

# 25<sup>th</sup> International Conference on Horizons in Hydrogen Bond Research

11-15 September 2023, Bologna, Italy



## Programme





# 25<sup>th</sup> International Conference on “Horizons in Hydrogen Bond Research”

11-15 September 2023 Bologna, Italy

## WELCOME TO BOLOGNA

Welcome to the 25<sup>th</sup> International Conference on “Horizons in Hydrogen Bond Research” (HBOND2023) and Graduate Research Day (GRD).

This edition is the twenty-fifth in the series of conferences on hydrogen bonding which was started by Prof. Lucjan Sobczyk in Poland in 1977 and was held biannually across Europe.

This edition is organized and supported by the Department of Chemistry “G. Ciamician” at the University of Bologna and will be hosted in the teaching buildings of the University (via Andreatta, 8, 40126 Bologna). Financial support from our sponsors is also acknowledged.

The aim of the conference is to bring together scientists working in the field of hydrogen bond and other weak interactions, who study virtually all states of matter by a multitude of experimental and theoretical methods. Non-covalently bonded systems are extremely important in many fields like biology, chemistry, astrophysics and materials sciences.

The scientific programme is organized in different sections introduced by 5 keynote plenary lectures and complemented by 10 invited talks that aim at showing the different fundamental aspects and applications of hydrogen and non-covalently bonded systems. 26 oral contributions and a poster session complete the programme.

The meeting is preceded by a Graduate Research Day (GRD) with a programme specially designed for PhD students. A conference dinner and visit to the University of Bologna Museums complement the programme and will make your stay more enjoyable.

We welcome you to the conference for interesting and entertaining discussions and experiences and we hope it will be an inspiring event that will provide plenty of opportunities for interaction and networking!



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**Supported by**



ALMA MATER STUDIORUM  
UNIVERSITÀ DI BOLOGNA  
DEPARTMENT OF CHEMISTRY  
“GIACOMO CIAMICIAN”





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## Committees

### INTERNATIONAL ADVISORY BOARD

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## **CONFERENCE SITE**

The conference will take place in the Teaching Complex in via Andreatta, 8, Bologna Italy.

The registration desk, coffee breaks and lunches will be located on the ground floor while the conference rooms are on the first floor.

The sessions will be held in **ROOM B** while **ROOMS C** and **D** can be used by the participants in case they need a quiet place during the breaks.

## **REGISTRATION DESK**

The registration desk will be located at the conference site: via Andreatta 8. It will be open on Monday, September 11<sup>th</sup> and Tuesday September 12<sup>th</sup> from 8:30 to 10:00.

It will also be open throughout the conference before and after the sessions and during lunch.

## **SOCIAL DINNER**

Thursday, September 14<sup>th</sup>, 2023, at 20:00 at SYMPO', Via delle Lame, 83, 40122 Bologna BO.

## **GUIDED TOUR TO THE UNIVERSITY OF BOLOGNA HISTORICAL MUSEUMS**

For participants who requested it, we offer a free guided tour to the University of Bologna Historical Museums during the free afternoon on September 14<sup>th</sup> at 14:00 right after lunch.

The visit will take place in groups of twenty and the cost will be covered by the organization.

Please note that the climb up the Tower requires considerable physical effort. Please talk to the organizers if you feel you could have a heart condition or suffer from dizziness and claustrophobia.

## **INSTRUCTIONS FOR AUTHORS**

### *Oral contributions*

The following times are associated with the different types of talk:

- Keynote 45 minutes, 35 for presentation and 10 for discussion.
- Invited 30 minutes, 25 for presentation and 5 for discussion.
- Contributed 20 minutes, 15 for presentation and 5 for discussion.

Speakers presenting a speech are requested to arrive at least 30 minutes before the start of their oral session. Please do consider that the use of your own laptop is highly discouraged. Presentation file format includes .pptx and .pdf.

Authors are required to have a copy of their presentation on a USB drive to be able to upload it to the PC of the corresponding session. If you don't have a USB flash drive available, you can send your presentation by email to [spectrameet@unibo.it](mailto:spectrameet@unibo.it) by the evening before your scheduled talk. This way, the organizers of the event will have the presentation ready for your presentation slot.

### *Poster contribution*

Poster grids will be located at the conference site. Poster size 70 x 100 cm vertical (portrait) orientation.

