



XVI CONFERENCE OF YOUNG RESEARCHERS IN ATOMIC AND MOLECULAR PHYSICS

**University of Valladolid
24 - 27 February 2025**



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Universidad de Valladolid



This is the short version of the conference booklet. Full abstracts with all authors, references, and figures can be found at www.j2ifam2025.uva.es



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ABOUT

J2IFAM 2025 - VALLADOLID

Greetings to all young physical-chemistry community, It is with great pleasure that we welcome you to the XVI edition of the **J²IFAM2025 Conference** that will be held in Valladolid.

The first Symposium of Young Researchers on Atomic and Molecular Physics was held in **Madrid in December 2008**. Organized by the Atomic and Molecular Physics and Aggregates Department of the Instituto de Física Fundamental (CSIC), the symposium aimed to provide young researchers with a platform to share their investigations.

The 1st edition brought together 18 participants. Since then, the conference has expanded to different cities across Spain, welcoming an ever-growing number of young scientists.

We are excited to welcome you to this XVI Edition, taking place in Valladolid for the second time (2016, 2025), and we hope you enjoy the conference.

SCIENTIFIC COMMITTEE

Prof. Dr. Jens-Uwe Grabow - Institut für Physikalische Chemie und Elektrochemie Leibniz, Universität Hannover

Prof. Dr. Martin K. Beyer - Institute for Ion Physics and Applied Physics, Universität Innsbruck

Prof. Dr. Jochen Küpper - Deutsches Elektronen-Synchrotron DESY, Universität Hamburg

Prof. Dr. Assimo Maris - Dipartimento di Chimica “G. Ciamician”, Università di Bologna

Prof. Dr. Elias Neeman - Physique des Lasers Atomes et Molécules (PhLAM), Université de Lille

Prof. Dr. Julia Contreras-García - Centre national de la recherche scientifique (CNRS), Sorbonne Université

Prof. Dr. Vincenzo Barone - Dipartimento di Chimica Teorica e Computazionale Scuola Normale Superiore di Pisa.

LOCAL ORGANIZING COMMITTEE

Andrés Verde
Ricardo Morán
Roger Castillo
Wenqin Li

Domingo Heras
Marcos Juanes
Sergio Mato
Zhen Wang

Farha Sajeev
Pratyush Ranjan
Sofia Municio

USEFUL INFORMATION

VENUE

The conference will be held over four days at two key venues: the Aula Mergelina of the Law Faculty (24th and 25th) and the Aula Magna of the Faculty of Sciences (26th and 27th).

REGISTRATION DESK

The **registration desk** is located in the entrance of both venues and will be open on:

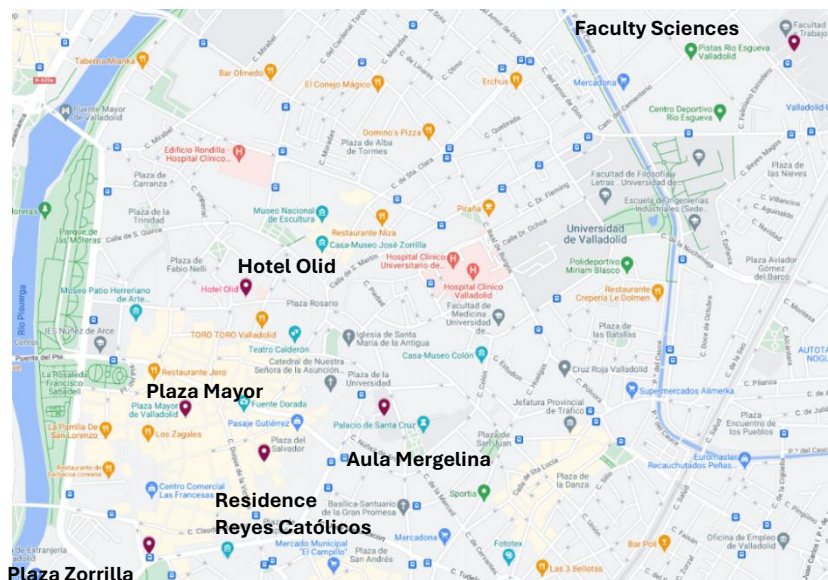
- Monday 24th February from 14:00 to 16:30.
- Throughout the conference during the breaks.

