XVI CONFERENCE OF YOUNG RESEARCHERS IN ATOMIC AND MOLECULAR PHYSICS

University of Valladolid
24 - 27 February 2025

Welcome to Valladolid

Welcome to the 16th International Conference of Young Researchers in Atomic and Molecular Physics.

We are delighted to welcome you to the 2025 edition of our conference, hosted by the University of Valladolid, one of Spain's most prestigious academic institutions. Organised and supported by the Department of Physical and Inorganic Chemistry, the event will take place in the University's facilities, providing a stimulating environment for the exchange of scientific knowledge. We extend our gratitude to the sponsors whose generous support makes this meeting possible.

The aim of the conference is to bring together young scientists working in atomic and molecular physics, fostering the exchange of knowledge across disciplines. The meeting will cover fundamental and applied research on the structure, dynamics, and interactions of atoms and molecules in different environments, with contributions from both experimental and theoretical perspectives. These studies are essential for advancing our understanding of chemical reactivity, spectroscopy, quantum phenomena, and their applications in fields such as astrophysics, nanoscience, and materials science.

The scientific programme will feature two plenary lectures, four invited talks on fundamental and applied aspects of hydrogen bonding, 31 oral talks, 19 flash presentations, and two poster sessions, offering a dynamic platform for the dissemination and discussion of innovative research.

Beyond the scientific sessions, participants will have the opportunity to explore the rich cultural and historical heritage of Valladolid. The social programme includes a conference dinner, a guided tour of scientific facilities, including the molecular spectroscopy laboratories and the Supersonic Plasma Spectroscopy and Jet Spectroscopy Group laboratories. Additionally, a guided visit to the city's most emblematic historical landmarks will provide a relaxed and inspiring atmosphere for meaningful interactions.

We look forward to welcoming you to an exciting and enriching meeting.

The Organizing Committee

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USEFUL INFORMATION

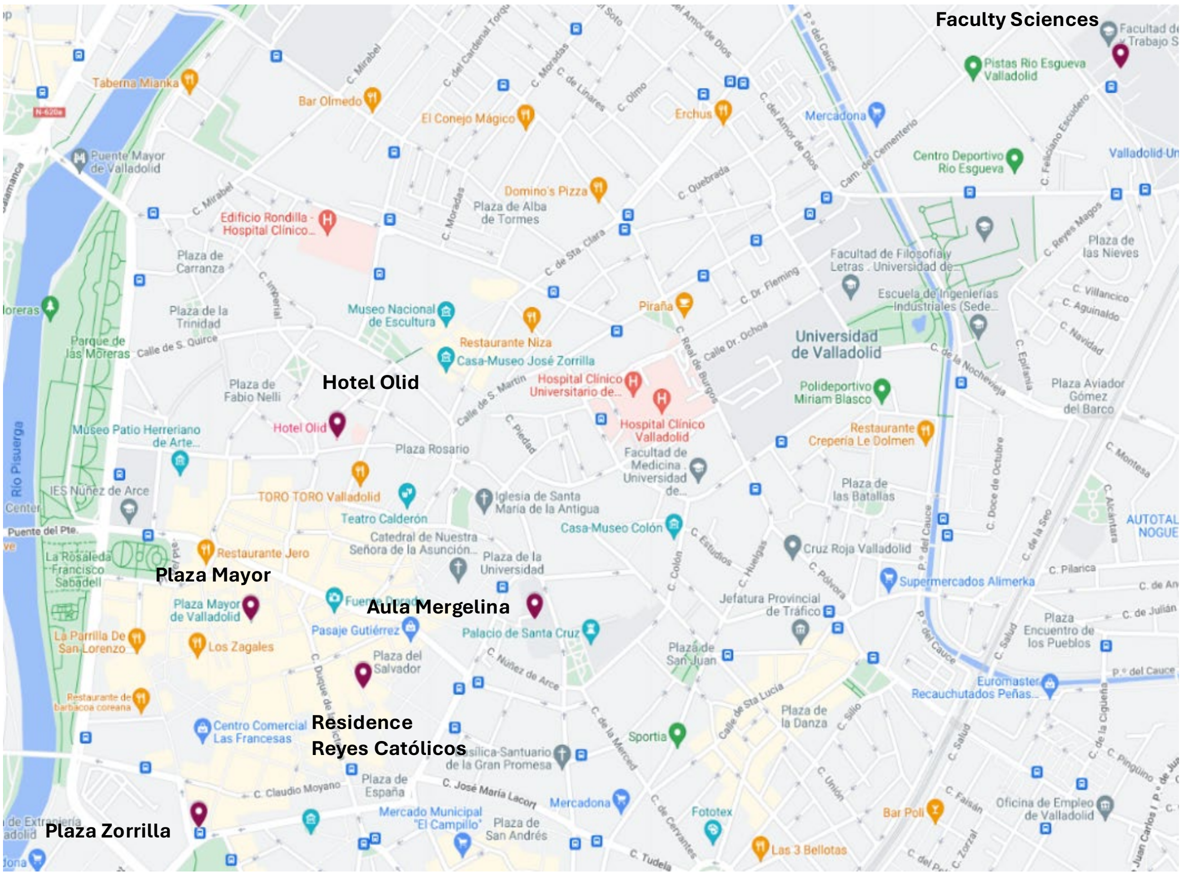
Venue

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 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

Beyond the scientific sessions, we invite you to enjoy two special activities designed to enhance your conference experience:

🌆 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

INSTRUCTIONS FOR AUTHORS

Oral contributions

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

- Oral communications, 12 min for presentation and 3 min for discussion.
- Flash communications, 3 min for presentation.

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 j2ifam2025@uva.es 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 “A0” (84,1 x 118,9 cm) vertical 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.

DETAILED PROGRAM AND SPEAKERS

This section presents the contributions of all participants, organized according to the scheduled order of presentations in the conference program. Each abstract offers a concise overview of the research and topics that will be discussed, reflecting the diversity and depth of the ideas being shared at this event.

We invite you to explore these abstracts as a preview of the insightful discussions and exchanges that will take place throughout the conference.

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) + H3+ ($^1A''$): 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-proponal in space by studying its rotational spectrum

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

Rotational Spectroscopic Study of a Weakly Bond 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-butanona 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 $HOCH_2CP$ *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 1

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**

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 Mahnaee**

Molecular Dynamics and DFT Simulations of CO_2/CH_4 *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

SPEAKERS

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

Sérgio R. Domingos

CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal
email: *sergio.domingos@uc.pt*

In the gas phase, molecular recognition relies on the ability of molecules to selectively identify and bind to their targets without the stabilizing influence of a solvent. While the absence of solvation simplifies the environment, recognition processes often remain highly dependent on conformational changes. In some cases, molecules can even become kinetically trapped in non-ideal conformations, potentially hindering efficient binding or slowing down recognition. By leveraging high-resolution rotational spectroscopy experiments paired with advanced quantum chemistry calculations, we gain a unique vantage point to explore molecular contacts and the intermolecular forces governing recognition. Key factors such as chirality, steric effects, and the dynamic coordination of micro-solvating agents emerge as crucial determinants in these processes. These investigations not only deepen our understanding of molecular structure and recognition but also provide critical insights into the operational constraints of molecular motors and other functional molecular systems. In this lecture, we will present an overview of our latest efforts in this arena, and discuss how gas-phase studies offer fresh perspectives on spectroscopic explorations of molecular structure and dynamics.

Acknowledgments: FCT Portugal through grants UIDB/04564/2020 (https://doi.org/10.54499/UIDB/04564/2020) and UIDP/04564/2020 (https://doi.org/10.54499/UIDP/04564/2020). This work was funded by the European Union (ERC, 101040850 - MiCRoARTiS). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

Explainable Chemical AI (XCAI): Moving Beyond Accurate Predictions.

Miguel Gallegos[1], Valentín Vassilev-Galindo[2], Igor Poltavsky[3], Ángel Martín Pendás[1], Alexandre Tkatchenko[3]

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[2] IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain.
[3] Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg.

The rise of Artificial Intelligence (AI) has brought about highly accurate yet opaque black-box models, limiting their ability to enhance our understanding of chemical phenomena. To address this, we present Explainable Chemical AI (XCAI), integrating physically rigorous theories like the Atoms in Molecules framework[1] with advanced AI kernels. Using a modified SchNet architecture,[2] our approach (SchNet4AIM, **Fig. 1**) accurately estimates local (atomic and pairwise) properties while ensuring precise reconstruction of molecular quantities. We demonstrate intrinsic explainability through the study of a supramolecular binding phenomenon, where SchNet4AIM provides quantum chemically consistent insights into the forces driving complexation and identifies the most dominant pairwise contributions. This approach combines numerical accuracy with chemical interpretability, expanding the reach of computationally demanding theories to previously inaccessible domains.

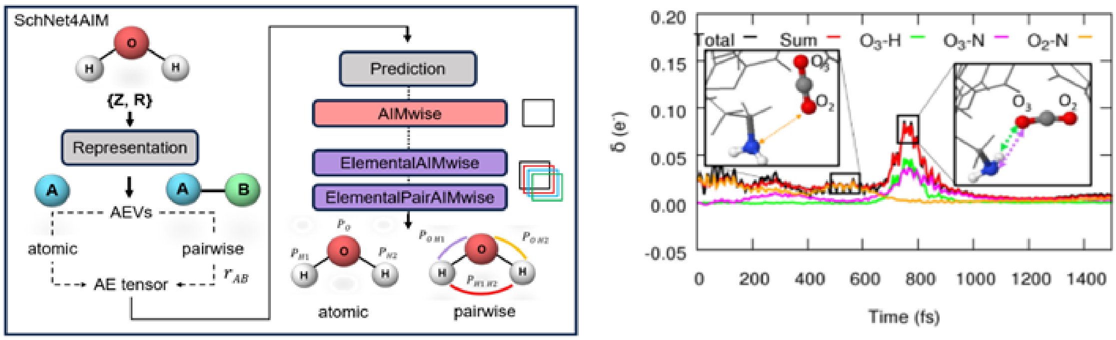

Figure 1. (Left) Schematic representation of SchNet4AIM. (Right) Evolution of SchNet4AIM group predictions during a Molecular Dynamics simulation.

Acknowledgments: We acknowledge the Spanish MICIU (No. PID2021-122763NB-I00 to A.M.P. and M.G., Nos. FPU19/02903 and EST22/00100 to M.G.) for financial support.

References

[1] Bader R.F.W., *Atoms in Molecules:_ A Quantum Theory.* International Series of Monographs on Chemistry. Clarendon Press, Oxford. **1990**.
[2] Sauceda K.T., Kindermans H.E., Tkatchenko P.-J., Müller K.-R., *J. Chem. Phys.*, **2018**, *148*, 241722–241722.

Inelastic collision of hydrogen atoms on tungsten surfaces with hydrogen coverage

Raidel Martin Barrios[1], Oihana Galparsoro[2], Cédric Crespos[1] and Pascal Larregaray[1]

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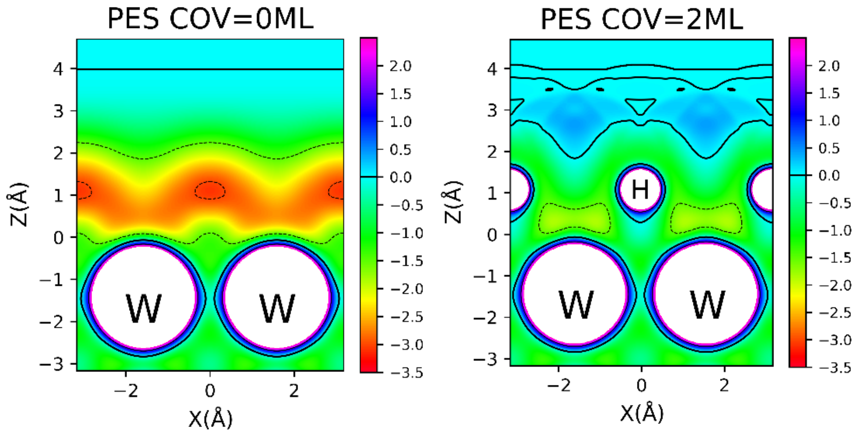
[2] DIPC, Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain.

Recent studies have shown that when hydrogen atoms collide with metal surfaces at energies of a few electron volts, the loss of translational energy is mainly due to electron-hole pair excitations [1]. In the case of hydrogen atoms interacting with a tungsten surface covered with hydrogen atoms, theoretical studies have only examined the energy lost under specific conditions of incident energy, azimuthal angle and polar angle [2,3]. Quasi-classical trajectory simulations were here carried out to investigate the energy transfer during the scattering of hydrogen atoms from hydrogen-covered tungsten surfaces, W(110) and W(100). The theoretical approach investigates the effect of hydrogen coverage, collision energy and direction of incidence on the energy loss. The scattering can be explained by three different dynamical mechanisms, the contribution of which varies depending on scattering conditions. These results help to explain why the energy loss spectra significantly differs if they are analysed in the whole space or only at the scattering plane. Furthermore, a previously unknown reflection channel at low energy and grazing incidence is suggested at high coverage, resulting from by modifications in the potential energy surface illustrated in Figure 1.


PES COV=0ML

PES COV=2ML

Figure 1. Potential energy surface in the Y=0 A plane for the W(100) for two scenarios: a clean surface (left panel) and a surface with a coverage of 2ML (right panel).

References

[1] O. Bunnermann, H. jiang, Y.Dorenkamp, A. Kandratsenka, S.M. Janke, D.J. Auerbach, and A. M. Wodtke, *Science,* **2015,** *Vol. 350***,** no. 6266, pp. 1346-1349.

[2] R. Martin-Barrios, O. Galsparsoro, A. Martínez-Mesa, L. Uranga-Piña, C. Créspos, and P. Larregaray. *J. Phys. Chem. C,* ***2021****, Vol. 125*, no. 26, pp. 14468-14473.

[3] R. Martin-Barrios, O. Galsparsoro, A. Martínez-Mesa, L. Uranga-Piña, C. Créspos, and P. Larregaray. Eur. Phys. J. Spec. Top., **2023**, *Vol. 232*, no. 12, pp. 1985-19993.

Reactive Collisions of S (^{3}P) + H3+ (^{1}A''): Force-Field approach to the ab initio Potential Energy Surface.