## **Internet Wi-Fi access**

Participants can access the Wi-Fi infrastructure by using their personal Eduroam account. Please check the service has been activated on your devices.

If a participant does not have access to Eduroam, we can provide them with complimentary registration using the Unibo network (an identification document is required for initial access).



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## Programme

### Monday session – 11 September

9:00 Opening Graduate Research Day

#### **Morning Session 1 9:15-11:10**

**Chair W. Caminati**

9:15 Keynote Talk (KTa) **D. Fazzi**

*The fine interplay between weak interactions and response properties in molecular materials*

10:00 Invited Talk (ITa) **S. Alessandrini**

*Ab initio modeling of Noncovalent System in the gas-phase: Interaction Energy and Geometry*

10:30 Contributed Talk (CTa) **S. Schweer**

*Chirality and isotope effects in acid-alcohol complexes*

10:50 Contributed Talk (CTb) **H. Singh**

*Unravelling the solvent role in the catalysis of the bio-renewable chemical, 6-*amyl- $\alpha$ -pyrone*, using rotational spectroscopy.*

11:10 Coffee break

#### **Morning Session 2 11:40-13:00**

**Chair T. Chakraborty**

11:40 Contributed Talk (CTc) **T. L. Fischer**

*Vibrational Spectroscopy of Hydrate Complexes for Benchmarking with Gas Recycling*

12:00 Contributed Talk (CTd) **A. Verde**

*The Duplication of the Microsolvated Complexes of *p*-Anisaldehyde*

12:20 Contributed Talk (CTe) **F. Torres Hernández**

*Conformational study of 2-phenylethylamine and its aggregates using laser spectroscopy in jets*

12:40 Contributed Talk (CTf) **F. Sun**

*Conformations of monochloropropionic acid in isolated and solution phase*

13:00 Lunch



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**Afternoon Session 1 14:30-16:00**

**Chair R. Paciotti**

14:30 Invited Talk (ITb) **A. Caracciolo**

*Gas-phase and gas-surface interactions of atomic oxygen relevant for terrestrial and extra-terrestrial atmospheres*

15:00 Contributed Talk (CTg) **E. Sennert**

*Halogenated alcohols microsolvating closed-shell and open-shell molecules*

15:20 Contributed Talk (CTh) **M. Barp**

*Gas-Phase Vibrational Spectroscopy of Halide – Hexafluoroisopropanol Complexes: Hydrogen Bond Strength vs. GasPhase Basicity and Anion Proton Affinity*

15:40 Contributed Talk (CTi) **P. Pinillos Pinedo**

*Finding the favored interaction spots of glucose and galactose by using phenol as a probe*

16:00 Coffee break

**Afternoon Session 2 16:20-17:20**

**Chair B. Hartwig**

16:30 Invited Talk (ITc) **A. Camiruaga**

*Insights into the role of water in sugar-peptide molecular recognition: a gas-phase vibrational spectroscopy study of micro-hydrated mannoside-peptide complexes*

17:00 Contributed Talk (CTj) **C. V. Jensen**

*Infrared Spectroscopy of Room Temperature Methanol Clusters*

17:20 Contributed Talk (CTk) **E. Pizzano**

*Near Infrared Spectroscopy as tool for the H-Bond investigations*





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**Tuesday session – 12 September**

9:00 Opening HBOND2023

**Morning Session 1 9:15-11:10**

**Chair P. Ugliengo**

9:15 Keynote Talk (KT1) **P. Hobza**

*Hydrogen Bonding with Hydridic Hydrogen – Experimental Low-Temperature IR and Computational Study: Is A Revised Definition of Hydrogen Bonding Appropriate?*

10:00 Invited Talk (IT1) **F. Zerbetto**

*Hydrogen bonds in molecular knots*

10:30 Contributed Talk (CT1) **S. Gómez**

*Modeling Hydrogen Bonding in Resonance Raman Spectroscopy*

10:50 Contributed Talk (CT2) **V. Zhaunerchy**

*Competition between folded and extended conformers of gas-phase chromophore-free peptides*

11:10 Coffee break

**Morning Session 2 11:40-13:10**

**Chair M. Suhm**

11:40 Invited Talk (IT2) **G. Bistoni**

*Computational Insights into the Role of Hydrogen Bonding in Highly Selective Catalytic Reactions*

12:10 Contributed Talk (CT3) **K. Müller-Dethlefs**

*Non-covalent Interactions: The Synergy of Experiment and Theory Viewed over Two Decades*