UNIVERSITY RESIDENCE: REYES CATÓLICOS

The **Reyes Católicos University Residence** is conveniently located, providing easy access to the conference locations.

MEALS

The lunch of days 26th and 27th of February will be provided by the organization at the **Campus Cafeteria**, located next to the Faculty of Sciences. Several meal options will be available, including choices for attendees with dietary restrictions.



SOCIAL PROGRAM



Guided Tour of Valladolid

Discover the rich history and charm of Valladolid on a guided city tour. Stroll through its historic streets, admire its stunning architecture, and immerse yourself in the cultural heritage of this vibrant city.

Meeting point: Plaza Zorrilla

Time: Tuesday, February 25th, at 16:30



Research Lab Visit

Get an exclusive behind-the-scenes look at the cutting-edge research conducted by the university's scientific teams. This guided visit will take you through the laboratories of the research groups at the Faculty of Sciences, where you will learn about their latest projects and innovations.



Gala Dinner

Join us for an unforgettable Gala Dinner, where attendees will have the opportunity to enjoy an exquisite meal in a refined setting while socializing with colleagues and speakers. This evening will be the perfect occasion to celebrate the conference in a relaxed and elegant atmosphere.

Venue: Restaurante La Raiz, Calle Recondo 3

Time: Thursday, February 27th, at 21:00

DETAILED PROGRAM

Monday Session – 24th February 2025

14:00-16:00 REGISTRATION

16:00-16:45 OPENING CEREMONY

Afternoon Session A 17:00-18:15

Chair: Isabel Peña

17:00-17:45 Plenary Talk (PT1): **Sérgio R. Domingos**

Molecular Structure and Recognition in the Gas Phase: A Rotational Expedition

17:45-18:15 Coffee Break

Afternoon Session B 18:15-19:15

Chair: Alberto Lesarri

18:15-18:45 Invited Talk (IT1): **Miguel Gallegos**

Explainable Chemical AI (XCAI): Moving Beyond Accurate Predictions

18:45-19:00 Contributed Talk (CT1): **Raidel Martin Barrios**

Inelastic collision of hydrogen atoms on tungsten surfaces with hydrogen coverage

19:00-19:15 Contributed Talk (CT2): **Daniel Félix González**

*Reactive Collisions of $S(^3P) + H_3^+$ ($^1A''$): Force-Field approach to the *ab initio* Potential Energy Surface*

Tuesday Session – 25th February 2025

Morning Session A 9:15-11:30

Chair: Teresa Belmonte

9:15-10:00 Plenary Talk (PT2): **Christian Clear**

The Power of Precision: Improving Atomic Data for Astrophysical Discoveries

10:00-10:15 Contributed Talk (CT3): **Javier Dominguez-Calvo**

Hooke's atom: A toy model for DFT

10:15-10:30 Contributed Talk (CT4): **Lorenzo Paoloni**

Characterization of ultrafast photoinduced molecular processes: modeling of transient X-ray Photoelectron Spectroscopy

10:30-10:45 Contributed Talk (CT5): **Zhen Wang**

Rotational study on ortho-/meta-bromopropionic acid and their monohydrated clusters

10:45-11:30 Coffee break

Morning Session B 11:30-13:30

Chair: Pablo Pinacho

11:30-12:00 Invited Talk (IT2): **Javier Ortín-Fernández**

Nextmol: a computational chemistry platform to build, characterize and predict in the specialty chemical industry.

12:00-12:15 Contributed Talk (CT6): **Martino Napoli**

Density functional theory simulations of Skaergaardite (CuPd) using Quantum Espresso

12:15-12:30 Contributed Talk (CT7): **Nuno M. Campos**

Quantum Tunneling Dynamics in a Molecular Sandwich

12:30-12:45 Contributed Talk (CT8): **Jiarui Ma**

A Broadband Rotational Spectroscopic Study of Tetrahydro-2h-pyran-2-ol and its micro-hydration

12:45-13:00 Contributed Talk (CT9): **Guillem Vila-Siles**

Shedding Light on Nonlinear Optical Properties: A Comparative Computational Analysis