Daniel Félix González[1], Alfredo Aguado Gómez[1], Octavio Roncero Villa[2]

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[2] Instituto de Física Fundamental (IFF-CSIC), C.S.I.C., Serrano 123, 28006 Madrid, Spain

As it has been reported in previous studies[1], sulfur hydrides play a key role in the chemistry of the interstellar medium (ISM), as they are among the first molecules to form in diffuse interstellar clouds and photodissociation regions. Interstellar sulfur-containing species are still an open discussion topic in astrochemistry, since the observed abundance of species like H_2S or SH^+ cannot be fully explained by means of direct hydrogen abstraction reactions involving H_2. In view of this, our research group aims to model the collisions of the four-atom system SH_3^+, with special attention on the S (^{3}P) + H_3^+ (^{1}A'') channel. Initially, we are developing an accurate fit to the *ab initio*[2] Potential Energy Surface (PES)[2] for its ground electronic state (^{3}A) via force-field with four-body corrections[1] (FF+4C) - we have considered the three lowest lying asymptotes, as shown in Fig. 1. This fitted PES will be used in Quasi-Classical Trajectory (QCT) calculations to properly model the reactive dynamics of the system.

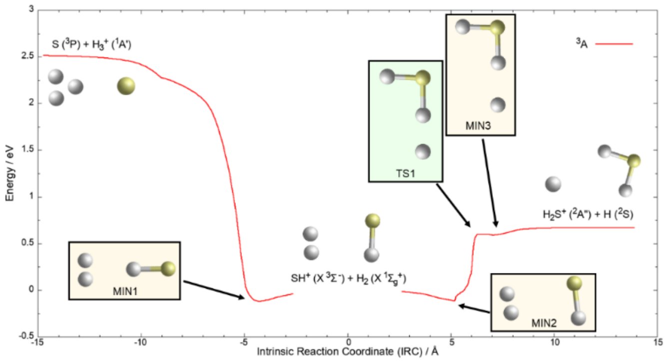

Figure 1. Computed *ab initio* minimum energy paths (MEP) connecting the three studied asymptotes of the ^{3}A adiabatic electronic state of the SH_3^+ system.

References

[1] Goicoechea J. R. et al., *Astronomy & Astrophysics*, **2021**, *647*, A10.
[2] Werner H. J. et al., *J. Chem. Phys*, **2020**, *152*, 14.

The Power of Precision: Improving Atomic Data for Astrophysical Discoveries

Christian Clear[1]

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Modern advancements in ground and space-based telescopes, such as the Very Large Telescope and the James Web Space Telescope, have revolutionised our ability to acquire high-resolution astronomical spectra across the infrared, visible, and ultraviolet regions. These spectra provide unprecedented insights into the chemical composition, dynamics, and physical conditions of distant celestial objects, enabling us to probe the structure and plasma processes within stars, galaxies, and nebulae—unlocking the mysteries of the universe's formation and the fundamental processes driving its evolution. However, the reliability of these discoveries is entirely dependent on the availability of accurate atomic data to interpret astrophysical spectra.

Poor quality atomic data are often the limiting factor in modern astronomical spectral analyses, and significant improvements are needed for many species. The Imperial College Spectroscopy group is addressing this challenge by using Fourier transform spectroscopy to measure atomic spectra of key astrophysical elements, resulting in significant advancements in atomic data accuracy and breadth. As the demand for precise atomic data grows with the emergence of next-generation telescopes, such as the Extremely Large Telescope, these efforts are becoming even more essential to advancing our understanding of the universe.

Hooke's atom: A toy model for DFT

Javier Dominguez-Calvo[1], Rubén Ferradás[1] and Eduard Matito[1,2]

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The analytical solution of many-electron quantum systems presents a fundamental challenge in quantum mechanics. Harmonium Atom (HA) [1,2], or Hooke's Atom, emerges as a rare exactly solvable case under some conditions. Such a system is defined as electrons tied to a massless center by harmonic interactions and repelled from each other by the Coulomb force. This is just a theoretical model as no real electron actually behaves this way. However, HA densities resemble molecular interactions, with peaks of probability of finding electrons at certain positions in space. Having exact solutions makes HA a perfect toy model for use to simulate other non-analytical counterparts.

The system is defined by the confinement parameter, or in other words, the strength of the harmonic interaction. For the two-electron system, exact wave functions can be obtained for specific, countable values of this parameter. In all those cases, an analytical expression of the wave function can be obtained, giving rise to many DFT related properties in analytical form, such as electron densities or even exchange-correlation potentials for different values of electron-electron interaction.

This work dwells on the systematic retrieval of exact electronic densities across multiple harmonic strengths regimes. It's analytical accessibility provides crucial insights into quantum physical phenomena, in particular those regarding electronic correlation effects that remain elusive in real molecular systems. Our findings establish a rigorous framework for benchmarking correlation models, and design density functional approximations; bridging the gap between theoretical exactly solvable systems and practical molecular applications.

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

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Pump-probe spectroscopies enable us to characterize the reaction mechanisms of photoinitiated chemical processes. In the context of chemical and material sciences, static X-ray photoelectron spectroscopy (XPS) is an invaluable technique for the characterization of several systems, in a broad range which goes from isolated molecules to complex materials. Recent advancements in the development of Free Electron Lasers (XFELs) pave the way for the employment of XPS as a probe (i.e. the measurement of transient XPS spectra), giving access to a unique combination of very high temporal resolution (up to few femtosecond) and high sensitivity to local changes of the molecular structure[1,2].

The development of suitable computational tools is crucial to interpret the experimental results and to model the physical-chemical processes involved. In this contribution, the modeling of the fragmentation process of the CH3F$^+$ molecular system is described and discussed as an example of the results which can be obtained combining an advanced quantum chemical modeling (mainly through the employment of XPS calculations and non-adiabatic molecular dynamics) with the measurement of ultrafast transient XPS spectra.

The scientific protocol employed will be discussed, especially with regards to its potentialities and limitations for future studies (e.g. involving more complex molecular systems).

The results support the usefulness of transient XPS spectroscopy for the direct observation of fast and localized structural changes following the photoexcitation of a molecular system.

Acknowledgments: The authors acknowledge the Red Española de Supercomputación (RES) for the computational resources and the scientific teams of the Small Quantum Systems beamline (European XFEL) and of the Maloja beamline (SwissFEL) at which all the experimental measurements were performed.

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

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Halogenated carboxylic acids, classified as emerging Persistent and Mobile Organic Chemicals (PMOCs), have drawn scientific concern owing to their environmental persistence, intrinsic mobility, and ecotoxicological potential. These properties are closely related to the molecular polarity, which in turn depends on intrinsic structural characteristics, as well as intermolecular interactions including those involving solvents. Therefore, investigating the conformational behavior and interactions (both intra- and inter-molecular) of halogenated carboxylic acids is crucial for elucidating their environmental fate mechanisms. High-resolution spectroscopic methods coupled with quantum chemical calculations enables quantitative characterization of the dynamic equilibrium between intramolecular and intermolecular interactions, offering a molecular paradigm for predicting PMOC environmental trajectories.

In this study, *ortho*-/*meta*-bromopropionic acid (2-BrPA/3-BrPA) were selected as model systems. Chirped-pulse Fourier Transform Microwave spectroscopy was employed within 2-8 GHz to investigate their gas-phase conformational behavior. Experimental results revealed that both isomers exhibit differences in their behavior: while the population of the 2-BrPA is centered in a single species, the 3-BrPA shows two abundant species in isolation conditions (See Fig.1) Additionally, ^{79}Br/^{81}Br isotopic effects and hyperfine splittings induced by the quadrupole coupling of the bromine nucleus were observed. Further rotational spectroscopic analysis of their monohydrate complexes showed that the water molecule preferentially forms bidentate hydrogen bonds with the carboxyl group (O_w–H_w···O=C and O_w···H–O) rather than interacting with the bromine atom. Detailed spectral analysis, along with spectroscopic and computational results, will be presented.

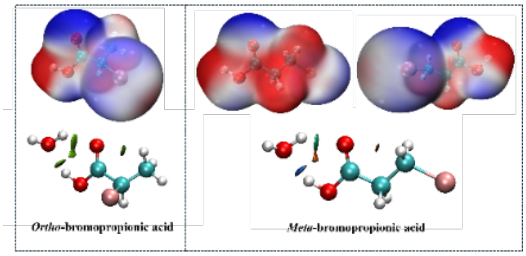

Figure 1. The detected conformers for 2-BrPA/3-BrPA and their monohydrated complexes.

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

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The chemical industry faces new challenges with the regulations that are being approved by administrations all over the world. Today's industry must evolve towards greener chemistry, limiting waste production and reducing its carbon footprint in the process[1]. Such requirements are greatly benefited by the implementation of computational chemistry procedures in the R&D processes. *In silico* simulations allow to study a wide range of chemical systems, screening out unsuitable candidates for the project of study before stepping into the wet lab, importantly reducing costs and research time. In this context, Nextmol provides a Software-as-a-Service platform that allows users with no previous experience in computational modeling or classical molecular dynamics to build models of their systems of interest, to propagate classical molecular dynamics and to predict their properties. This communication focuses on the study of the glass transition temperature of 546 polymers in the Nextmol platform, which were used to train a machine learning model[2]. This approach allows to predict the glass transition temperature of thousands of polymers in a matter of seconds just from their molecular structure, providing a framework that drastically accelerates research in the chemical industry.

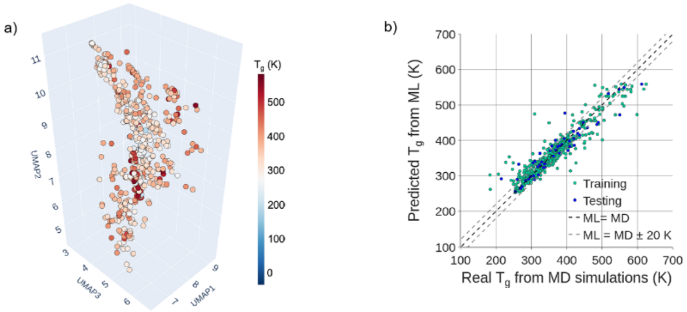

Figure 1. a) Representation of the chemical space along with the glass transition temperature of 546 polymers and b) assessment of the performance of the machine learning model.

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

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The present study investigates the electronic and vibrational properties, of Skaergaardite (CuPd) using density functional theory (DFT) as implemented in Quantum ESPRESSO. Skaergaardite is a Copper Palladium alloy found in Skaergaard intrusion with a simple cubic structure (CsCl-like). Due to its porous structure, it presents a large surface area available for interactions, which makes it a promising catalyst for CO2 reduction. The PBE functional with a Hubbard-like localized term (DFT+U) was used in combination with both ultrasoft pseudopotentials (USPP) and norm-conserving pseudopotentials (NCPP). A conventional approach with a dense Monkhorst-Pack grid of k-points (9x9x9) was applied. The obtained electronic bands, shown in Figure I, exhibit a dense overlap of the *d*-orbitals of both Cu and Pd in the conduction band. The phonon dispersion bands are consistent with those of the pure metals components as well as the fcc CuPd polymorph.
These results highlight the reliability of DFT+U in studying complex alloy systems with scarce experimental benchmarks, offering insights into the behaviour of Skaergaardite and its potential applications in material science.

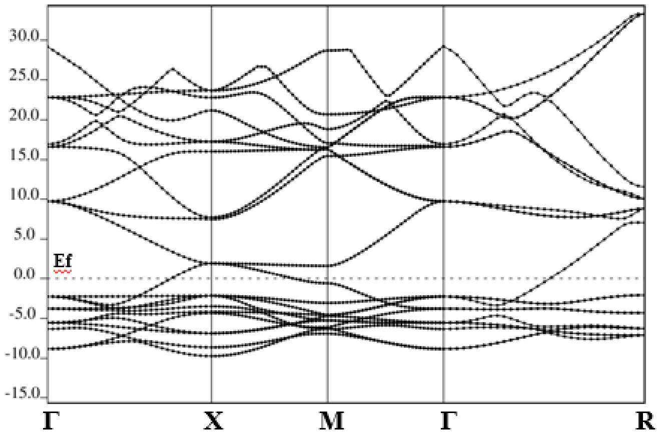

Figure I. Electronic dispersion bands (USPP) of Skaergaardite (CuPd).

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Quantum tunneling dynamics in a molecular sandwich

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Metallocenes, consisting of two nearly parallel units surrounding a central metal atom, which can rotate relative to reach other, are often regarded as sandwich compounds.[1] The simplest and most widely known example in this class of molecules is ferrocene. In ferrocene based rotors, the cyclopentadienyl rings can rotate around the Fe(II) metallic center adopting staggered and eclipsed configurations. The energy barrier for this rotational motion is highly dependent on the substituents inserted into the rings. The addition of bulky groups, like tert-butyl substituents, generally increases the rotation barrier, usually locking the rotor into specific configurations,[2] while the addition of phenyl groups leads, unexpectedly, to concerted rotary motion of the rings.[3] In our recent attempts to understand the dynamics in a metallocene molecular sandwich using rotational spectroscopy, we observed spectral signatures of quantum tunneling in the rotational spectrum of 1,1'-ferrocenedimethanol, a ferrocene-based rotary system which can exist in locked staggered and eclipsed conformations. In this contribution, we will present the results of our broadband microwave experiments, and discuss our strategy for the analysis, supported by quantum chemistry calculations.

Acknowledgments: This work received financial support from FCT through grants UIDB/04564/2020, UIDP/04564/2020, 2022.15813.CPCA, and 2023.10981.CPCA.A2. N.M.C. acknowledges FCT scholarship 2023.00840.BD. The authors acknowledge the computational resources provided by the Laboratory for Advanced Computing at University of Coimbra. This work was funded by the European Union (ERC, 101040850–MiCRoARTiS). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

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

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2

Tetrahydro-2H-pyran-2-ol (THP) is an alcohol containing a pyranose ring, lacking substituents, which results in reduced conformational flexibility and fewer intramolecular non-covalent interactions compared to pyranoses such as glucose. This makes THP a valuable prototype for studying various phenomena and dynamics in carbohydrate chemistry.[1] Such phenomena include the anomeric effect, which describes the preference for the axial conformation over the less sterically hindered equatorial conformation. In solution, the cyclic forms of THP exists in equilibrium with an open-chain intermediate, 5-hydroxypentanal.[2]

We analyzed the rotational spectra of THP and its micro-hydrated complexes at the 2–6 GHz and 6–18 GHz frequency ranges. The gas-phase experimental structures for both the axial and equatorial conformations of THP were determined, providing intrinsic structural insights into the anomeric effect. The open-chain intermediate of THP was also detected in the molecular jet. The preliminary results of the ring-opening reaction dynamics will be presented. Additionally, we will also discuss how micro-hydration affects the conformational preference of THP.