12:30 Contributed Talk (CT4) **A. Fernández-Ramos**

*The role of the hydrogen-bonded complexes in bimolecular reactions involving OH at ultra-low temperatures*

12:50 Contributed Talk (CT5) **A. Maris**

*Intra and intermolecular interactions in hydroxylamine derivatives*

13:10 Lunch



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**Afternoon Session 1 14:30-16:20**

**Chair J. Lundell**

14:30 Invited Talk (IT3) **J. Waluk**

*Nuclear Quantum Effects in Intra- and Intermolecular Hydrogen Bonds*

15:00 Contributed Talk (CT6) I. Shenderovich

*Experimentally Proven but Not Yet Explained: Examples of Obscure Mechanisms of Protonation and Proton Transfer*

15:20 Contributed Talk (CT7) **I. Bakó**

*Nuclear quantum effects: their relevance in topology of hydrogenbonded network and diffraction studies of hydrogen bonded liquids*

15:40 Contributed Talk (CT8) **S. Blanco**

*Hydrogen bond cooperativity in the pyridine... $(\text{H}_2\text{O})_n$  ( $n=2-4$ ) adducts generated in a supersonic jet: a rotational spectroscopy study*

16:00 Coffee break

**Afternoon Session 2 16:50-17:40**

**Chair J. Lundell**

16:30 Invited Talk (IT4) **C. Cappelli**

*Hydrogen Bonding: a big challenge for computational spectroscopy*

17:00 Contributed Talk (CT9) **S. D'Agostino**

*Enabling Proton Conduction in Solid Acids Via Supramolecular Complex Formation: The Case of Crown Ethers and Alkali Hydrogensulfates*

17:20 Contributed Talk (CT10) **B. Hartwig**

*Combining microwave and vibrational spectroscopy: The asymmetry parameter of the nuclear quadrupole coupling constants as a possible probe for hydrogen bond strength*



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**Wednesday session – 13 September**

**Morning Session 1 9:15-11:10**

**Chair D. Braga**

9:15 Keynote Talk (KT2) **P. Metrangolo**

*Orthogonal Hydrogen and Halogen Bonding in Peptide Self-Assembly*

10:00 Invited Talk (IT5) **F. Grepioni**

*Nature inspired crystal engineering: from interactions to applications*

10:30 Contributed Talk (CT11) **E. Mendez-Vega**

*Understanding Solvent Polarity: Micro- vs Macrosolvation in Reichardt's Dyes*

10:50 Contributed Talk (CT12) **K. Hermansson**

*Water in and on crystals – a database for ML and a knowledge-base for spectroscopic prediction*

11:10 Coffee break

**Morning Session 2 11:40-13:10**

**Chair N. Walker**

11:40 Keynote Talk (Kt3) **H. Fielding**

*Liquid-microjet photoelectron spectroscopy with UV light pulses*

12:30 Contributed Talk (CT13) **T. Chakraborty**

*Site specific nonradiative decay of halo- and polyphenols: Hydrogen bonding effects*

12:50 Contributed Talk (CT14) **J. A. Fernández**

*Experimental Determination of the Strength of Non-Covalent Interactions in Dimers*

13:10 Lunch



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**Afternoon Session 1 14:30-16:20**

**Chair E. Arunan**

14:30 Invited Talk (IT6) **A. Das**

*Sequence Dependent Folding Motifs of Peptides: A Comprehensive Picture from Condensed and Gas Phase Studies*

15:00 Contributed Talk (CT15) **P. Carçabal**

*When solvated molecules shape the solvent: sugar water interaction in the gas phase*

15:20 Contributed Talk (CT16) **J. C. López**

*Hydrogen Bond Interaction with Water Influence Antioxidant Properties of Flavone*

15:40 Contributed Talk (CT17) **N. Walker**

*Internal Rotation and Isomerisation in Monohydrates of Heteroaromatics: Insights from Rotational Spectroscopy*

16:00 Contributed Talk (CT18) **J. Lundell**

*Revisiting vibrational spectroscopy of the  $H_2O \cdots CO$  complex*

16:20 Coffee break

16:50 Poster Session

18:00 Meeting International Advisory Board

**Thursday session – 14 September**

**Morning Session 1 9:15-11:10**

**Chair K. Hermansson**

9:15 Keynote Talk (KT4) **M. Mas-Torrent**

*Morphology and polymorphism control in organic semiconductor thin films as a tool to optimize the device performance*

