

HBOND 2022

12 - 15 SEPTEMBER 2022

24th International Conference on Horizons in Hydrogen Bond Research

PROGRAMME

Bilbao, September 2022

www.hbond2022bilbao.com



MONDAY 12

08.00 – 09.00

REGISTRATION

09.00 – 09.15

OPENING

SESSION 1 – Chairman: **Elanganan Arunan**

09.15 – 10.00

PLENARY LECTURE 1: Mischa Bonn

A molecular view of water interfaces.

10.00 – 10.30

INVITED TALK 1: Eric Borguet

The impact of hydrogen bonding on vibrational relaxation at aqueous interfaces.

10.30 – 11.00

SELECTED TALK 1: Timothy Zwier

Single-Conformation Spectroscopy and Electronic Energy Transfer along a H-bonded Peptide Scaffold.

11.00 – 11.30

COFFEE BREAK

SESSION 2 – Chairman: **Emilio J. Cocinero**

11.30 – 12.00

IT 2: Tapas Chakraborty

Hydrogen Bonding Effects on Excited and Ionic State Dynamics of Binary Phenolic.

12.00 – 12.20

ORAL COMMUNICATION 1: Mario Gutiérrez

Proton Transfer Dyes Encapsulated within MOFs: A Promising Approach for Detecting Vapors of Acids and Bases.

12.20 – 12.40

OC 2: Ilya Shenderovich

Adduct under Field – Modeling the Effects of Solvent and Matrix on Hydrogen Bonding.

12.40 – 13.00

OC 3: Manuel Monge-Palacios

The Effect of Hydrogen Bonding on the Reactivity of OH Radicals with Prenol and Isoprenol: Multistructural Torsional Variational Transition State Theory Calculations and Shock Tube Experiments.

13.00 – 14.30

LUNCH BREAK

SESSION 3 – Chairman: **Asier Longarte**

14.30 – 15.00

IT 3: Edit Matyus

Exact quantum dynamics developments for molecular complexes and floppy molecular systems.

15.00 – 15.30

IT 4: Sławomir Grabowski

Interactions that should be classified as hydrogen bonds but are not by accepted definitions.

15.30 – 16.00

IT 5: Poul Erik Hansen

Intra-molecular Hydrogen bonding in NH...X Systems. New Insights.

16.00 – 16.30

COFFEE BREAK

16.30 – 16.50

OC 4: Imanol Usabiaga

Large difference in Binding Energy despite molecular similarity. Computational modeling and laser spectroscopy experiments of Theophylline-DNA complexes.

16.50 – 17.10

OC 5: Camilla Calabrese

Probing non covalent interactions by means of rotational spectroscopy in fluorinated aromatic rings.

17.10 – 17.30

OC 6: Taija Lena Fischer

The HyDRA Blind Challenge.

17.30 – 19.30

POSTER SESSION 1

TUESDAY 13

SESSION 4 – Chairman: **Sonia Melandri**

09.00 – 09.45

PL 2: **Melanie Schnell**

Probing the growing hydrogen-bond networks in microsolvated complexes using broadband rotational spectroscopy.

09.45 – 10.15

IT 6: **Pierre Çarçabal**

Interactions of sugars with biomolecules and water in the gas phase.

10.15 – 10.45

IT 7: **Yoshiteru Matsumoto**

Microscopic chiral-recognition in propylene oxide dimer induced by H-bond of an achiral pyrrole molecule.

10.45 – 11.05

OC 7: **Ander Camiruaga**

Spectroscopic study of intermolecular interactions between mannose and receptor models.

11.05 – 11.30

COFFEE BREAK

SESSION 5 – Chairman: **Martin Suhm**

11.30 – 12.00

IT 8: **Naresh Patwari**

Reaction Fields in Proton Transfer Reactions.

12.00 – 12.20

OC 8: **Nanna Falk Christensen**

Equilibrium constants of hydrated complexes at room temperature.

12.20 – 12.40

OC 9: **Marcos Juanes**

Hydrogen bonding involving oxygen, sulfur and nitrogen in six membered-ring aggregates by microwave spectroscopy.

12.40 – 13.00

OC 10: **Sumitra Vishram**

Dipole moment enhanced π - π stacking in fluorophenylacetylenes.

13.00 – 14.30

LUNCH BREAK

SESSION 6 – Chairman: **Nick Walker**

14.30 – 15.15

PL 3: **Otto Dopfer**

Geometric and Electronic Structure of Silane-Based Cation Clusters: Charge-Inverted Ionic H-Bonds, 3c-2e Bonds & Silicon Hydride Wires.

15.15 – 15.45

IT 9: **Bruno Martínez-Haya**

On the manifold proton bonding of H₃O⁺ in polyether ring cavities.

15.45 – 16.15

IT 10: **Oleg Boyarkine**

Identification of isomeric biomolecules by spectroscopy of non-covalent ionic complexes.

16.15 – 16.45

COFFEE BREAK

SESSION 7 – Chairman: **Francisco Basterretxea**

16.45 – 17.15

IT 11: **Wouter Herrebout**

Assessing a neural network based approach for vibrational circular dichroism spectroscopy: the impact of intramolecular hydrogen bonding.