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Shedding light on nonlinear optical properties: a comparative computational analysis

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Great attention has been paid to materials characterized by a large nonlinear optical (NLO) response due to their applications as optical switches or three-dimension fluorescence microscopy, among others. One example of an NLO process is the second harmonic generation, a physical process where photons with frequency ω interact with a non-centrosymmetric material, causing the combination of two photons and resulting in the refraction of a photon with double frequency. Despite the interest arisen by nonlinear optical properties (NLOPs), most of the quantum chemistry methods were designed to calculate thermodynamic reactions and barrier energies, whereas only few methods are designed to compute molecular properties.

In the presence of the so-called nondynamic correlation, only a few methods can be applied, the most popular of them is the complete active space self-consistent field (CASSCF) method.

This project focuses on the computational analysis of different lengths polyacetylene (PAs) chains using HF, MP2, CASSCF and CCSD methods with different basis (aug-cc-pVTZ, aug-cc-pVDZ, cc-pVTZ, cc-pVDZ and Sadlej's POL). Our goal is to compare the methods and their reliability to compute NLOPs.

The Partitioning of NLOPs into Orbital Contributions (PNOC) tool was used to analyse the results[1]. This is a new tool to measure the contribution of the different molecular orbitals to the (hyper)polarizabilities.

The results obtained show that, for polyacetylene (PAs) chains, MP2 can predict accurately the total values of the NLOPs and their orbital contributions. Nonetheless, we found that CASSCF significantly underestimates the NLOPs, giving larger errors with respect to CCSD than HF. The latter finding suggests caution using CASSCF to compute NLOPs, and opens the question of which method should be used to compute NLOPs for multireference systems.

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

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Rotational spectroscopy has been a vital tool in identifying most of the 241 molecular species currently detected in space.[1] Ethanolamine is one such complex molecule, recently identified in the molecular cloud G+0.693-0.027.[2] By introducing an additional methyl (CH_3) group, ethanolamine forms 1-amino-2-propanol (1-a-2-p), a molecule that holds potential for astronomical detection, as illustrated in Figure 1. Previous studies have investigated one conformer of 1-a-2-p in the frequency range of 26.5–39.7 GHz using conventional absorption spectroscopy. It reports the internal rotation barrier height of the methyl group and the spectroscopic rotational constants of the ground and vibrationally excited states.[3]

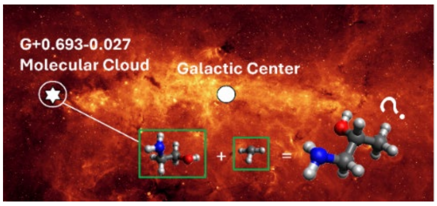

Figure 1. Infrared view of the galactic center and molecular cloud G+0.693, a promising site for the detection of 1-amino-2-propanol. Image credit: modified from NASA/JPL-Caltech/S. Stolovy (Spitzer Science Center/Caltech)

This work expands upon the previous study by extending the measured frequency ranges and providing accurate quartic and sextic distortion constants. The rotational spectra of 1-a-2-p were recorded using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy in the frequency ranges of 12–26.5 GHz and 75–110 GHz[4] using home-built spectrometers. This approach provides broadband, high-resolution rotational spectra with high sensitivity.[5] The employed frequency ranges align with those of the Effelsberg and the Atacama Large Millimeter/Submillimeter Array (ALMA) telescopes. Measurements were performed at ~10 K in the lower frequency range using a supersonic jet expansion and at ~300 K in the higher frequency range. In addition to the lowest energy conformer of 1-a-2-p, a second conformer predicted 4.9 kJ/mol higher than the previously reported conformer has been observed for the first time in this study. The rotational constants for both the ground and vibrationally excited states of both conformers were determined and will be presented. Additionally, nuclear quadrupole hyperfine splitting arising from the ^{14}N nucleus was resolved in the lower frequency range measurements. These high-resolution spectra for 1-a-2-p will help perform a search for it in astrophysical environments.

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

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We present a jet-cooled rotational spectroscopic study of a binary complex made of furfural and n-hexane. Six different dimeric conformers were experimentally identified. The experimental conformational cooling studies with different carrier gases have been coupled with associated DFT calculations to analyze the intricate conformational landscape, which is characterized by multiple minima that are close in energy. The combined experimental and theoretical results provide a qualitative picture of the conformational interconversion landscape, the relative stability of the observed conformers, and importantly, an unusual surface-confined chirality enrichment in the binary aggregates of furfural and n-hexane (Figure 1).

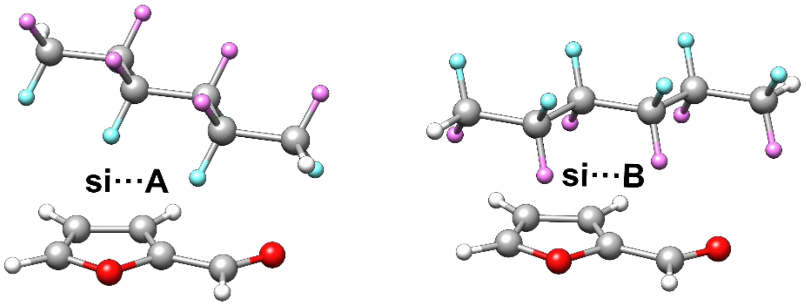

Figure 1. Two conformers of furfural and n-hexane complex experimentally observed using chirped-pulse Fourier transform spectrometer.

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

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The convergence of experiment and theory at the atomic scale has reached unprecedented accuracy, driven by advancements in experimental setups, high spatial and energy resolution, increased computing power, high-performance computing (HPC), and the integration of machine learning. These developments now enable the modelling of realistic solids with near ab initio accuracy, even for large and complex systems.

This talk will explore the transformative role of machine learning in investigating the structural, electronic, and vibrational properties of two specific silicon-based systems. Despite decades of extensive study, silicon remains central to semiconductor research, particularly in emerging applications such as qubits[1] and novel nano-opto-electro-mechanical systems (NOEMS)[2]. Understanding its perfect crystallinity under stress and the influence of controlled defects—such as grain boundaries—is crucial for optimizing device performance.

The presentation will outline a multi-scale theoretical workflow that integrates density functional theory with empirical models and high-resolution electron microscopy data, all enhanced by machine learning techniques. This approach provides a comprehensive understanding of how nanoscale structures influence material properties, offering new insights into the design and optimization of next-generation silicon-based devices.

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

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Around 70% of Earth's surface is covered by the ocean. Marine aerosols are thus one of the most important naturally occurring aerosols.[1] Through direct as well as indirect interaction with solar radiation they influence Earth's climate. They consist of inorganic salts such as sodium chloride, as well as organic materials like saccharides, peptides or acids. One of these acids is pyruvic acid, which originates from the degradation of isoprene and acetone. Pyruvic acid is the most abundant alpha-keto carboxylic acid in the atmosphere and upon irradiation with UV light, it undergoes a C-C bond photolysis releasing neutral CO_2.[2,3] This study addresses now the question whether photochemistry changes when pyruvic acid is embedded in a salt cluster. Therefore UV/Vis spectra were recorded for sodium pyruvate salt clusters $[Na_n Pyr_{(n-1)}]^+$ and pyruvate embedded in a sodium chloride cluster $[Na_n Cl_{(n-1)} Pyr]^+$. The experiments were conducted on an APEX 9.4 T FTICR mass spectrometer and the ions were produced using an electrospray ionization source. The comparison of the two systems showed that chloride causes a new intense absorption at around 400 nm that is not observed for pure pyruvate or pyruvic acid. The same products are observed as for the energetically higher lying absorptions. Also, the intensity distribution does not change significantly. Indications for the influence of halides on the photochemistry of carboxylic acids are found in the literature for other systems further strengthening our hypothesis that chloride is responsible for the occurrence of this new absorption.

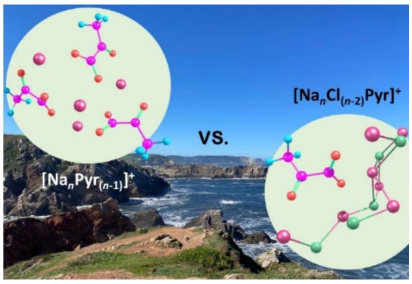

Figure 1. Artistic depiction of the comparison of the two salt systems.

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The concerted dynamics of water molecules around a chiral molecular switch

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Although cold gas phase molecular clusters are usually thought of as static systems, this is not always the whole story. Recent studies on the micro-solvation of molecules using rotational spectroscopy show significant dynamics involving the enclosing water networks. If symmetry allows, these dynamic rearrangements of the solvating water molecules occur through quantum tunneling.[1] Destroying this local symmetry with a chiral subspace creates a vantage point to capture large-amplitude motions of the solvating network; multi-minima potential energy surfaces with low-energy transient barriers emerge from these hydrated topologies, pushing the observables towards vibrationally-averaged molecular conformations.

In this scope, we investigated the stepwise growth of a solvation layer around a chiral molecular switch, camphorquinone oxime, using broadband Molecular Rotational Resonance (MRR) spectroscopy in the 2-8 GHz range. Whereas quantum chemistry calculations confirmed an almost barrierless landscape, isotopic data on ^{18}O species revealed that the position of water molecules was most compatible with transition-state geometries. These findings support the existence of a concerted dynamic motion of water molecules around this molecular system.

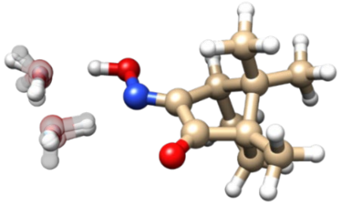

Figure 1. The concerted dynamics of di-hydrated camphorquinone oxime.

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Kinetic modelling of interstellar hydrocarbons: cyano derivatives of propene

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In the last few years, astrochemistry has experienced an incredible growth due to the improvement of the sensitivity of radiotelescopes, allowing the detection of a wide variety of molecules in the interstellar medium (ISM). One of the target sites of study is TMC-1, a dense molecular cloud where several hydrocarbons have been detected, among other species. Five different cyano derivatives of propene were detected towards TMC-1 in 2022 with the QUIJOTE line survey.[1] An accurate quantum chemical characterization of the system with a further kinetic analysis has been performed to discern the isomer-specific reaction channels.

The rate constants for all the feasible reaction pathways to form the cyano derivatives are computed, finding that the calculated abundances for each isomer match reasonably the observed ones and the results of previous theoretical calculations.[2] Furthermore, the incorporation of these accurate rate constants into already existing chemical models improves the efficiency of such models to describe the hydrocarbon chemistry in TMC-1.

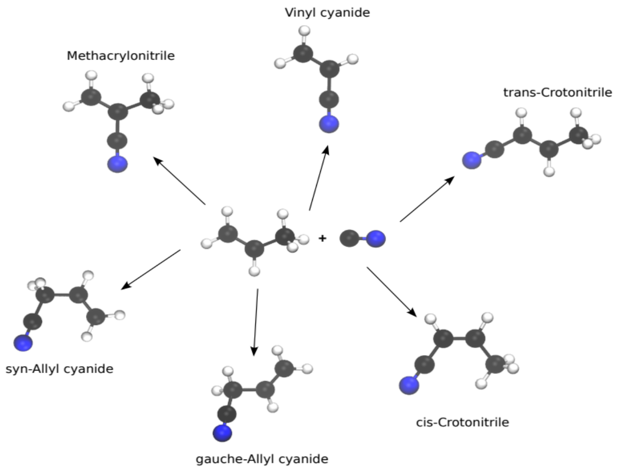

Figure 1: Structures of the six cyanoderivatives of propene.

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

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Presented here is a custom python user interface designed to manage and control the cavity portion of Tennessee Tech's brand new, custom-made combined chirp pulse and Fabry Perot cavity L-shaped FTMW spectrometer. The cavity setup consists of a Fabry Perot cavity, a microwave circuit, and a molecular beam source, which will be used to record rotational spectra of astrochemical species. This script allows for efficient operation and automation of cavity selection and spectra collection. Spectra collection also includes taking a background each before each run to eliminate known noise, ensuring proper identification of spectral lines. To do this, communication with four devices in the FTMW setup is essential: a Valon Synthesizer, an SRS Pulse Delay Generator, a Tektronix Oscilloscope, and a Zaber XNA08A25-E09 actuator. The Valon Synthesizer, controlled via USB and Serial API through valonController.py, generates microwaves with string commands converted to UTF-8. The SRS Pulse Delay Generator sets the trigger rate and controls multiple devices via GPIB and pyVISA API through SRSController.py, with crucial timing managed by the startTrig() function. The Tektronix Oscilloscope, controlled via GPIB and pyVISA through oscilloscopeController.py, digitizes analog microwave signals with various data acquisition methods stored in NumPy arrays. The Zaber actuator managed via USB and ASCII through zaberController.py, precisely controls the Fabry-Perot cavity length. Performance is optimized using the Time API for function speed checks and the Threading API for concurrent data acquisition and GUI management. Data analysis and plotting are handled by NumPy and Matplotlib, with position and intensity data synchronized to ±0.007 seconds accuracy. Threading API is used along with a calibration curve developed from our instrument's initial data, to allow for quick and automated selection of a cavity. A subprogram developed in parallel allows for cavity mapping and tracking across the frequency range, 8-18 GHz. This allows for a thorough look into the different cavity modes to ensure maximum molecular signal strength. The script presented offers a comprehensive automation of the FTMW setup to enhance the spectrometer's efficiency, making it more user-friendly and streamlined for operators.

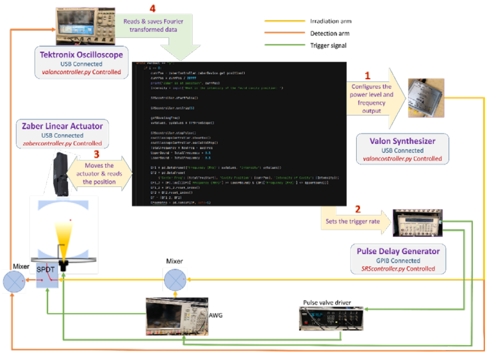

Figure 1: Illustrated schematic of python code integration with Cavity FTMW Setup at TN Tech.

Inspiring Women in STEM

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Historically, women have made significant contributions to science, technology, engineering and mathematics (STEM). Yet they remain underrepresented in these fields, making up just 28% of the global STEM workforce and just 22% of AI professionals.

