



# IBER 2025

XVIII IBERIAN JOINT MEETING ON  
ATOMIC AND MOLECULAR  
PHYSICS

## PROGRAM

| MONDAY      |                                     | JULY 21 |
|-------------|-------------------------------------|---------|
| 17:30-18:30 | REGISTRATION                        |         |
| 18:30-20:30 | WELCOME RECEPTION<br>POSTER SESSION |         |

| TUESDAY     |                                                                                                                                               | JULY 22 |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------|---------|
| 8:45-9:00   | OPENING SESSION                                                                                                                               |         |
| Session     | 1<br>Chair: José Andrés Fernández                                                                                                             |         |
| 9:00-9:40   | PLENARY P1: Frédéric Merkt<br>Precision tests of fundamental physical theory in few-electron atoms and molecules                              |         |
| 9:40-10:05  | INVITED I1: Andrea Lombardi<br>Nanoporous $\gamma$ -Graphynes for Selective CO <sub>2</sub> Capture: Modeling Adsorption and Storage Dynamics |         |
| 10:05-10:20 | ORAL O1: Emilio J. Cocinero<br>High-Resolution Spectroscopies for Unravelling Molecular Mechanisms Across Disciplines                         |         |
| 10:20-10:35 | ORAL O2: Domingo Heras Elvira<br>Gas-Phase Structure of Riluzole Revealed by High-Resolution Microwave Spectroscopy                           |         |
| 10:35-10:50 | ORAL O3: Jorge Miguel Sampaio<br>Atomic Calculations for Modelling Kilonova Spectral Evolution                                                |         |
| 10:50-11:20 | COFFEE BREAK                                                                                                                                  |         |
| Session     | 2<br>Chair: Saulo Vázquez                                                                                                                     |         |

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| 11:20-12:00    | <b>PLENARY P2: Luis G. Arnaut</b><br>FLASH Therapies: How the Saturation of Light Absorption Enables Selectivity in Oncology                                                   |
| 12:00-12:25    | <b>INVITED I2: Juan J. Nogueira</b><br>Intermolecular Interactions in Membrane Permeation and Protein Bindings                                                                 |
| 12:25-12:40    | <b>ORAL O4: Harry J. Stroud</b><br>Developing an iMD-VR+SMD protocol for sampling complex reaction coordinates defined using interactive molecular dynamics in virtual reality |
| 12:40-12:55    | <b>ORAL O5: Raúl Lago Saavedra</b><br>Automatization protocol for computational reconstruction of the time-evolution of biomolecular processes                                 |
| 12:55-13:10    | <b>ORAL O6: Lorena Ruano de Domingo</b><br>Molecular Insights into the Interactions between Bioactive Molecules and Membranes                                                  |
| 13:10-13:25    | <b>ORAL O7: Alberto Martín Santa Daría</b><br>Intersystem crossing in enzyme catalysis: the cases of glucose oxidases                                                          |
| 13:25-15:00    | <b>LUNCH</b>                                                                                                                                                                   |
| <b>Session</b> | <b>3</b><br><b>Chair: Juan J. Nogueira</b>                                                                                                                                     |
| 15:00-15:40    | <b>PLENARY P3: Nadia Balucani</b><br>Reactive collisions of atomic oxygen and aromatic compounds in crossed-beam experiments                                                   |
| 15:40-16:05    | <b>INVITED I3: Ángel Martín Pendás</b><br>Chemical Machine Learning with Real-Space Chemical Descriptors                                                                       |
| 16:05-16:20    | <b>ORAL O8: Ion Mitxelena</b><br>NOFT: An efficient method for Strong Correlation                                                                                              |
| 16:20-16:35    | <b>ORAL O9: David Ferro Costas</b><br>Semi-Automated Workflow for Contaminant Degradation Mechanisms: Bisphenol A under Fenton-Type Conditions                                 |
| 16:35-16:50    | <b>ORAL O10: Omar López Rodríguez</b><br>Cutting-edge Machine Learning Approaches for efficient and accurate reaction network analysis                                         |
| 17:20          | <b>TOURISTIC ACTIVITY</b><br>Visit to the Martín Códax Albariño<br>Wine Cellars and Tasting                                                                                    |