10:00 Invited Talk (IT7) **M. R. Chierotti**

*Walking along hydrogen bonds by means of solid-state NMR*

10:30 Contributed Talk (CT19) **P. Hapala**

*Designing photosensitive hydrogen bonded polymer templates for molecular nanofabrication*

10:50 Contributed Talk (CT20) **A. Krawczuk**

*Influence of hydrogen bond formation on prediction of dipole moments of proteins – GruPol database approach*

11:10 Coffee break

**Morning Session 2 11:40-13:10**

**Chair J. A. Fernández**

11:40 Invited Talk (IT8) **C. Fonseca Guerra**

*Discovering in silico the uniqueness of hydrogen bonding*

12:10 Contributed Talk (CT21) **S. Pothoczki**

*Hydration of monosaccharide molecules*

12:30 Contributed Talk (CT22) **M. Paolantoni**

*Hydration properties of sugars revisited*

12:50 Contributed Talk (CT23) **D. Obenchain**

*Exploring the different ortho/para effects in the binding of H<sub>2</sub> in gas-phase complexes*

13:10 Lunch

14:00 Guided tour to the UniBo Historical Museums / Free afternoon

20:00 Social dinner at SYMPO', via delle Lame 83



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**Friday session – 15 September**

**Morning Session 1 9:15-11:10**

**Chair M. Schnell**

9:15 Keynote Talk (KT5) **H. Kjærgaard**

*Hydrogen Bonds in Atmospheric Compounds and Complexes*

10:00 Invited Talk (IT9) **S. Coussan**

*Study of  $CH_3I \cdots (H_2O)_n$  complexes. From  $CH_3I \cdots H_2O$  to  $CH_3I$  in interaction with amorphous, cubic and hexagonal water ice. Atmospheric implications and nuclear risks*

10:30 Contributed Talk (CT24) **S. Sobanska**

*Investigation of interactions between water and organic molecules of atmospheric interest – Implication in aging of secondary organic aerosols*

10:50 Contributed Talk (CT25) **E. Vogt**

*The First OH-stretching Overtone Region of Water Dimer*

11:10 Coffee break

**Morning Session 2 11:40-13:10**

**Chair P. E. Hansen**

11:40 Invited Talk (IT10) **P. Bolognesi**

*Cyclic dipeptides as intermediates “seeds of life”? An experimental and computational model*

12:10 Contributed Talk (CT26) **R. Paciotti**

*DFT calculations and IRMPD spectroscopy: the relevant role of H bond for structure assignment*

12:30 Poster Prizes – HBOND2023

12:50 Closing Remarks

13:10 Lunch



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**HIDEN**  
ANALYTICAL

# Instruments for Advanced Science

Mass spectrometers for vacuum, gas, plasma and surface science

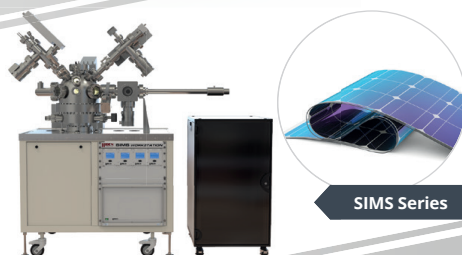
## Residual Gas Analysis

Perform RGA at UHV/XHV. Our RGA configurations include systems for UHV science applications including temperature-programmed desorption and electron/photon stimulated desorption.



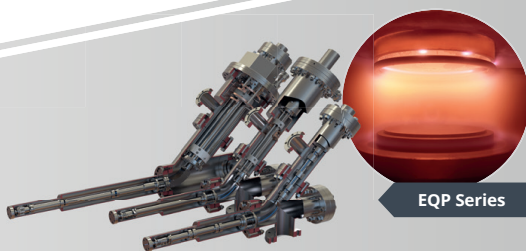
## Thin Film Surface Analysis

Conduct both static and dynamic SIMS analysis with a choice of primary ions for full chemical composition and depth profiling. Our SIMS solutions include complete workstations and bolt-on modules.



## Plasma Characterisation

Fully characterise a range of plasmas: RF, DC, ECR and pulsed plasmas, including neutrals and neutral radicals. Extend your analyses to atmospheric pressure processes using the HPR-60, with time-resolved mass/energy analysis.