The journeys of trailblazing women will be profiled, from historical figures who defied the odds to contemporary innovators who are revolutionizing industries. Figures such as Marie Curie, the first woman to win a Nobel Prize in Physics, and Mae Jemison, the first African-American woman in space, exemplify the impact of female pioneers in these fields. By fostering mentorship, increasing visibility and creating inclusive environments, it is possible to unleash the full potential of women in science, technology, engineering and mathematics (STEM). By highlighting their achievements and resilience, the challenges women face in STEAM today will be addressed.

Not only will I explore the lives and legacies of notable women who have transformed these fields, but I will also share my own experience as a researcher and science communicator. My story will serve as an example of how passion for science and perseverance can open doors and overcome barriers.

Electronic and magnetic properties of triangulene monomer and its oligomers

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Triangular zig-zag nanographenes, including metal-free magnetic systems such as triangulene,[1] have acquired considerable scientific attention since their theoretical conception. These compounds, possessing an inherent spin polarization,[2] emerge as promising systems holding substantial importance for innovative magnetic and electronic devices. Here, we investigate the electronic and magnetic properties of several structures including the triangulene monomer and its oligomers using density functional theory (DFT) and multireferencial methods. We evaluate the magnetic coupling, spin-polarization energies, and spin Hamiltonian parameters using a variety of electronic structure approaches, with a discussion on the of the suitability and limitations of the different methods employed. Moreover, the magnitude of the computed properties is demonstrated via molecular orbital diagrams, fractional occupation density and natural transition orbitals between ground and excited states. In this context, we further achieve electron spin localization by diabatizing spin-adapted eigenstates of the molecular electronic Hamiltonian using the spin permutation operator, which enables the decomposition of spin-pure electronic states into spin-localized states, facilitating the evaluation of spin exchange couplings. By combining the diabatization scheme with these electronic structure methods, we proved a clear framework that improves understanding of spin interactions in triangulene compounds.

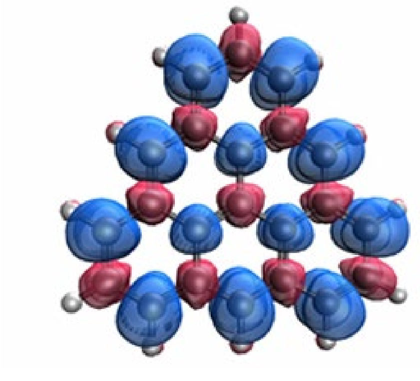

Figure 1. Spin density of a triangulene.

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

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In this communication we present how ionizing radiation influences the formation of peptide bonds in clusters of amino acids in the gas phase. In the past, simulations and experiments were carried out in parallel to understand the possible mechanisms involved[1,2]. Due to these promising previous results, we have expanded the study, including clusters of other amino acids. The main objective of this study is to evaluate the conditions of peptide bond formation in pure clusters of glycine, threonine, valine, serine and cysteine in the gas phase induced by collisions with alpha particles.

Experimentally, mass spectrometry is used to analyze the charged species formed after the collision with the highly charged ions. From the theoretical point of view, first the search for conformers is carried out using the CREST program[3], and then the structures obtained are further reoptimized with the Gaussian16 software[4] using the density functional theory DFT. The second stage of the work was to make an analogous study, but on protonated clusters, since these species are believed to play the key role in the experiments. Finally, we have explored the potential energy surfaces to locate the transition states that explain the mechanism for peptide bond formation from the protonated clusters, also using DFT.

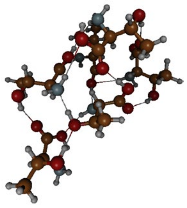

Figure 1. Most stable conformer obtained from CREST for a cluster with 6 threonine molecules.

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

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Hydrogen storage remains a critical challenge for advancing clean energy technologies. Solid-state materials such as Graphdiyne (GDY), a carbon-based two-dimensional structure, have shown promise as storage media due to their high surface area, especially when doped with transition metal clusters[1]. Using simulations based on Density Functional Theory (DFT) within the QUANTUM ESPRESSO[2] framework, the adsorption of hydrogen molecules on V_6 doped GDY, that is, on vanadium clusters containing six atoms supported on GDY, was analysed under two doping regimes: high and low coverage of the layer with V_6. The V_6 clusters bind to the GDY layer with an adsorption energy of 10.46 eV, forming a very stable configuration.–On the other hand, the first and second hydrogen molecules adsorb on V_6 in the dissociated form with 1.86 eV and 1.53 eV adsorption energies, respectively, in the high coverage regime. No significant differences were found between the two regimes. A study of the electronic charge density and the electronic density of states revealed that the dissociated hydrogen molecules bind to the vanadium atoms via hydride-type bond. Hydrogen can also be adsorbed on V_6 in molecular form through a polarization type of bonding. This work highlights the potential of vanadium-doped GDY to serve as an efficient hydrogen storage material, advancing safer, more efficient storage solutions for renewable energy.

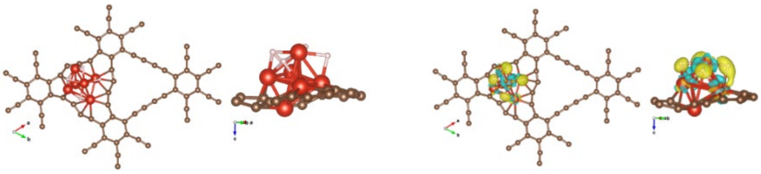

Figure 1. V_6-doped GDY with two adsorbed dissociated hydrogen molecules (left) and the system's charge density (right) with positive density charge in yellow and negative in blue.

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Water Complexes on a Cyclic Thioether from Broadband rotational Spectroscopy

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Cyclic thioethers (also called thiacrowns) are macrocyclic or small-ring compounds that contain sulfur atoms within a ring structure. They are structurally similar to crown ethers but contain one or more sulfur atoms instead of oxygen. In the presence of water, thioethers can form hydrogen bonds. When water molecules interact with thioether groups, the hydrogen atoms of water (from the O-H bond) may form weak bonds with the sulfur atom, resulting in a hydrogen bond network. The hydrogen bonding interaction in this case is often weaker compared to the typical hydrogen bonding involving oxygen, but it still affects the structural properties and dynamics of the complex, especially in the gas phase.

In this study, we employ chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) in the 2-8 GHz frequency range to investigate the complexation of 1,4,7-trithiacyclononane (TTCN) with water molecules supported by quantum chemical calculations. By using CP-FTMW, we were able to obtain high-resolution, broadband rotational spectra, which allows us to examine the structural and dynamic interactions between TTCN and water in the gas phase. The gas-phase conformational analysis of TTCN has been previously reported[1]. However, in this study, we have identified an additional stable conformer of the TTCN molecule.

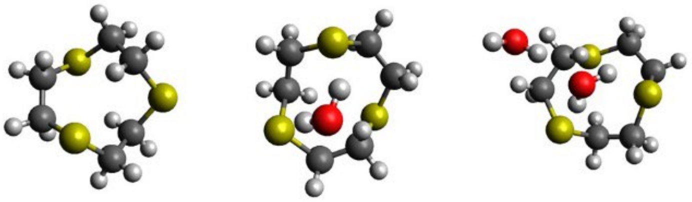

Figure 1. The newly identified conformer of TTCN molecule and the detected isomers of water complexes from quantum chemical calculation

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Ultrafast excited-state dynamics of anisole and its methyl substitutes

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Photochemical processes driven by ultraviolet (UV) light play a vital role in nature. The molecular building blocks of life efficiently absorb UV radiation but resist damage due to ultrafast non-radiative relaxation mechanism[1,2]. Dissociative $^1\pi\sigma^*$ states are key to the photo-resistive properties of aromatic amino acids[3]. Simpler molecular analogues are often used in order to explore the interplay between $^1\pi\pi^*$ and $^1\pi\sigma^*$ states. Anisole (Fig. 1a), featuring a methoxy group on a benzene ring, serves as a model for studying electron-donating substituents on aromatic systems.

We present here time-resolved photoelectron spectroscopy measurements with sub-20 fs temporal resolution to investigate the electronic relaxation pathways and coupled electron-nuclear dynamics in anisole ($CH_3OC_6H_5$) and its methyl-substituted derivatives (*o*-, *m*-, *p*-methyl anisole). Using tunable UV pump pulses between 258 and 287 nm, we prepare electronically excited neutral states, which are probed with 25 eV pulses from a high-order harmonic source equipped with a time-delay-compensated monochromator. By recording photoelectron kinetic energy distributions as a function of UV-XUV time delay (Fig. 1b), we achieved universal detection of transient molecular structures and energy relaxation processes[4].

Previous theoretical studies[5,6] have predicted that conical intersections between ground and excited states, separated by small barriers, act as non-adiabatic pathways for radiation-less decay. Our results show a wavelength-dependent rise time followed by decay with oscillatory features, which we attribute to the energetic barrier predicted in the literature.

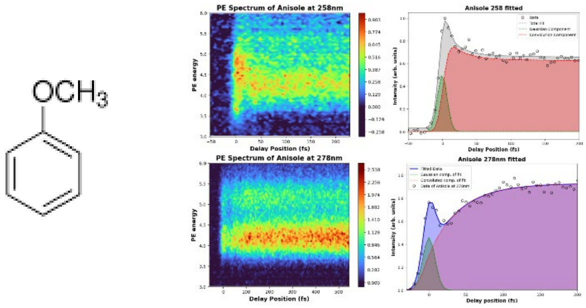

Figure: a) Anisole molecule, b) photoelectron kinetic energy signal of anisole as a function of the delay at 258 nm, and c) fitted temporal evolution of the data.

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

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The study of non-covalent interactions (NCIs) is essential for understanding the behavior and properties of biomolecules. Among these interactions, hydrogen bonding stands out as one of the most important NCI, as it plays a fundamental role in determining the structure of proteins and DNA.[1] Mass-resolved laser spectroscopy in combination with computational methods has been successfully applied to investigate NCIs, providing valuable information regarding the molecular conformation and binding energies.[2,3]

Following our previous investigations on the aggregation of 2-phenylethanol (PEAL),[4] in this work we focus on the study of NCIs present in homo and hetero-dimers derived from 2-phenylethanethiol (PET) and 2-phenylethylamine (PEA), using time-of-flight mass spectrometry (TOF-MS) in combination with resonant multiphoton ionization spectroscopy (REMPI) and ion dip infrared spectroscopy (IDIR). Our experimental results, combined with quantum chemical calculations, provide important insights into the molecular interactions involved in the aggregation of PET, PEAL and PEA (Figure 1).

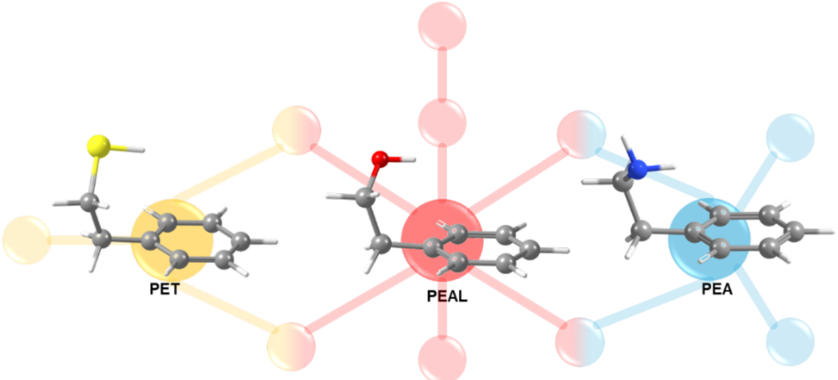

Figure 1. Dimerization pathways of PET, PEAL and PEA

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

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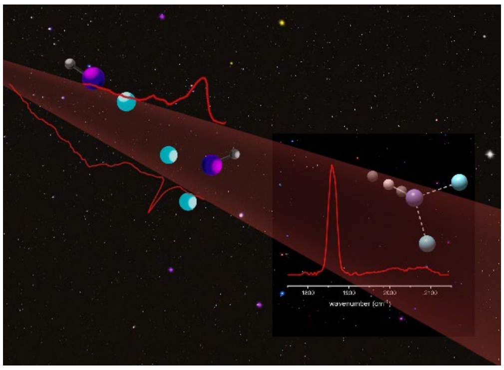
Iron is one of the most abundant metals in the universe, the iron hydride cation (FeH^+) is considered to exist in the interstellar medium (ISM). However, it has not been identified by spectral observation in the ISM due to the lack of laboratory data.

Our research aims to fill this gap by providing spectroscopic data on FeH^+ to aid its identification in the interstellar medium. Ions of interest were generated using a laser vaporization source targeting ^{56}Fe-enriched iron and analyzed with a Fourier Transformation Ion Cyclotron Resonance Mass Spectrometer (FT-ICR-MS) after irradiation. We investigated the vibrational spectroscopy of Argon-tagged FeH^+, observing the Fe-H fundamental stretching mode[1] and its first overtone[2]. High-level quantum chemical calculations are indispensable for accurate explanations of natural phenomena on the molecular level.

In the study, we present detailed theoretical and experimental investigations on the vibrational transition of argon-tagged FeH^+, its deuterated analogs, and electronic transitions to low-lying excited states. according to the comparison between experiment and theory, the Fe-H fundamental stretching and its first overtone in bare FeH^+ is expected in the 1790-1840 cm^{-1} and 3525-3619 cm^{-1} region, respectively.



Acknowledgments: This research was funded in part by the Austrian Science Fund (FWF), Grant DOIs 10.55776/w1259 (DK-ALM, SJ, AE, NP, MKB) and 10.55776/P35013 (MO). MJ thanks the Ministerio de Universidades of Spain and the Universidad de Valladolid (UVa) for a "Margarita Salas" postdoctoral contract (CONREC-2021-265).

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Glycolic acid microsolvation in gas phase

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Glycolic acid (CH_2-OH-COOH), the simplest hydroxyacid, is thought to have prebiotic significance in interstellar chemistry, potentially contributing to the origins of life in the universe. From a biological point of view, it is involved in the glyoxylate cycle, an anabolic alternative of the Krebs cycle taking place in plants and other systems.[1] Two low energy conformers have been identified by microwave spectroscopy,[2,3] and its one monohydrated complex by infrared spectroscopy.[4] Other studies are limited to theoretical calculations.

The present study investigates glycolic acid hydrates (GW_x) in gas phase using a broadband chirped-pulse Fourier transform microwave spectrometer (CP-FTMW) coupled to a supersonic jet expansion. We have identified the first tree hydrated complexes ($GW_{1–3}$) and detected the ^{18}O monosubstituted water isotopologues for all the hydrated complexes, allowing the determination of their r_s structure. In the trihydrated complex (see Figure 1) a splitting of transitions is observed, which is attributed to the presence of two states with nearly identical rotational constants. The experimental results are complemented by theoretical calculations to provide a deeper understanding of the stabilizing forces in these complexes and to explore the relationship between hydration number, structure and cooperative effects.