| WEDNESDAY JULY 23 |                                                                                                                                                                       |
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| Session           | 4<br>Chair: Alberto Lesarri                                                                                                                                           |
| 8:55-9:40         | <b>PLENARY P4 (Miguel Catalán Talk): Timothy S. Zwier</b><br>Single-Conformer Spectroscopy and Photodynamics of Cryo-cooled Gas-Phase Ions                            |
| 9:40-10:05        | <b>INVITED I4: Bruno Martínez Haya</b><br>Freezing protons: proton bonding at cryogenic temperatures                                                                  |
| 10:05-10:20       | <b>ORAL O11: Belén Maté</b><br>Infrared optical constants and band strengths of 10 K H <sub>2</sub> O, CO <sub>2</sub> and CO porous ice mixtures                     |
| 10:20-10:35       | <b>ORAL O12: Rita Roque</b><br>Breaking temperature barriers: unlocking new molecular libraries for jet-cooled spectroscopy                                           |
| 10:35-10:50       | <b>ORAL O13: Pongpanot Pongworasuwanna</b><br>UV Photochemistry of Molecular Clusters as Model Systems for Building a Bottom-up Understanding of New Particle Systems |
| 10:50-11:20       | <b>COFFEE BREAK</b>                                                                                                                                                   |
| Session           | 5<br>Chair: Jorge Miguel Sampaio                                                                                                                                      |
| 11:20-12:00       | <b>PLENARY P5: Vincent Lorient</b><br>Ionization time delay from molecules of increasing size                                                                         |
| 12:00-12:25       | <b>INVITED I5: Helder Crespo</b><br>Seeing inside a femtosecond laser pulse: practical routes to single-cycle light                                                   |
| 12:25-12:40       | <b>ORAL O14: Alexandre Zanchet</b><br>The H <sub>2</sub> +CN reaction dynamics                                                                                        |
| 12:40-12:55       | <b>ORAL O15: Pablo del Mazo Sevillano</b><br>The destruction of CH <sup>+</sup> with atomic hydrogen at low temperature understood: a non-adiabatic dynamical study   |
| 12:55-13:10       | <b>ORAL O16: Pedro Recio</b><br>Photodissociation dynamics of methyl- nitrite (CH <sub>3</sub> ONO) in the A band                                                     |
| 13:10-13:25       | <b>ORAL O17: Lola González Sánchez</b><br>Relevant anions in Astrochemistry: Computational simulation of inelastic collisions in gas phase                            |

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| 13:25-15:00    | <b>LUNCH</b>                                                                                                                                                                                                 |
| <b>Session</b> | <b>6</b><br><b>Chair: Ángel Martín Pendás</b>                                                                                                                                                                |
| 15:00-15:40    | <b>PLENARY P6: Wybren Jan Buma</b><br>Tailoring photon converters                                                                                                                                            |
| 15:40-16:05    | <b>INVITED I6: André Filipe Cortez</b><br>Enhancing Light Collection of next-generation Dark Matter detectors: From wavelength-shifters to novel hybrid optical structures                                   |
| 16:05-16:20    | <b>ORAL O18: Luca Mancini</b><br>Insights from Atomistic Molecular Dynamic Simulations into Intermolecular Forces in Graphene-like Materials                                                                 |
| 16:20-16:35    | <b>ORAL O19: Luis Sustelo</b><br>Prospects of Quantum Computing of Atomic Energies                                                                                                                           |
| 16:35-16:50    | <b>ORAL O20: Sara Gil Guerrero</b><br>Decoding the Architecture of Molecular Diodes: Toward Rational Design for Ideal Rectification                                                                          |
| 16:50-17:20    | <b>COFFEE BREAK</b>                                                                                                                                                                                          |
| <b>Session</b> | <b>7</b><br><b>Chair: Marta Manso</b>                                                                                                                                                                        |
| 17:20-18:00    | <b>PLENARY P7: Arne Senftleben</b><br>Chiral dynamics in crystals and molecules                                                                                                                              |
| 18:00-18:25    | <b>INVITED I7: Stefan Gerlich</b><br>Advancing High-Mass Matter-Wave Interferometry with Metal Clusters and Biomolecules                                                                                     |
| 18:25-18:40    | <b>ORAL O21: Elena Jiménez Martínez</b><br>Gas-phase Reaction Kinetics of Interstellar Radicals with H <sub>2</sub> S and CH <sub>3</sub> CH <sub>2</sub> SH at Ultra-Low Temperatures down to 11.7 K        |
| 18:40-18:55    | <b>ORAL O22: Germán Molpeceres</b><br>The isomerism of interstellar formic acid. A story told in three acts.                                                                                                 |
| 18:55-19:10    | <b>ORAL O23: Miguel Jiménez Redondo</b><br>Reaction rate coefficients of the deuterated Hx <sup>+</sup> + H <sub>2</sub> and HCl <sup>+</sup> + H <sub>2</sub> systems studied in a low-temperature ion trap |