HBOND2023						
Graduate Research Day		Tuesday 12/09/23	Wednesday 13/09/23	Thursday 14/09/23	Friday 15/09/23	
9:00	<b>Monday 11/09/23</b>	9:00				
	<b>Opening GRD</b>	<b>Opening HBOND2023</b>				
	<b>Chair W. Caminati</b>	<b>Chair P. Ugliengo</b>	<b>Chair D. Braga</b>	<b>Chair K. Hermansson</b>	<b>Chair M. Schnell</b>	
9:15	<b>KTa D. Fazzi</b>	<b>KT1 P. Hobza</b>	<b>KT2 P. Metrangolo</b>	<b>KT4 M. Mas-Torrent</b>	<b>KT5 H. Kjærgaard</b>	
10:00	<b>ITa S. Alessandrini</b>	<b>IT1 F. Zerbetto</b>	<b>IT5 F. Grepioni</b>	<b>IT7 M. R. Chierotti</b>	<b>IT9 S. Coussan</b>	
10:30	<b>CTa S. Schweer</b>	<b>CT1 S. Gómez</b>	<b>CT11 E. Mendez-Vega</b>	<b>CT19 P. Hapala</b>	<b>CT24 S. Sobanska</b>	
10:50	<b>CTb H. Singh</b>	<b>CT2 V. Zhaunerchy</b>	<b>CT12 K. Hermansson</b>	<b>CT20 A. Krawczuk</b>	<b>CT25 E. Vogt</b>	
11:10	<b>Coffee break</b>	<b>Coffee break</b>	<b>Coffee break</b>	<b>Coffee break</b>	<b>Coffee break</b>	
	<b>Chair T. Chakraborty</b>	<b>Chair M. Suhm</b>	<b>Chair N. Walker</b>	<b>Chair J.A. Fernández</b>	<b>Chair P. E. Hansen</b>	
11:40	<b>CTc T. L. Fischer</b>	<b>IT2 G. Bistoni</b>	<b>KT3 H. Fielding</b>	<b>IT8 C. Fonseca Guerra</b>	<b>IT10 P. Bolognesi</b>	
12:00	<b>CTd A. Verde</b>	<b>CT3 K. Müller-Dethlefs</b>		<b>CT21 S. Pothoczki</b>	<b>CT26 R. Paciotti</b>	
12:20	<b>CTe F. Torres Hernández</b>	<b>CT4 A. Fernandez-Ramos</b>	<b>CT13 T. Chakraborty</b>	<b>CT22 M. Paolantoni</b>	<b>Poster prizes - HBOND2023</b>	
12:40	<b>CTf F. Sun</b>	<b>CT5 A. Maris</b>	<b>CT14 J. A. Fernández</b>	<b>CT23 D. Obenchain</b>	<b>Closing remarks</b>	
13:00	<b>Lunch</b>	<b>Lunch</b>	<b>Lunch</b>	<b>Lunch</b>	<b>Lunch</b>	
	<b>Chair R. Paciotti</b>	<b>Chair J. Lundell</b>	<b>Chair E. Arunan</b>			
14:30	<b>ITb A. Caracciolo</b>	<b>IT3 J. Waluk</b>	<b>IT6 A. Das</b>	<b>FREE</b>		
15:00	<b>CTg E. Sennert</b>	<b>CT6 I. Shenderovich</b>	<b>CT15 P. Çarçabal</b>	<b>or</b>		
15:20	<b>CTh M. Barp</b>	<b>CT7 I. Bakó</b>	<b>CT16 J. C. López</b>			
15:40	<b>CTI P. Pinillos Pinedo</b>	<b>CT8 S. Blanco</b>	<b>CT17 N. Walker</b>	<b>Guided tour to University of Bologna Historical Museums (1h)</b>	<b>DEPARTURE</b>	
16:00	<b>Coffee break</b>	<b>Coffee break</b>	<b>CT18 J. Lundell</b>			
	<b>Chair B. Hartwig</b>	<b>Chair J. Lundell</b>	<b>Coffee break</b>			
16:30	<b>ITc A. Camiruaga</b>	<b>IT4 C. Cappelli</b>				
17:00	<b>CTj C. V. Jensen</b>	<b>CT9 S. D'Agostino</b>	<b>Poster session</b>			
17:20	<b>CTk E. Pizzano</b>	<b>CT10 B. Hartwig</b>	<b>Meeting IAB</b>			
				<b>Social Dinner</b>		