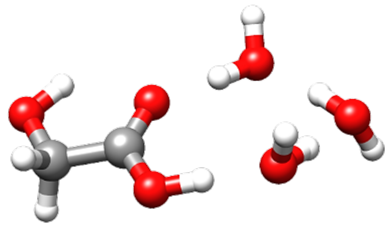

Figure 1. Structure of the lowest energy GW_3 conformer at B3LYP-D3BJ/6-311++G(2d,p).

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Photodissociation initiated by sunlight of 2-butanona in the troposphere.

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Ketones, such as 2-butanone, are emitted into the atmosphere from both natural sources and anthropogenic activities, including industrial processes and vehicular emissions[1]. These compounds play a significant role in atmospheric chemistry, contributing to the formation of ozone and secondary organic aerosols through photochemical and oxidative processes[2]. Among the various atmospheric degradation pathways, photolysis induced by ultraviolet solar actinic radiation ($\lambda > 290$ nm) and reactions with atmospheric oxidants like hydroxyl (OH) radicals are critical mechanisms for ketone removal [3,4].

In this study, the gas-phase photolysis of 2-butanone was evaluated under controlled conditions using a solar simulator. Experiments were conducted both in the presence and absence of light to differentiate photolytic effects from other potential loss mechanisms. A Pyrex cell containing diluted 2-butanone in air was irradiated various exposure times, and the temporal evolution of the sample was monitored using Fourier Transform Infrared (FTIR) spectroscopy. The concentration of 2-butanone was quantified before and after irradiation to assess sample loss and to determine whether photolysis occurred.

This approach enabled the determination of photolysis rate coefficients (J) and provided insight into the atmospheric degradation of 2-butanone. The implications of 2-butanone photolysis on its atmospheric fate will be discussed.

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

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Transition metals (TM) are often used as excellent catalysts in many reactions because of their different oxidation states, activity, selectivity, and unfilled d-orbitals. Supported TM catalysts have been strongly investigated in the last decades since a fine dispersion of the metal catalyst on the support reduces amount of catalyst needed while retaining the same catalytic effect. Carbon-based materials are proposed as efficient support platforms for catalysis due to their excellent electronic and mechanical properties, high superficial area, and low cost. Along with the metal-support interactions, the performance of the catalysts can be adjusted by varying the size of the supported metal nanoparticles[1]. Structural deformations of the supports can be triggered depending on the selected metal and support and on the nanoparticle coverage.

We have performed DFT calculations to study the structural and electronic properties of single atom and single cluster catalyst of cobalt, palladium, and vanadium adsorbed on Graphdiyne (GDY) and Boron-graphdiyne (BGDY) layers. The main goal is to investigate the competition between atomic and cluster dispersion in building up stable catalytic platforms, depending on the coverage of the substrate. Our results suggest a strong dependence on the specific metal and the support.

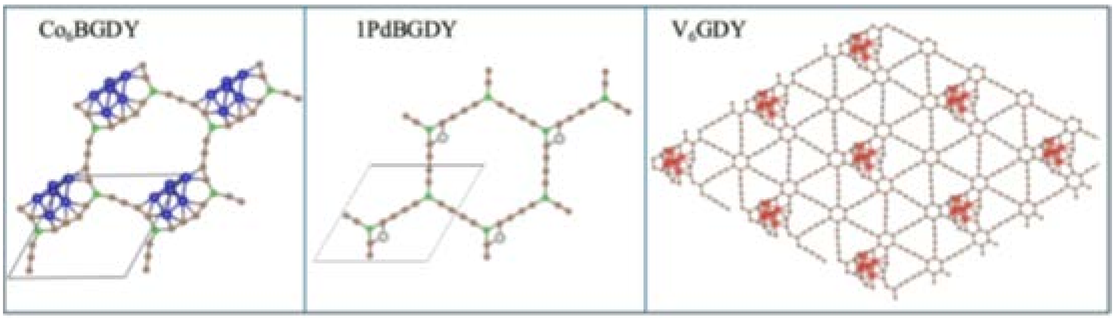

Figure 1. TM catalysts supported on BGDY and GDY layers.

Acknowledgments: Work supported by Grant PID2022-138340OB-I00 funded by MCIN/AEI/ 10.13039/501100011033 and FSE+. J.S. acknowledge the doctoral grant from The Schlumberger Foundation, Faculty for the Future.

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

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The substituent effects in the catalyst-free [3+2] cycloaddition (32CA) reaction between azides and nitriles has been studied using molecular electron density theory at the M06-2X/6-311+G(d,p) computational level. In this study, the theoretical scale of reactivity was explained by the electrophilic activation/deactivation effects that promoted by electron-withdrawing and electronreleasing substituents in both azide and nitrile components. The most electron-withdrawing and electron-releasing substituents in components were selected to study the regioselectivity of the expected correspondent tetrazole products by the global electron density transfer (GEDT) analysis at the transition state structure (TS) (Figure 1).

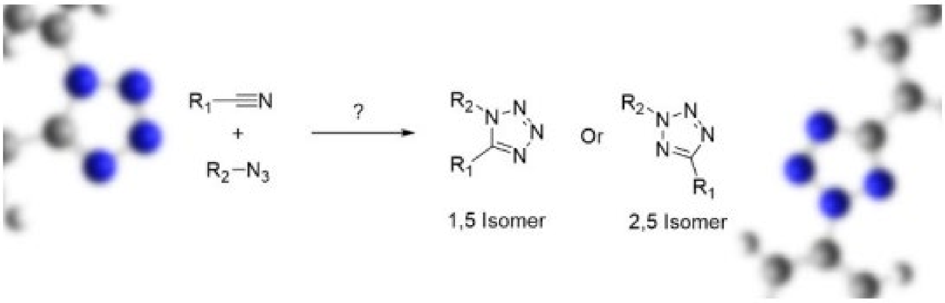

Figure 1. The [3+2] cycloaddition (32CA) reaction between azide and nitrile.

Optical response of a binary atomic system with gain

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We study the optical response of a binary atomic system in which one of the atoms is incoherently pumped while the system is continuously illuminated by a quasi-resonant beam [1]. Based on a fully time-dependent QED approach we analyze, and eventually optimize, the coherent manipulation of the system [2]. Using a diagrammatic representation, we identify all the radiative processes, namely, scattering, absorption, stimulated emission and spontaneous emission, along with the excitation transfer rate. We find that, for certain values of the pump rate and the interatomic distance, the collective part of the extinction cross section vanishes and eventually becomes negative. PT-symmetry signatures such as that of an asymmetrical response with respect to the direction of the illumination are also analyzed [4]. In a prospective work this study will be extended to atomic arrays, with the aim of optimizing the scalability of multiple-atom qubits [3].

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Rotational Spectroscopic Study of Cis-Stilbene and its Water Complexes

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Molecular photoswitches have promising applications in controllable drug delivery within the field of photopharmacology, typically characterized by extended hydrophobic aromatic systems. While the application of molecular photoswitches to photopharmacology in biological systems is appealing, a significant challenge lies in their poor water solubility, as biological systems operate in aqueous environments.[1] Cis-stilbene (CS) is one of the most important motifs found in many molecular photoswitches, as it undergoes cis-trans photoisomerization upon exposure to UV light. It is widely used as a benchmark for theoretical models. Understanding the interaction between CS and water is crucial for accurately modeling photoisomerization in aqueous solutions.

Here, we present a broadband rotational spectroscopy study of cis-stilbene and its 1-2 water complexes, combined with theoretical calculations. The rotational spectra of cis-stilbene and its hydrates were recorded using a newly arranged chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer at the University of Alberta, covering 2-8 GHz spectral range. The experimentally observed elusive CS-$(H_2O)_2$ cluster is predicted to be stable by only a few, less commonly used quantum chemistry methods. Extensive quantum chemistry investigations at various levels of theory were performed to identify the conformational carrier of the CS-$(H_2O)_2$ cluster.

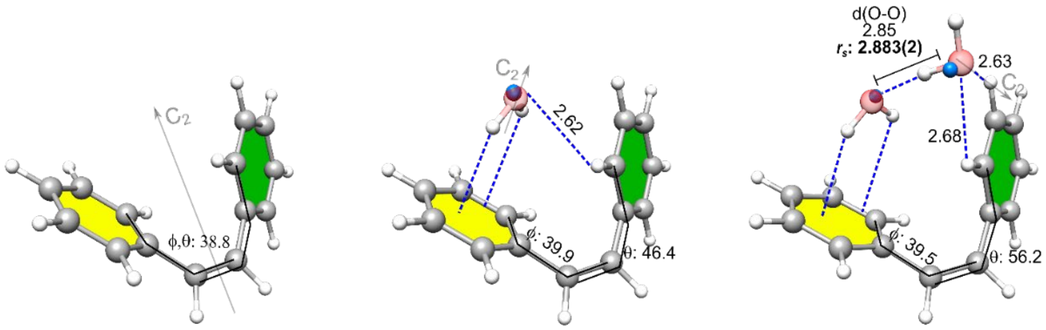

Figure 1. Experimentally observed CS and its 1-2 water complexes.

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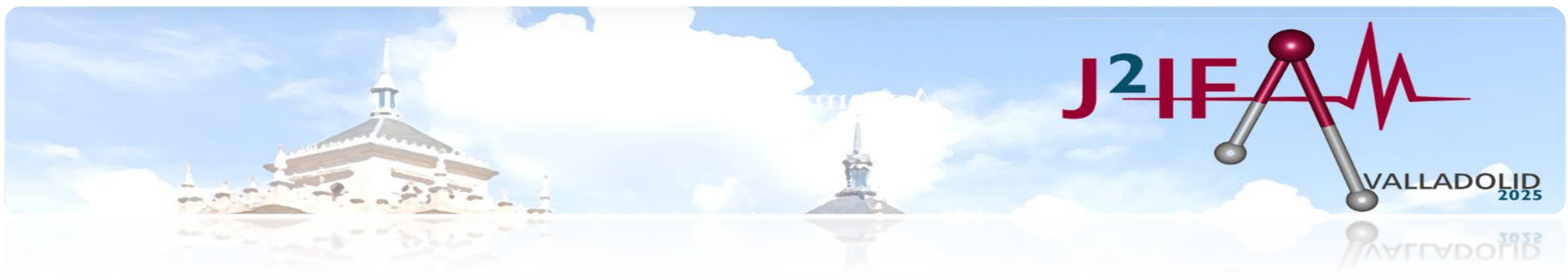

Theoretical study of reactions in the interstellar medium with phosphorus radicals

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The field of astrochemistry is based on the detection of chemical species and modelling of their possible formation and transformation reactions in the interstellar medium (ISM). Several nitrogen-containing molecules have been identified. However, only a limited number of simple phosphorus-containing molecules have been detected in space, including phosphorus carbide (CP) and phosphorus monoxide (PO).

The aim of this work is to analyse the formation possibility of more complex phosphorus-containing molecules in the ISM from the simple molecules already detected. Specifically, we focus on the reactions between simple unsaturated hydrocarbons acetylene (C_2H_2) and ethylene (C_2H_4) with PO and CP radicals. Analogous reactions of CN with these hydrocarbons[1,2] as well as C_2H_2 with CP[3] have been previously studied.

Results show a clear correlation between the presence of an oxygen atom and endothermic reactions. Therefore, only one reaction was studied: $C_2H_4 + CP$. The analysis of its potential energy surface shows several intermediates that, through some transition states, result in the formation of two products.

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A High-Level Quantum Chemical Study on the Structure and Spectroscopic Properties of $HOCH_2CP$ Conformers

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The search for phosphorus-bearing species in the interstellar medium (ISM) has become a compelling topic in the last years due to its significance in prebiotic chemistry[1]. Following the recent detection of the glycolonitrile molecule ($HOCH_2CN$) in the interstellar medium[2], we employed high-level quantum chemistry methodologies to predict the structure and spectroscopic properties of the potential conformers of $HOCH_2CP$, the phosphorus-bearing analogue of glycolonitrile.

Using the B2PLYPD3 functional and the explicitly correlated coupled cluster method, CCSD(T)-F12b, we computed the relative energies and rotational parameters of the $HOCH_2CP$ conformers. Furthermore, we proposed possible reactions that could lead to the formation of this molecule in the ISM. Our study suggests that the most stable structure is the gauche conformer, regardless of the level of theory employed. We also studied transition states and the interconversion barrier between the conformers.

The analysis of its rotational spectrum is anticipated to be challenging due to the double-minimum interconversion effect between the gauche conformers. The comprehensive set of spectroscopic constants and vibrational frequencies provided here will aid future laboratory or astronomical searches.

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

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This study investigates the physical mechanisms underlying the detection of Cu(II) using an azophenyl-substituted ortho-vanillin Schiff base (HL) probe. Its electronic and optical properties were analyzed using atomic spectroscopy and theoretical modelling. Upon interaction with Cu(II), the probe exhibits a distinct color change, confirmed through UV-Vis, FTIR, and EPR spectroscopy. The study of electronic transitions, particularly the blue shift and changes in absorption maxima, indicates a stable 1:2 stoichiometry between Cu(II) and the probe. These findings are supported by Job's plot and X-ray crystal structure analysis. Theoretical investigations based on Density Functional Theory (DFT), utilizing X-ray crystal structure data, provide detailed insights into electronic density redistribution and molecular orbital energy levels (HOMO-LUMO). During the formation of Cu(II) complexes, the observed decrease in the HOMO-LUMO gap reflects the physiochemical mechanism of electronic transitions and internal charge transfer. This process significantly alters the optical characteristics of the probe, highlighting its importance in metal ion detection and in understanding electronic charge dynamics. The HL probe demonstrates significantly low cytotoxicity towards cancer cells, making it suitable for live-cell imaging of Cu(II) ions in MDA-MB 231 cell line. The probe is employed to detect cancer cells in the presence of normal cells. Its spectroscopic shifts, combined with theoretical analysis, offer a comprehensive model for studying electronic structures, energy level transitions, and molecular dynamics. This research underscores the probe's potential not only in ion detection but also in advancing materials development and theoretical modelling for cellular and molecular processes.