13:00-13:15 Contributed Talk (CT10): **Prachi Misra**

Facilitating the search of 1-amino-2-propanol in space by studying its rotational spectrum

13:15-13:30 Contributed Talk (CT11): **Aran Insausti**

Rotational Spectroscopic Study of a Weakly Bonded Furfural and n-Hexane Binary Complex

13:30-16:00 Free lunch

16:30 SOCIAL ACTIVITY: Guided Tour (Spanish and English)

Meeting point: Plaza Zorilla



Wednesday Session – 26th February 2025

Morning Session A 9:15-11:30

Chair: Laura Palacio

9:15-9:30 WOMEN IN SCIENCE: GEMF-RSEF

9:30-10:00 Invited Talk (IT3): **Catalina Coll**

Theoretical study of realistic silicon nanostructures: structural, electronic and vibrational properties

10:00-10:15 Contributed Talk (CT12): **Sarah J. Madlener**

The Influence of Chloride on the Photochemistry of Pyruvate in Salt Clusters

10:15-10:30 Contributed Talk (CT13): **Rita J.C. Roque**

The concerted dynamics of water molecules around a chiral molecular switch

10:30-10:45 Contributed Talk (CT14): **María Mallo Álvarez**

Kinetic modelling of interstellar hydrocarbons: cyano derivatives of propene

10:45-11:00 Contributed Talk (CT15): **Cadence Miller**

Custom Python Code for Operating Tennessee Tech's New L-shaped FTMW Spectrometer

11:00-11:30 Coffee Break

Morning Session B 11:30-15:00

Chair: Elena Alonso

11:30-12:15 SCIENCE FOR EVERYONE: **Clara Inés Alcolado**

Inspiring Women in STEM

12:15-12:30 Contributed Talk (CT16): **Alicia Omist**

Electronic and magnetic properties of triangulene monomer and its oligomers

12:30-12:45 Contributed Talk (CT17): **Mariana Leiferman Tamames**

Role of ionization and protonation in the formation of peptide bonds in clusters of amino acids in the gas phase

12:45-13:00 Contributed Talk (CT18): **Irene Belloso**

Simulation of Hydrogen Adsorption on Single-Cluster Vanadium Catalysts Supported on Layered Materials

13:00-13:15 Contributed Talk (CT19): **Farha Sajeev**

Water Complexes on a Cyclic Thioether from Broadband rotational spectroscopy

13:15-15:00 Lunch

Afternoon Session A 15:00-17:20

Chair: Sergio Mato

15:00-15:15 Contributed Talk (CT20): **Kushal Shaw**

Ultrafast excited-state dynamics of anisole and its methyl substitutes

15:15-15:30 Contributed Talk (CT21): **Fernando Torres-Hernández**

Spectroscopic Analysis of Non-Covalent Interactions in 2-Phenylethanethiol, 2-Phenylethanol and 2-Phenylethylamine Dimers

15:30-15:45 Contributed Talk (CT22): **Shan Jin**

Toward detection of FeH^+ in the interstellar medium: infrared multiple photon dissociation spectroscopy of argon-tagged FeH^+

15:45-16:00 Contributed Talk (CT23): **Roger Castillo Delgado**

Glycolic acid microsolvation in gas phase

16:00-16:05 Flash Talk (FT1): **Azahara Ortiz**

Photodissociation initiated by sunlight of 2-butanone in the troposphere

16:05-16:10 Flash Talk (FT2): **Johanna Y. Sandoval**

Single atom and single cluster transition metal catalysts supported on GDY and BGDY layers

16:10-16:15 Flash Talk (FT3): **Noura Aflak**

Unveiling the Role of Substituents in [3+2] Cycloaddition Reactions Between Azides and Nitriles: Insights from Molecular Electron Density Theory (MEDT)

16:15-16:20 Flash Talk (FT4): **Lorena Acevedo**

Optical response of a binary atomic system with gain

16:20-16:25 Flash Talk (FT5): **Jiarui Ma**

Rotational Spectroscopic Study of Cis-Stilbene and its Water Complexes

16:25-16:30 Flash Talk (FT6): **Álvaro de la Fuente Villanueva**

Theoretical study of reactions in the interstellar medium with phosphorus radicals