| THURSDAY JULY 24 |                                                                                                                                                                                                               |
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| Session          | 8<br>Chair: Luis Bañares                                                                                                                                                                                      |
| 9:00-9:40        | <b>PLENARY P8: Helen Fielding</b><br>UV Photoelectron Spectroscopy of Aqueous Solutions                                                                                                                       |
| 9:40-10:05       | <b>INVITED I8: Eva Marguí Grabulosa</b><br>Enhancing analytical performance of XRF: Cutting-edge sample treatment strategies and chemometric tools                                                            |
| 10:05-10:20      | <b>ORAL O24: Asier Longarte</b><br>Time-resolved Photoionization of Aromatic Molecules in Solution                                                                                                            |
| 10:20-10:35      | <b>ORAL O25: Roger Yulier Bello Romero</b><br>An Orbital Basis Set for Double Photoionization of Atoms and Molecules                                                                                          |
| 10:35-10:50      | <b>ORAL O26: Celso Manuel Gonzalez Collado</b><br>Electronic coherences in molecules with XFAIMS                                                                                                              |
| 10:50-11:20      | <b>COFFEE BREAK</b>                                                                                                                                                                                           |
| Session          | 9<br>Chair: José Pires Marques                                                                                                                                                                                |
| 11:20-12:00      | <b>PLENARY P9: Alberto Ruiz Jimeno</b><br>Future Higgs Factories: Advances in Physics, Viability and Sustainability                                                                                           |
| 12:00-12:25      | <b>INVITED I9: María J. López</b><br>Metal-fullerene complexes for hydrogen energy technologies                                                                                                               |
| 12:25-12:40      | <b>ORAL O27: Rita Prosimi</b><br>Confining He atoms in diverse ice-phases: Stability and energetics of hydrate crystals                                                                                       |
| 12:40-12:55      | <b>ORAL O28: Marta I. Hernández</b><br>Separation of hydrogen isotopologues through adsorption on a sodium-decorated graphene prototype: a quantum-mechanical study                                           |
| 12:55-13:10      | <b>ORAL O29: Cristina Maria Bernardes Monteiro</b><br>Scintillation yield from MPGD avalanches in He-40%CF <sub>4</sub> admixtures with few percent of molecular additives for directional Dark Matter search |
| 13:10-13:25      | <b>ORAL O30: José Campos Martínez</b><br>Quantum sieving and isotopic separation by two-dimensional membranes                                                                                                 |

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| 13:25-15:00    | <b>LUNCH</b>                                                                                                                                                          |
| <b>Session</b> | <b>10</b><br><b>Chair: Sérgio Domingos</b>                                                                                                                            |
| 15:00-15:40    | <b>PLENARY P10: Henrik G. Kjærgård</b><br>OH-stretching vibrations in molecular complexes - from cold to warm                                                         |
| 15:40-16:05    | <b>INVITED I10: Cristóbal Pérez</b><br>Rotational Spectroscopy for Structural Elucidation of Complex Molecular Aggregates                                             |
| 16:05-16:20    | <b>ORAL O31: José A. Fernández</b><br>Interaction Energies of Molecular Aggregates: Predictive Models vs. Experimental Data                                           |
| 16:20-16:35    | <b>ORAL O32: Aran Insausti</b><br>Evolution of Solute–Water Interactions in the Methyl Benzoate-(H <sub>2</sub> O) <sub>1–5</sub> Clusters by Rotational Spectroscopy |
| 16:35-16:50    | <b>ORAL O33: Sergio Mato</b><br>Deciphering the Molecular Basis of HIV Treatment: Gas-Phase Analysis of Lamivudine and Emtricitabine                                  |
| 16:50-17:20    | <b>COFFEE BREAK</b>                                                                                                                                                   |
| <b>Session</b> | <b>11</b><br><b>Chair: José Manuel Hermida</b>                                                                                                                        |
| 17:20-17:35    | <b>ORAL O34: Ana Filomena Botelho Isabel</b><br>Measurement of Dual-Component Attenuation Length in Square BCF-92 Wavelength-Shifting Fibers                          |
| 17:35-17:50    | <b>ORAL O35: Pedro Alberto Oliveira Costa e Silva</b><br>A large area gas proportional scintillation counter with annular geometry for x- and gamma-ray spectroscopy  |
| 17:50-18:05    | <b>ORAL O36: Fernando Domingues Amaro</b><br>NeuThin - Neutron Position Sensitive Detectors using Ultra-Thin Converter Layers                                         |
| 18:05-18:20    | <b>CLOSING CEREMONY</b>                                                                                                                                               |
| 18:20-19:00    | <b>GEFAM MEMBERS ASSEMBLY</b>                                                                                                                                         |
| 21:00          | <b>GALA DINNER</b><br>DELGADO-BARRIO AWARD                                                                                                                            |