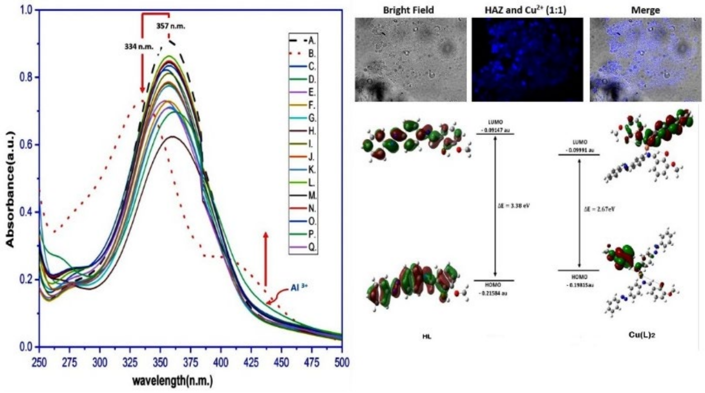

Figure 1. (a) Absorbance Spectral change of HL in addition of copper. (b) Cancer cell sensing in MDA-MB 231 cell line. (c) Theoretical study of Hl and complex $Cu(L)_2$.

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Low-Energy Electron Impact Ionization of Water Molecules

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Collisions between charged and neutral particles play a central role in atomic physics, as they lead to a variety of phenomena such as ionization and excitation of atoms and molecules. In particular, the study of single ionization by electron impact has been a focus of research due to its relevance in understanding the behavior of electrons and ions in the presence of external fields. This process commonly referred as (e,2e), involves the interaction of an incident electron with an atomic or molecular target. Specifically, the water molecule serves as a captivating focal point of study. Given that water comprises over 80% of biological materials, there exists significant interest in exploring cross-section data for electron-impact ionization of water. In our current investigation, we employ the M3CWZ model to examine the ionization of the orbitals 1b1+3a1 of the H_2O molecule, specifically focusing on low impact energies. Our results are presented in Figure.1 as a sum TDCS's of $1b1$ and $3a1$ orbitales at a low impact energy 65 eV, our theoretical results are compared with the MCTDW [1] and M3DW [2] models, showing comparable accuracy to both the available theories and the experimental data.

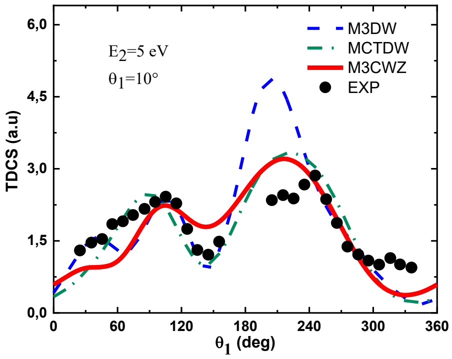

Figure 1. Absolute summed TDCS for the ionization of 1b1 and 3a1 orbitals of H2O as a function of the ejection angle at 65 eV impact energy. Theoretical results are red solid line (M3CWZ), blue dashed line (M3DW) [2] and green dashed-dotted line (MCTDW) [1]. The absolute experimental data are black circles taken from [3].

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The Conformational Panorama of gabapentin

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Gabapentin is an anticonvulsant drug used to treat epilepsy, neuropathic pain, and anxiety disorder. It was initially though that, because of the structural similarities that gabapentin shares with the neurotransmitter GABA, by developing gabapentin as a GABA analogue it would show an enhanced ability to cross the blood-brain barrier, creating a more effective therapeutic agent for neurological conditions. Nevertheless, it has been proved that its mechanism of action is distinct. Instead of directly influencing GABA receptors, gabapentin inhibits the $\alpha 2\delta 1$ subunit of calcium channels on presynaptic neurons. In this work we characterize the most stable conformers of gabapentin in isolated conditions using Laser Ablation Chirped Pulse Fourier Transform Microwave (LA-CPFTMW) spectroscopy. The experimental results, complemented with computational methods, show that there are five predominant conformers of gabapentin based on the intramolecular interactions and in the configuration of the cyclohexane ring. The detected structures differ in the intramolecular interactions between the different functional groups and are stabilized mainly through N-H•••O=C, O-H•••N, and N-H•••O-H intramolecular interactions.

The results are also contrasted with those of GABA, highlighting structural insights relevant to gabapentin's efficacy as a therapeutic agent. As it will be shown, the incorporation of a ring I GABA to form gabapentin entails drastic differences in their conformational panorama.

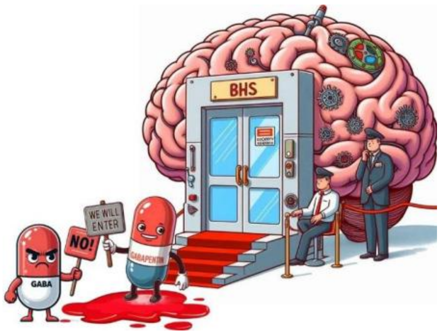

Figure 1. Representation of GABA and gabapentin interacting with the blood-brain barrier (BBB), highlighting structural and functional differences that influence their therapeutic roles.

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Shedding light on atmospheric photochemistry by means of computational methods

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Sunlight chemistry plays a key role in the global dynamics of atmospheric compounds. Understanding the photochemical processes that these species may undergo is essential to assess their role and fate in our planet's atmosphere. In this regard, atmospheric models can simulate the atmospheric cycle of these species and analyse their global distribution and accumulation. However, the limited information on the photochemical properties of certain atmospheric compounds sometimes leads to models and simulations that do not align with observational data. Taking that into account, in recent years we have studied the photochemical reactivity of atmospheric mercury,[1-3] a potent neurotoxin of global concern, and of key sulphur species involved in the formation of sulphate aerosols, a chemical process of great importance in solar geoengineering plans to reduce global temperatures.[3-6] These studies, carried out using quantum chemical methods and in collaboration with atmospheric scientists, shed light on the importance of light-induced reactivity in the atmospheric cycling of mercury and sulphur compounds.

Acknowledgments: The content of this contribution is related to my PhD thesis entitled "*Atmospheric chemistry of mercury and sulfur induced by sunlight: Quantum-chemical modelling and environmental implications*", supervised by Dr. Daniel Roca Sanjuán, PDI member of the Department of Physical Chemistry, and Dr. Alfonso Saiz López, Research Professor at the Institute of Physical Chemistry Blas Cabrera (CSIC) in Madrid. The project that gave rise to these results received the support of a fellowship from "la Caixa" Foundation (ID 100010434); the fellowship code is LCF/BQ/DR20/11790027. This work was also supported by the Spanish Agencia Estatal de Investigación of the Ministerio de Ciencia e Innovación (MICINN) and the European Regional Development Fund (FEDER) through project PID2021-127199NB-I00 and by the Generalitat Valenciana through project CIAICO/2022/121.

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

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The astrochemical studies of the P-bearing molecules have attracted great interest in the latest years, since the increase of observations of these kind of molecules in several astrophysical objects. However, the chemistry of the P atom is neither very well-known nor well understood, making it difficult to develop chemical models to understand the origin of these molecules.[1] One of the possible triggers for the chemistry of the P atom are the phosphorous hydride molecules, supported by the great abundance of the H_2 of H_3^+ molecules.[2] To test this hypothesis and gather data on P chemistry, the main goal of this project is to study the formation and destruction processes, as well as, the physical properties of the different phosphorous hydrides and their cations. To study the processes leading to the formation of PH_2^+, it is necessary to describe the potential energy surfaces of all the states involved. Focusing on dissociation into the lowest-energy channels, $P^+ + H_2$ and $PH^+ + H$, the study begins with the characterization of the triplet states of PH_2^+. We have calculated the three triplet states associated with these dissociation channels and the non-adiabatic couplings between them. The PES will allow us to calculate the absorption and photoionization spectra related of PH_2^+ and study the reaction dynamics of atomic dissociation channels, which will be crucial to understand the processes to interpret the data from the astrophysical media.

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

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α-Pinene ($C_{10}H_{16}$) is considered one of the most important global secondary organic aerosol (SOA) sources. In the last years, intense studies have been conducted to unveil the chemical composition of α-pinene SOA. Some experiments as those reported by *Ye et al.* [1] have shown that pinanediol ($C_{10}H_{18}O_2$), an oxidation product of α-pinene, can be an important contributor to new particle formation. Understanding its interactions with atmospheric molecules is essential to elucidate the early stages of molecular aggregation in aerosol formation. Here, we present an investigation of pinanediol (PD) and its hydrates using a chirped-pulse Fourier transform microwave spectrometer (CP-FTMW) in the 2-8 GHz frequency range and supported by quantum chemical calculations. The parent species and all heavy atom isotopologues (^{13}C and ^{18}O) of PD have been observed in their natural abundance. The resulting experimental rotational constants have been used to determine the substitution structure (r_s) of PD. The rotational spectroscopy investigation has been extended to hydrates of PD, and two complexes with one molecule of water have been observed. The two adducts are stabilized by intramolecular O−H···O hydrogen bonds in a clockwise or counter-clockwise arrangement forming a six-membered ring. This work enrichs our knowledge of the structure of PD and its possible interactions in the atmosphere opening new perspectives for the study of other monoterpenoids.

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

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The conformational landscape of small organic acids and their complexes provides valuable insights into their behavior in various environments. One of the most important carboxylic acids is pyruvic acid, a simple alpha-keto acid, which plays a significant role in atmospheric chemistry, influencing aerosol formation, cloud properties, and ultimately, climate.[1] Using chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy,[2] we have studied the structural behavior of pyruvic acid after the addition of individual solvent molecules (water and 2,2,2-trifluoroethanol). This technique allows for the detection of a large number of conformations in an isolated environment, facilitating the unambiguous identification of conformers, tautomers, isotopologues, and enantiomers. Based on the previous rotational study of the structures of the pyruvic acid-water complexes,[3] our investigation has been instrumental in elucidating the intermolecular interactions involved, revealing a greater tendency for water molecules to bind to a single hydration site, specifically the hydroxyl and carbonyl groups of the ketone. The cluster with 2,2,2-trifluoroethanol is estabilized by interactions with the carbonyl and methyl groups. This study underscores the importance of microwave spectroscopy as a tool for the experimental structural elucidation of microsolvated complexes in the gas phase.[4]

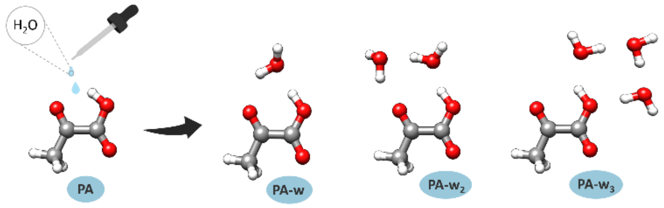

Figure 1. The addition of water molecules to pyruvic acid.

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Kinetic Study of CN with H_2S and CH_3CH_2SH at the Ultra-Low Temperatures of the Interstellar Medium.

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Ultra-low temperature conditions of the coldest parts (~10-100 K) of the interstellar medium (ISM) are very difficult to achieve to study the gas-phase reaction kinetics. The CRESU (*Cinétique de Réaction en Ecoulement Supersonique Uniforme*) technique[1] was developed for that purpose avoiding the gas condensation onto the reactor walls. This technique employs the supersonic gas expansion at speeds much higher than the speed of sound (Mach number = 5.26-8.58, depending on the temperature conditions). In interstellar molecular clouds, such as Orion Nebula, sulfur compounds have been detected[2], while cyano (CN) radicals are ubiquitous in the ISM[3]. The knowledge of the gas-phase kinetics of radical-molecule reactions is important to develop molecular models of the ISM to understand the evolution of the universe. For that reason, in this work, the gas-phase kinetics of the reactions of CN with H_2S (hydrogen sulfide) and CH_3CH_2SH (ethanethiol) have been studied between 11.7 K and 45.5 K. The Pulsed Laser Photolysis – Laser Induced Fluorescence (PLP-LIF) technique[1] was employed to generate CN radicals by ultraviolet PLP of ICN and to monitor the LIF exponential decay as a function of the reaction time (165-760 μs, depending on the temperature conditions).

The results of this investigation will be discussed in terms of the CN-reactivity and the potential impact on the modelled abundances of H_2S and CH_3CH_2SH in an interstellar dark cloud.

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Simple Ionization of Molecular Nitrogen.

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Collisions between charged and neutral particles play a central role in atomic and molecular physics. A significant area of investigation lies in the study of electron and positron impact single ionization of atomic and molecular targets, known as (e,2e) processes, which shed light on the behavior of electrons and positrons during their interaction with the target in the entry channel, as well as their interactions with all resulting particles in the exit channel. This phenomenon provides valuable insights into fundamental atomic and molecular processes. The ionization of the nitrogen molecule (N_2) is particularly important to study, as nitrogen is a key component of biological materials, including proteins and DNA. Understanding its ionization process offers critical insights into both fundamental physics and its applications in biological and medical research.

In this study, we present theoretical triple differential cross sections (TDCS) for the ionization of nitrogen molecule (N_2) induced by both electron and positron impact, in the intermediate energy regime. Calculations are performed using three coulomb waves with variable charge model which was successfully applied for atoms [1] and H_2O molecule [2] and extended here for N_2 molecule. The model, called M3CWZ, also incorporates the post-collisional interaction (PCI). The TDCS results are obtained in asymmetric coplanar geometry for the outermost molecular orbital $3\sigma_g$ and compared with the previous theoretical result of DWBA model [3] as well as the experimental data taken from [4] De Lucio et al 2016 Physical Review. A. The comparison indicates an overall good agreement between our results and the experimental observations.

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Charge effect on the single ionization of Argon

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This study investigates the ionization of argon 3p by positron and electron impact at an incident energy of 200 eV, using 3CWZ model. This approach utilizes Coulomb waves with variable effective charges, Z(r), to describe the continuum states of all particles involved in the ionization process. The 3CWZ model incorporates key physical phenomena, such as post-collision interaction (PCI) and exchange effects, which are crucial for accurately modeling ionization dynamics. Triple differential cross sections (TDCS) are calculated for various kinematic conditions and compared with recent experimental data from Dubois and de Lucio [1], as well as with predictions from other theoretical frameworks. The results show that the 3CWZ model provides a reliable representation of the ionization process, aligning well with experimental observations. Notably, it effectively accounts for the influence of the projectile charge (positron versus electron) on ionization dynamics, outperforming other models in this aspect. This work highlights the critical importance of including variable effective charges, PCI, and exchange effects in theoretical models to achieve more accurate descriptions of ionization processes, especially when different projectiles are involved. These findings provide valuable insights into the fundamental interactions between charged particles and atoms, advancing both theoretical and experimental research in atomic collision physics.