16:30-16:35 Flash Talk (FT7): **Ángel Damián de Castro**

A High-Level Quantum Chemical Study on the Structure and Spectroscopic Properties of HOCH₂CP Conformers

16:35-16:40 Flash Talk (FT8): **Samrat Dev**

Azophenyl-substituted Schiff Base as a Cu(II) Sensor: A Molecular Spectroscopy and DFT-Based Study

16:40-16:45 Flash Talk (FT9): **Ayoub Tamin**

Low-Energy Electron Impact Ionization of Water Molecules

16:45-16:50 Flash Talk (FT10): **Sofía Municio San José**

The Conformational Panorama of gabapentin

16:50-17:30 Coffee Break

Afternoon Session B 17:30-18:30

17:30-18:30 Poster Session I

Thursday Session – 27th February 2025

Morning Session A 9:15-11:30

Chair: Celina Bermúdez

9:15-9:45 Invited Talk (IT4): **Javier Carmona-García**

Shedding light on atmospheric photochemistry by means of computational methods

9:45-10:00 Contributed Talk (CT24): **Jorge Alonso de la Fuente**

Unveiling the Role of Phosphorus Hydrides in Astrochemistry: Formation, Destruction and Reaction Dynamics

10:00-10:15 Contributed Talk (CT25): **Ricardo Morán**

Probing the structure of the atmospheric aerosol precursor pinanediol and its water complexes with microwave spectroscopy

10:15-10:20 Flash Talk (FT11): **Andrea Vázquez**

Investigating Gas-Phase Microsolvation and Conformational Behavior of Pyruvic Acid Using High-Resolution Rotational Spectroscopy

10:20-10:25 Flash Talk (FT12): **Francisco Martínez**

Kinetic Study of CN with H₂S and CH₃CH₂SH at the Ultra-Low Temperatures of the Interstellar Medium.

10:25-10:30 Flash Talk (FT13): **Mekhalfa Sana**

Simple Ionization of Molecular Nitrogen.

10:30-10:35 Flash Talk (FT14): **Omar Zaidi**

Charge effect on the single ionization of Argon

10:35-10:40 Flash Talk (FT15): **Kushal Shaw**

Mapping Charge Transfer Dynamics in nitroaniline and derivatives

10:40-10:45 Flash Talk (FT16): **Shan Jin**

Spectroscopy of Ionic Iron Compounds with Astrochemical Relevance

10:45-10:50 Flash Talk (FT17): **Domingo Heras Elvira**

Decoding the 1,4 N...S interaction of biomolecules using rotational spectroscopy

10:50-10:55 Flash Talk (FT18): **Sara Llorente**

Integration and Calibration of a CMOS Camera for high-resolution spectroscopy of Nd III

10:55-11:00 Flash Talk (FT19): **Munavvar Husain**

Exploring the Excitation Effects of Fluorine and Cobalt Substitution on Porphine Using Quantum Chemistry Topology

11:00-11:05 Flash Talk (FT20): **Gh. Saleh**

A New Approach to Explaining Electron Cloud Formation in Various Element

11:05-11:30 Coffee Break

Morning Session B 11:30-15:00

Chair: Domingo Heras

11:30-12:30 Poster Session 2

12:30-12:45 From University to Industry: CURIA

12:45-13:00 Contributed Talk (CT26): **Paul Pinillos**

Study of the hydration of aspartame with IR-UV spectroscopy

13:00-13:15 Contributed Talk (CT27): **Santiago Pérez-Hernando**

Stereodynamics of cold molecular collisions

13:15-13:30 Contributed Talk (CT28): **David San Andrés**

First detection in space of the high-energy isomer of cyanomethanimine: H₂CNCN

13:30-15:00 Lunch

Afternoon Session 15:00-18:00

Chair: Farha Sajeev

15:00-15:30 Invited Talk (IT5): **Markel Ylla**

Machine Learning model for Multireference diagnostics based on Kohn-Sham energies