17.15 – 17.45

ST 2: **Abderrazzak Douhal**

Spectroscopy and Dynamics of Selected Hydrogen-bonded Organic Frameworks (HOFs).

17.45 – 18.05

OC 11: **Casper Vindahl Jensen**

Room Temperature Gas-phase FTIR Spectroscopy of tert-Butyl Hydroperoxide (TBHP) Dimer

18.05 – 18.25

OC 12: **Pablo Pinacho**

Hydrogen-Bonding Network and Geometries of Hydrogen Sulfide and Water Complexes.

18.25 – 18.45

OC 13: **Namitha Brijit Bejoy**

Outer-Valence Intermolecular Coulombic Decay in Hydrogen-Bonded Complex.

18.45 – 19.05

OC 14: **Fernando Torres Hernández**

Spectroscopic study of 2-Phenylethanethiol and its aggregates.

19.05 – 19.25

OC 15: **Sophie M. Schweer**

Acid vibrations in complexes with alcohols: Are the protons ready to jump?

WEDNESDAY 14

09.30 – 13.00

EXCURSION

13.00 – 14.30

LUNCH BREAK

SESSION 8 – Chairman: **Alberto Lesarri**

14.30 – 15.15

PL 4: **Sanjay Wategaonkar**

Dimethylsulfide/Ether Complexes Violate the Badger-Bauer Rule.

15.15 – 15.45

IT 12: **Cristóbal Pérez**

Revealing Hydrogen Bond Topologies from Broadband Rotational Spectroscopy.

15.45 – 16.15

IT 13: **Himansu S. Biswal**

Secondary Effects of Hydrogen Bonding with Sulfur and Selenium: Energy Transfer, Chemical Shielding, Aromaticity and Piezoelectricity.

16.15 – 16.45

COFFEE BREAK

16.45 – 17.05

OC 16: **Oleg Filippov**

The role of dihydrogen bond and tetrel bond in the dehydrocoupling of phenylsilanes/ alcohols.

17.05 – 17.25

OC 17: **Maidier Parra-Santamaría**

Challenging the limits of rotational spectroscopy: gas phase structural elucidation of multiconformational macrolactones.

17.25 – 17.45

OC 18: **Surabhi Gupta**

Ammonia@Crown Ether: Hydrogen bonds, inversion and tunnelling.

17.45 – 19.30

POSTER SESSION 2

THURSDAY 15

SESSION 9 – Chairman: G. Naresh Patwari

09.00 – 09.45

PL 5: **Ruth Signorell**

Intermolecular Interactions in Vapor Nucleation and Condensation.

09.45 – 10.15

IT 14: **Belén Maté**

Hydrogen bonds in ices of astrophysical and atmospheric interest.

10.15 – 10.45

IT 15: **Igor Reva**

Characterization of Hydrogen Bonds in Molecules with OH Group via Generation of Non-Hydrogen-Bonded Conformers.

10.45 – 11.05

OC 19: **Wenqin Li**

Hydrogen bonding, π -Stacking or both? Rotational Observation of Hydrogen-Bond Assisted Stacking in the Heterodimers of 1-Naphthol--1-Naphthalenethiol and 2-Naphthol--2-Naphthalenethiol.

11.05 – 11.30

COFFEE BREAK

SESSION 10 – Chairman: Ilya Shenderovich

11.30 – 12.00

IT 16: **Jon Matxain**

The importance of Hydrogen Bonding in Polymeric Materials.

12.00 – 12.20

OC 20: **Himanshi Singh**

Interplay between intra- and intermolecular H-bond interactions of alpha-methoxy phenylacetic acid and its complexes.

12.20 – 12.40

OC 21: **Sonia Melandri**

σ -hole activation and structural changes upon perfluorination of aryl halides: direct evidence from gas phase rotational spectroscopy.

12.40 – 13.00

Presentation of HBOND 2023: **Sonia Melandri**

13.00 – 14.30

LUNCH BREAK

SESSION 11 – Chairman: **Timothy S. Zwier**

14.30 – 15.00

IT 17: **Jan Rezáč**

Development of semiempirical quantum-mechanical methods targeting non-covalent interactions.

15.00 – 15.30

IT18: **Daniel Obenchain**

Agreeing that we disagree, a double-benchmark study of the complexes of 1-naphthol.

15.30 – 16.00

ST 3: **Asier Longarte**

Influence of H bonds in the photoionization of aqueous aniline.

16.00 – 16.30

COFFEE BREAK

16.30 – 16.50

OC 22: **Wutharath Chin**

Selective photoisomerisation of salicylic acid.

16.50 – 17.10

OC 23: **Barbara Golec**

The effect of hydrogen bonding on photophysics and photostability of indole derivatives.

17.10 – 17.30

OC 24: **Nick Walker**

Microwave spectra, molecular geometries, and internal rotation of CH₃ in N-methylimidazole...H₂O and 2-methylimidazole...H₂O Complexes.

17.30 – 17.50

OC 25: **Wolf D. Geppert**

Spectroscopic investigations of atmospherically relevant acrolein–water and acrolein-methanol complexes.

21.00

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Ercisa eventos & servicios

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