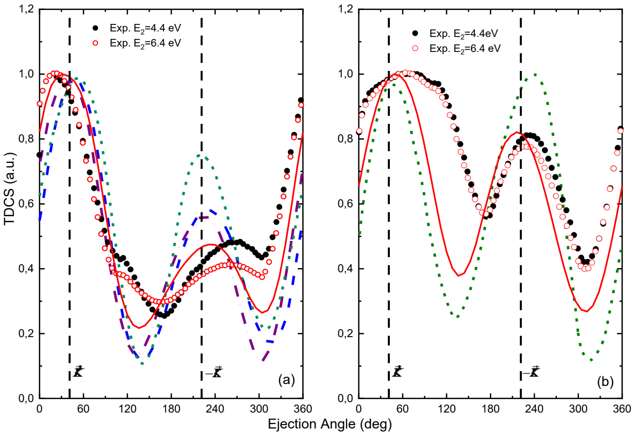

Figure 1. Theoretical and experimental TDCS results for argon 3p ionization by positrons (panel a) and electrons (panel b) are presented as functions of the ejection angle. 3CWZ (red solid line), CDW-EIS (green short-dashed line) [2], DWBA (blue dashed line) [3], and DWBA (purple dashed-dotted line) [4].

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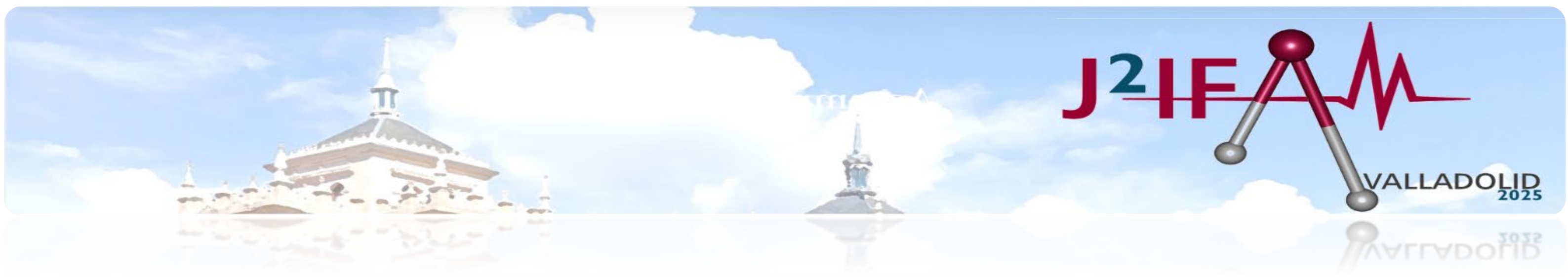

Mapping Charge Transfer Dynamics in nitroaniline and derivatives

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Photoinduced electron transfer (ET) and charge transfer (CT) processes are essential in natural and technological systems, governing mechanisms such as photosynthesis, photo-oxidation, and molecular damage, as well as photovoltaic devices that convert solar energy into clean electrical energy. These processes begin with the ultrafast formation of electron-hole pairs, occurring on attosecond to femtosecond timescales[1]. Beyond this ultrafast regime, slower nuclear dynamics interplay with electronic relaxation over femtoseconds to nanoseconds, driving structural changes in the system[2].

Push-pull molecules, characterized by donor ($-NH_2$) and acceptor ($-NO_2$) groups, serve as effective models for studying ET and CT dynamics. *para*-nitroaniline (PNA, $C_6H_6N_2O_2$) is particularly noteworthy due to its simple structure and strong CT behavior. UV photoexcitation in PNA initiates a charge transfer from the amino group to the nitro group, leading to electronic transitions and significant dipole moment changes[3]. The charge transfer state in PNA corresponds to a $^{1}\pi\pi^*$ transition involving the amino-to-nitro group charge migration. Additionally, the lowest triplet state corresponds to the $^{3}\pi\pi^*$ transition, providing insight into intersystem crossing and triplet state dynamics[3].

In this study, we present preliminary results from time-resolved transient absorption spectroscopy (TAS) experiments on PNA and derivatives, like 3-nitroaniline and N,N-dimethyl–4-nitroaniline. Structural modifications, such as altering the donor group's position, enable us to probe their effects on electronic relaxation and solvation dynamics. These findings highlight the role of structural and environmental factors in determining ET and CT mechanisms, offering insights into broader implications in photochemistry and energy conversion[4].

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Spectroscopy of Ionic Iron Compounds with Astrochemical Relevance

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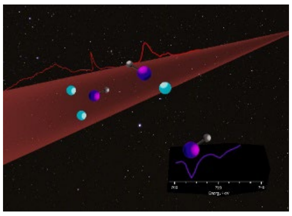
Understanding the atmospheric composition of low-mass stars and brown dwarfs is crucial for interpreting their spectra. Metal-bearing condensable clouds, such as those containing cationic iron hydride (FeH^+), are predicted to play significant roles in these environments, though FeH^+ has yet to be detected due to limited laboratory data. Our research aims to fill this gap by providing spectroscopic data on FeH^+ to aid its identification in the interstellar medium. Ions of interests were generated using a laser vaporization source targeting ^{56}Fe-enriched iron and analyzed with a Fourier Transformation Ion Cyclotron Resonance Mass Spectrometer (FT-ICR-MS) after irradiation. We investigated the vibrational spectroscopy of Argon-tagged FeH^+, observing the Fe-H fundamental stretching mode[1] and its first overtone[2]. We are also conducting UV-Vis spectroscopy of FeH^+ to further explore its astrophysical significance. High-level quantum chemical calculations are indispensable for accurate explanations of natural phenomena on the molecular level. In collaboration with Prof. Dr Tobias Lau at Helmholtz-Zentrum Berlin (HZB). we measured the first tag-free FeH^+ X-ray absorption spectroscopy[3], and the comparison between experimental data and the absorption of the interstellar medium in the iron L2,3 edge observed in the Cygnus X-1 spectrum enhances the potential for detecting FeH^+ in astrochemical environments. The tag-free spectroscopy of FeH^+ is coveted center in our research project. The UV-Vis spectroscopy of FeH^+ is also conducted coupled with state-of-art calculation methods.



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Decoding the 1,4 N···S intramolecular interaction in biomolecules using rotational spectroscopy

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Non-covalent interactions involving sulfur and nitrogen play a significant role in stabilizing molecular conformations and influencing electronic properties. This study focuses on two sulfur-containing heterocyclic compounds, 4-methyl-5-(2-pyrazinyl)-3-dithiolethione (Oltipraz) and 2-(2-Pyridyl)benzo[b]thiophene (PBT), to explore the impact of the 1,4 N···S intramolecular interaction using high-resolution rotational spectroscopy and quantum chemical calculations.

The molecular structures of both compounds were analyzed using broadband chirped-pulse Fourier transform microwave spectroscopy (2-8 GHz) in a supersonic jet expansion, allowing for a precise determination of their rotational constants and ^{14}N nuclear quadrupole coupling parameters. Density functional theory (DFT) calculations supported the spectroscopic findings and provided the electronic and conformational properties of these molecules.

In Oltipraz, preliminary spectral analysis suggests the presence of an intramolecular N···S interaction, influencing its preferred molecular conformation by stabilizing a specific twisted geometry. For PBT, the rotational spectrum revealed the presence of two conformers. The preference for the cis-locked geometry confirmed the role of N···S interactions in guiding molecular orientation.

The Non-Covalent Interaction (NCI) index analysis and Natural Bond Orbital (NBO) calculations provided further insights into the nature and strength of the 1,4 N···S interaction, confirming its conformational and electronic role. The computational results indicate that this interaction significantly lowers the energy barrier between conformers, stabilizing specific orientations.

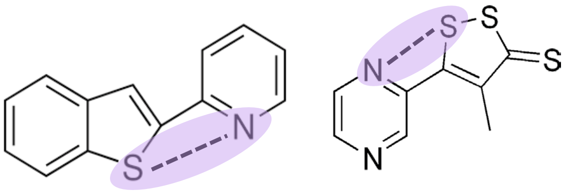

Figure 1. Molecular structure of PBT (left) and oltipraz (right).

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

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The study of stellar phenomena such as kilonovae is limited by the lack of accurate atomic data. Rare earth elements, like Nd III, play an important role in the study of such events. However, these elements remain significantly understudied[1], with limited information available in major atomic databases like NIST[2], VALD[3] or Kurucz[4].

Our experimental setup uses a hollow cathode lamp as a plasma source, based on a design developed at Imperial College London[5]. In this configuration, Doppler broadening, which is inversely proportional to atomic mass, is the dominant broadening mechanism. This results in narrow spectral lines for heavy elements such as Nd III[6], requiring a high-resolution detector with a small pixel size to minimize instrumental broadening and ensure accurate spectral measurements.

This work presents the calibration of our improved spectroscopic setup[7,8]. The system integrates a hollow cathode discharge lamp, a 1.5 m Jobin-Yvon monochromator with a 2400 lines/mm diffraction grating, and a newly installed CMOS camera with a pixel size of 6.5 microns. Calibration includes assessments of curvature, dispersion, and transmission to ensure accurate measurements of atomic parameters such as branching ratios.

Acknowledgments: I would like to express my gratitude to Maria Teresa Belmonte and Pratyush Ranjan Sen Sarma for their guidance and support during my undergraduate thesis project.

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

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Porphyrins are intriguing molecules with properties, which are important for biochemical, light-harvesting and other applications, especially if derivatization of the original macrocycle is performed. Their study will not be complete without the analysis of modifications of the electronic structure upon excitations. In this study we apply Quantum Chemistry Topology [1,2] to both the ground and excited states and show that the methodology used so far mostly for ground states of molecules could be applied for excited states as well. We present the analysis of the electronic density obtained from the CASSCF (complete-active-space self-consistent field) and TD-DFT (time-dependent density functional theory) calculations of porphin and cobalt(II) porphyrin and their derivatives with hydrogen atoms substituted by fluorine and show that several derivative quantities, like Laplacians or stress tensor of the density are sensitive to changes upon the excitations and derivatization and can be used to study these phenomena.

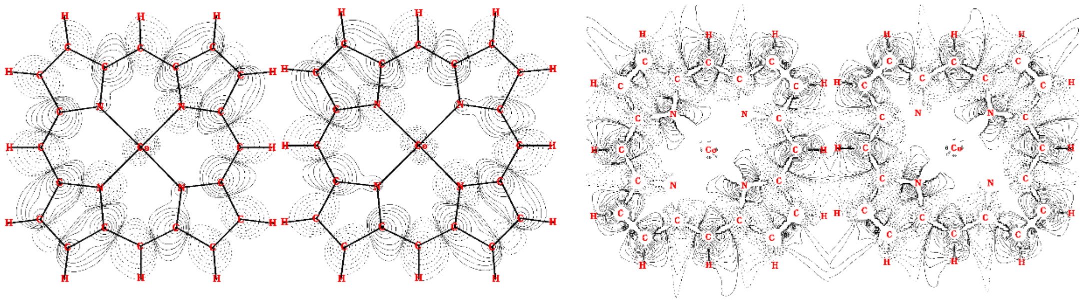

Figure 1. (Left) Laplacian Contour for 1st and 2nd Excited State Difference Density of $C_{20}H_{14}N_4Co$. (Right) Ellipticity of Stress Tensor 1st and 2nd Excited State Difference Density of $C_{20}H_{14}N_4Co$.

Acknowledgements

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A New Approach to Explaining Electron Cloud Formation in Various Elements

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When we consider an atom, we observe that it consists of a central structure (the nucleus) surrounded by electrons that orbit around it. An intriguing aspect of this system is that the electron moves in all directions around the nucleus, making it appear to exist simultaneously in every direction. In essence, the electron's motion is such that, although it is a single particle (as in the case of a hydrogen atom), its presence can be detected in all directions. This is because the path of its motion forms a spherical surface around the nucleus.

In this paper we will show that the trajectory of an electron can be described as a closed curved orbit around the nucleus. On its own, the electron cannot be present everywhere at the same time. However, the nucleus's rotation, combined with the interactive and cohesive forces between the electron and the nucleus, creates a dynamic relationship. This interaction causes the nucleus's rotation to influence the electron's trajectory, effectively broadening its presence. As a result, while the electron follows its primary orbit, it also appears to occupy other regions, giving rise to the perception of an electron cloud.

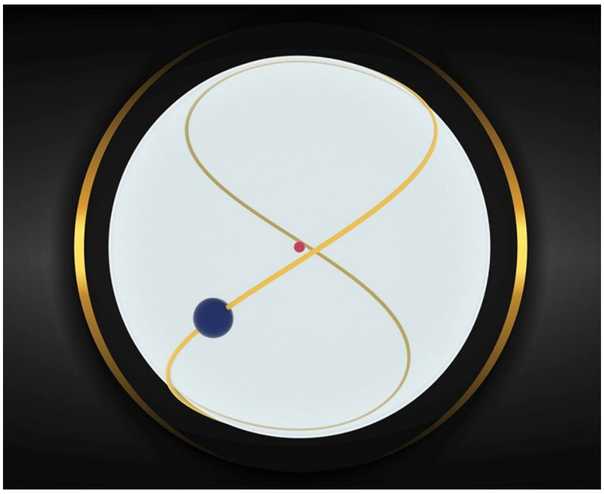

Figure 1. The path of electron motion around the nucleus

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Study of the hydration of aspartame with IR-UV spectroscopy

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Aspartame, a widely used artificial sweetener, owes its characteristic sweetness to its ability to act as an agonist of the tongue's sweet taste receptor. However, its structural conformation and interactions with the surrounding environment, particularly with water molecules, remain critical to understand its activity in diverse settings. To address these questions, we have explored how water molecules influence the conformational landscape of aspartame and identified which parts of the molecule are more likely to interact with the solvent.

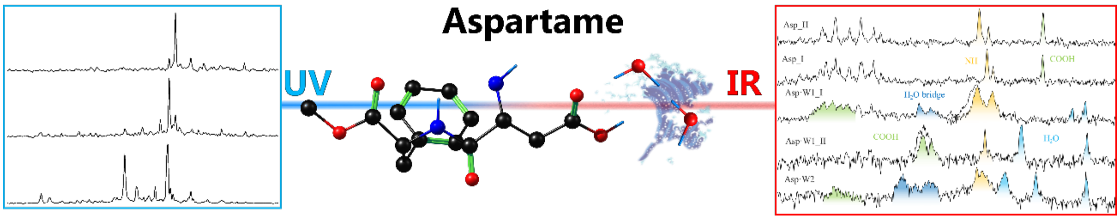

Figure 1. Representation of the electronic and vibrational spectrums obtained for aspartame·water$_{0\text{-}2}$.