15:30-15:45 Contributed Talk (CT29): **Javier Hernández-Rodríguez**

Unraveling spin-forbidden enzymatic peroxidation through quantum dynamics

15:45-16:00 Contributed Talk (CT30): **Andrés Verde**

Unravelling the structure of resveratrol through laser-ablation rotational spectroscopy and quantum chemical calculations

16:00-16:15 Contributed Talk (CT31): **Sahar Mahnae**

Molecular Dynamics and DFT Simulations of CO₂/CH₄ Separation Through Carbon-Based Nanoporous Membranes: Influence of Pore Size

16:15-16:30 Contributed Talk (CT32): **Antonio Cebreiro**

Magnetic analysis using efficient state-interaction approach

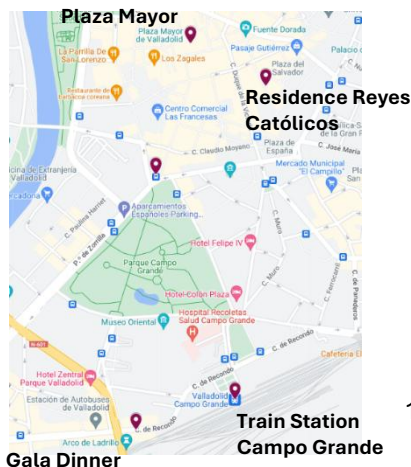
16:30-17:00 Closing Ceremony

17:00-18:00 SCIENCE ACTIVITY: Lab Tour

21:00 Gala Dinner

Venue: Restaurante La Raíz

Street Recondo, 3



MONDAY 24		TUESDAY 25		WEDNESDAY 26		THURSDAY 27	
9.15h		PLENARY 2: Christian Clear		WOMEN IN SCIENCE: Laura Palacio		INVITED 4: Javier Carmona	
9.30h				INVITED 3: Catalina Coll		Jorge Alonso	
9.45h				Sarah Madlener		Ricardo Morán	
10.00h				Rita Roque		FLASH 11-20: Andrea Vázquez, Francisco Martínez, Sana Mekhalifa, Omar Zaidi, Kushal Kumar, Shan Jin, Domingo Heras, Sara Llorente, Munavar Husain, Gh Saleh	
10.15h		María Mallo					
10.30h		Cadence Miller					
10.45h		COFFEE BREAK					
11.00h		COFFEE BREAK		COFFEE BREAK			
11.15h		INVITED 2: Javier Ortín		SCIENCE FOR EVERYONE: Clara Alcolado		POSTER SESSION 2	
11.30h							
11.45h							
12.00h							
12.15h	Martino Napoli						
12.30h	Nuno Campos						
12.45h	Ma Jiauri		Alicia Omist				
13.00h	Guillem Vila-Siles		Mariana Lieferman		From University to Industry: CURIA		
13.15h	Prachi Misra		Irene Belloso		Paul Pinillos		
13.30h	Aran Insausti		Farha Sajeev		Santiago Pérez		
13.45h					David San Andrés		
14.00h	REGISTRATION		LUNCH		LUNCH		
14.15h							
14.30h							
14.45h							
15.00h							
15.15h							
15.30h							
15.45h							
16.00h							
16.15h	SOCIAL ACTIVITY: FREE TOUR		Kushal Kumar		INVITED 5: Markel Ylla		
16.30h			Fernando Torres		Javier Hernández		
16.45h			Shan Jin		Andrés Verde		
17.00h			Roger Castillo		Sahar Mahmaee		
17.15h	PLENARY 1: Sergio Domingos		FLASH 1-10: Azahara Ortiz, Johanna Yasmin, Noura Attak, Cindy Lorena, Ma Jiauri, Álvaro de la Fuente, Ángel de Castro, Samrat Dev, Tamin Ayoub, Sofia Municio		Antonio Cebreiro		
17.30h			COFFEE BREAK		CLOSING CEREMONY		
17.45h			COFFEE BREAK				
18.00h			COFFEE BREAK				
18.15h	COFFEE BREAK		POSTER SESSION 1		SCIENCE ACTIVITY: LAB TOUR		
18.30h							
18.45h							
19.00h							
19.15h	INVITED 1: Miguel Gallegos						
19.30h	Raidel Martín Barrios						
	Daniel Félix González						
21.00h					GALA DINNER		