	11:00	Zbignew Sojka <i>Mechanistic steps of SCR reaction over Cu, Ni and Co zeolites investigated by EPR/HYSCORE and IR/2D COS techniques combined with DFT molecular modeling</i>	11:20	Mikhail Petukhov <i>2D Cuprous Fluoride on Copper Crystal</i>
10:55	Tony Famulari <i>Electronic and Structural Characterization of, Peroxygenase-Like Cytochrome P450, Cyp116b5hd</i>	11:40	Paolo Bruzzese <i>Determination of the Structure and Dynamics of Copper Single-Metal Sites in Zeolites by Means of 17O EPR and DFT Modelling</i>	11:40	Jürgen Behm <i>Electrocatalysis at the Atomic Scale: Nanostructured Bimetallic Electrodes</i>
11:15	Paracat Meeting	12:00	Angelika Brukner <i>Active surface sites in solid catalysts: Searching the needle in a haystack by EPR and friends</i>	12:20	Closing Remarks
		12:30	LUNCH Buffet	12:30	LUNCH Buffet
14:00	Chemistry at the Surface Registration	14:30	Luca Artiglia <i>Temperature and Reaction Environment Influence the Nature of Platinum Species Supported on Ceria</i>		
15:00	Opening of the Workshop	15:00	Piotr Pietrzyk <i>Role of surface reactive oxygen species in adsorption and removal of water toxicants by amorphous metal oxides in the presence of hydrogen peroxide</i>		
15:10	Gianfranco Pacchioni <i>Oxide Surfaces: in the Search of the Hidden Electrons</i>	15:20	Valeria Lagostina <i>CW and Pulse EPR Studies of Vanadium Species on Shape Controlled Anatase Nanocrystals.</i>		
15:50	Gabriele Deplano <i>Titration of Accessible Cu(I) Sites in Cu-Exchanged ZSM-5 by Volumetric CO Adsorption</i>	15:40	Cristiana Di Valentin <i>Modelling Complex Nanosystems for Drug Delivery, Targeting and Imaging.</i>		
16:10	Leonora Podvorica <i>Isolated Ti(III) Species on the Surface of a Pre Active Ziegler-Natta Catalyst</i>	16:10	Coffee-Break		
16:30	Coffee-Break	17:00	Thomas Risse <i>The role of radicals for the hydroxylation of a supported silica bilayer on Ru(0001)</i>		
17:00	Yu-Kai Liao <i>Unravelling the Nature of Cr5+ Species on Silica Surface in Phillips Catalyst by Advanced EPR Techniques</i>	17:30	Damien Murphy <i>Dual mode MW resonators for dielectric heating of radical reactions</i>		
17:20	Mathias Blanco <i>Endohedral Functionalization of Carbon Nanotubes with Enhanced Photocatalytic Activity</i>	18:00	Gaetano Granozzi <i>My scientific journey: encounters and sliding doors</i>		
17:40	Cristina Pavan <i>New Molecular Descriptors of Silica Surface: Towards a Revised Paradigm for Particle Toxicology</i>				
18:00	Jürg Osterwalder <i>Model systems for water splitting electrode surfaces</i>	18:20	Elio Giamello		
19:00	Welcome Party	19:30	Gala Dinner		