In this study, a combination of IR−UV spectroscopic techniques and computational simulations was employed to investigate aspartame·water$_{0\text{-}2}$ clusters (Figure 1). Our results reveal that the addition of water molecules simplifies aspartame's conformational panorama by stabilising folded structures through interactions with its polar regions. These findings provide deeper insight into the role of water in modulating aspartame's behaviour, contributing to a deeper understanding of its function in both biological and industrial contexts.

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Stereodynamics of cold molecular collisions

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Over the last few years there has been a great progress in the study of inelastic and reactive collisions at cold (<1K) and ultra-cold (<1mK) collision energies, making it possible to impose quantum control of chemical reaction dynamics. At such low collision energies, few partial waves partake in the scattering process and, through its appearance on the integral cross section, we can isolate the resonances. Such processes have been extensively studied from the experimental and theoretical points of view. In particular, Zare and coworkers have studied inelastic collisions rare gas atoms with H_2 at energies near 0.1-5 K extensively[1-3]. These experiments were carried out by co-expanding the collision partners in supersonic beams combined with selection of the initial alignment of the molecular rotational angular momentum through Stark-induced adiabatic Raman Passage (SARP). The SARP method allows stereodynamical control of the collision process by selecting a given projection (m_j) of the molecular rotational angular momentum *j* on the relative collision velocity vector or preparing a molecular state. We present here theoretical calculations for the rotational relaxation $v\, j=2 \rightarrow v\, j'=0$ for the Ne + D_2 system.

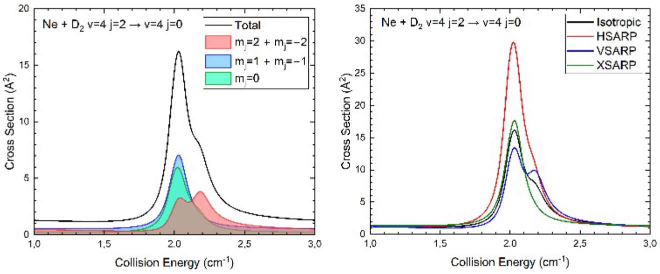

Figure 1. Contribution of different m_j to the total cross section (left) and the effect on the cross section of different SARP preparations (right) for the Ne + D_2 v=4 j=2 → v=4 j=0 transition.

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First detection in space of the high-energy isomer of cyanomethanimine: H_2CNCN

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We present the first detection in the interstellar medium (ISM) of *N*-cyanomethanimine (H_2CNCN), the stable dimer of HCN of highest energy[1] and the most complex organic molecule reported in space containing the prebiotically relevant NCN backbone. The detection is supported by the identification of a plethora of a-type rotational transitions with $3 \leq J_{\mathrm{up}} \leq 11$ and $K_{\mathrm{a}} \leq 2$ towards the Galactic Center G+0.693-0.027 molecular cloud, through its recently improved ultra-high-sensitivity spectral survey using the Yebes 40 m and IRAM 30 m radio telescopes. This cloud is the only interstellar source showing the three cyanomethanimine isomers thus far (including the *Z*- and *E*- isomers of *C*-cyanomethanimine[2], HNCHCN). Based on a Local Thermodynamic Equilibrium analysis, we derived a total molecular abundance with respect to H_2 of $(2.1 \pm 0.3) \times 10^{-11}$, which sets *N*-cyanomethanimine as one of the least abundant species detected thus far in this region. This demonstrates how the growing efforts in achieving a greater sensitivity on the observational data are pushing the limits of molecular species detectability in space. Moreover, it also provides evidence that high-energy isomers can also be found in the ISM, being equally important and necessary to obtain their spectroscopy to enable their identification.

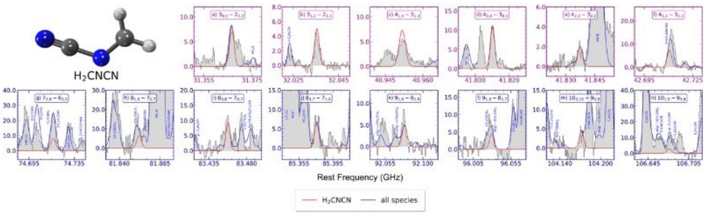

Figure 1. Lines of H_2CNCN detected towards G+0.693 using Yebes 40 m (magenta panels) and IRAM 30 m (blue ones) data. Observational spectra in grey, LTE fitting in red, rest of molecules detected in this cloud in blue (with labels). Panel labels denote the rotational transition plotted.

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

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Understanding molecules behavior relies on electronic structure methods, which are grouped by their ability to account for dynamic or nondynamic electron correlation effects. Accurately portraying molecular systems depends on wisely choosing a suitable electronic structure method. Specifically, when dealing with systems with predominant nondynamic correlation (known as multireference or MR), using single-reference methods can lead to major errors in describing the molecule's properties and energies. In an era dominated by the generation of extensive molecular datasets requiring computational treatment, there's a growing demand for affordable methods to identify multireference characteristics. Unfortunately, as far as we know, there are no cost-effective tools available for a quick assessment of a molecule's multireference nature.

Recently, we have conducted a thorough analysis of wavefunction theory based MR diagnostics using extensive datasets [1], identifying a single well-behaved representative metric of electron correlation that could be employed in single-reference wavefunctions. In this work, we present the extension of the multireference diagnostic to be applied in density functional theory. We used a supervised learning model to establish a map between Kohn-Sham orbital energies and the MR character of the molecule, achieving an excellent agreement with the predictions furnished by MP2 and CCSD calculations.

This work thus offers an economical approach requiring a single DFT calculation to assert the MR character of a molecular system, showcasing its potential as a cost-effective, high-accuracy solution for the detection of nondynamic correlation.

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Unraveling spin-forbidden enzymatic peroxidation through quantum dynamics

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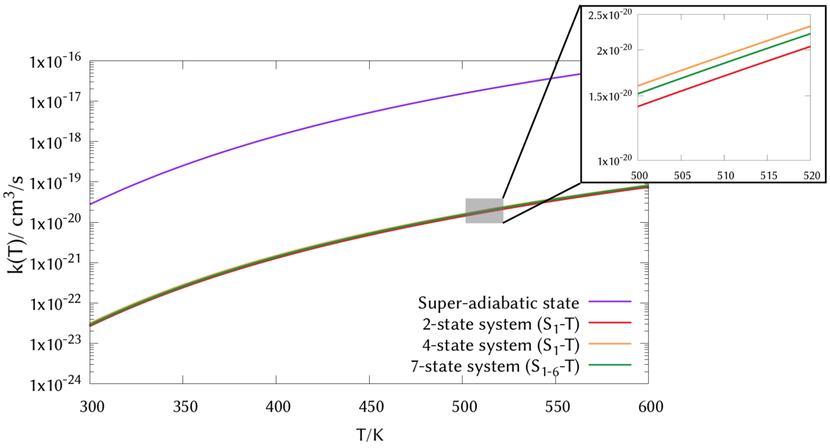
Reactions between molecular oxygen and closed-shell organic molecules leading to the formation of stable (closed-shell) adducts involve the change of the spin state of the system and accordingly should be slow at room temperatures. Nevertheless, enzymes are able to catalyze these reactions, even in the absence of cofactors that may promote the intersystem crossing.[1]

One of these reactions is the addition of O_2 to 3,5-dihydroxyphenylacetyl-CoA (DPA-CoA) that occurs in the active site of the DpgC enzyme. Previous studies showed that the intersystem crossing can be described employing reduced dimensionality and a model system.[2] To analyze the importance of the possible quantum dynamical effects, we report quantum scattering calculations on seven MRCI 2D PESs (six singlets and the triplet state), including the spin-orbit coupling. The MCTDH[3] method as implemented in QUANTICS[4] package, is used for the quantum dynamics calculations. Quantum integral cross-sections and thermal rate constants [Fig. 1] are presented, shedding light on the dynamics of the spin-forbidden process.

Figure 1. Thermal rate constants for the adiabatic and multi-state approaches.



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

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Polyphenols represent a significant class of natural products that have garnered significant research interest due to their wide range of biological activities, including antioxidant and anti-inflammatory properties. Among the extensive family of polyphenols, resveratrol is a flexible molecule with interesting chemical and biological properties. Investigation of the molecular structure and dynamics of this compound is essential to provide insights about its activities. In this work, we have employed a combination of broadband rotational spectroscopy and quantum chemical calculations to explore the conformational preferences of resveratrol. Laser ablation has been used to vaporize the sample instead of the traditional heating system to overcome the difficulties arising from the high boiling point and low vapour pressure of this compound. The detection of four spectra with similar rotational constants gave rise to different interpretations related to the most stable conformers. For all the detected species, the planar moment of inertia P_c shows the nearly planar skeleton of the molecule. The comparison of the gas-phase data obtained with structural information obtained from X-ray diffraction techniques in crystals and complexed with proteins gives relevant insights into the properties of resveratrol.

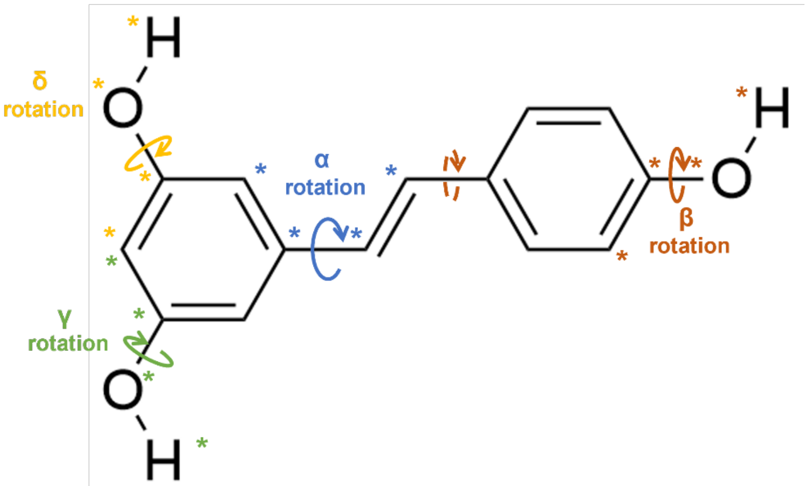

Figure 1. Molecular structure of resveratrol with the rotations that give rise to the potential conformers.

Molecular Dynamics and DFT Simulations of CO_2/CH_4 Separation Through Carbon-Based Nanoporous Membranes: Influence of Pore Size

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Efficient CO_2/CH_4 separation is crucial for reducing greenhouse emissions and improving natural gas quality[1]. This study uses Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations to evaluate CO_2 and CH_4 filtration through nanoporous monolayer graphdiyne (GDY) and boron-graphdiyne (BGDY) membranes. The pore sizes are smaller than the geometrical sizes due to the extension of the electron density. BGDY's larger pores allow non-selective gas passage, while GDY's smaller pores enable selective CO_2 permeation due to its orientation-dependent interaction with the membrane and lower activation barrier (0.28 eV for CO_2 vs. 0.51 eV for CH_4)[2]. MD simulations confirm that GDY's structure and pore size effectively reject CH_4 while facilitating CO_2 transport at both 0 K and 300 K. A funnel-like mechanism is found for the pore crossing. These findings establish GDY as a promising membrane for CO_2 capture and gas purification applications.

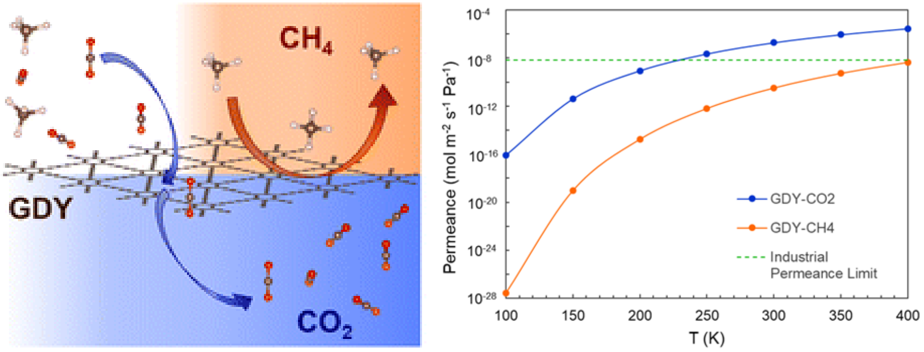

Figure 1. Comparative Study of CO_2 and CH_4 Permeation Through Graphdiyne-Based Membranes: Insights into Molecular Orientation and Energy Barriers.

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Magnetic analysis using efficient state-interaction approach

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The g-tensor (also expressed as g-shift Δg) is a magnitude that parametrizes the Zeeman effect, involving the interaction of the spin magnetic moment with a magnetic field. It provides significant information about the environment of unpaired electrons.

In this talk, I will present an efficient state-interaction approach for evaluating g-tensor [1, 2]. Using a spin-orbit-coupled effective Hamiltonian with a restricted active space configuration interaction (RASCI) wavefunction [3], this method captures key excited-state contributions to g-tensor (Figure I) without requiring large orbital spaces while maintaining computational efficiency. Additionally, we introduce a property-driven algorithm to automatically optimize the active space. Application to high-spin molecules demonstrates accuracy comparable to advanced methods, providing detailed insight into the origins of g-tensor. This methodology offers a flexible, efficient tool for exploring magnetic properties in complex molecules.

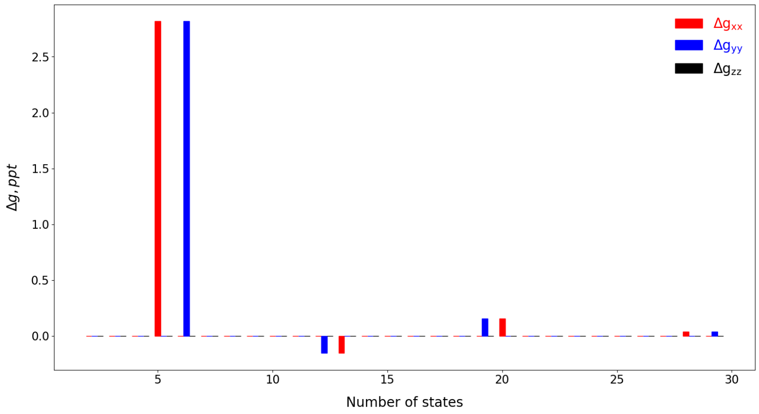

Figure I. Δg between the ground state (state 1)
and the corresponding excited states for O2 molecule

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Gh	Saleh	Saleh Research Centre	Netherlands
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Zhen	Wang	Universidad de Valladolid	Spain
Markel	Ylla	University of Basque Country	Spain
Omar	Zaidi	University Setif	Algeria

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