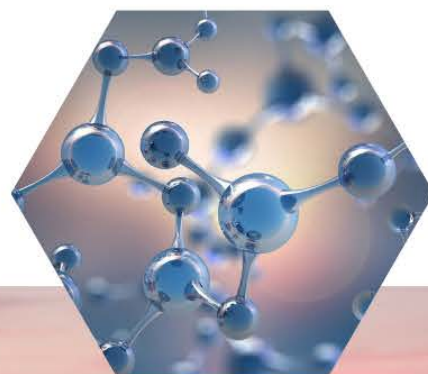


# IBER 2022

# XVI IBERIAN JOINT MEETING ON ATOMIC AND MOLECULAR PHYSICS

MÁLAGA (SPAIN)



September 21-23, 2022



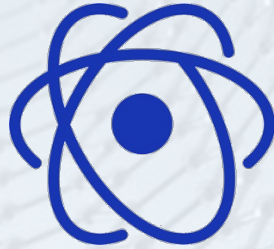
Facultad de Medicina - Universidad de Málaga

GEFAM@RSEQ.ORG

WWW.IBER2022.COM







# IBER 2022

## XVI IBERIAN JOINT MEETING ON ATOMIC AND MOLECULAR PHYSICS

Málaga (Spain), 21-23 September 2022

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# IBER 2022

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# Welcome

## Welcome to IBER 2022!

IBER 2022 constitutes the XVI Edition of the Series of **Iberian Joint Meetings on Atomic and Molecular Physics**, organized by the Spanish and Portuguese societies of Physics.

The IBER Conference Series brings together international researchers and scientists of the Iberian community dedicated to Atomic and Molecular Physics and related areas, facilitating the scientific interaction and exchange of knowledge between research groups.

The 2022 edition marks the first IBER Conference after the interruption of the COVID-19 pandemic. Future Conferences will return to the biannual periodicity of this event.

We thank everybody for your presence in Malaga and wish you a scientifically productive Conference.

Scientific Committee and Local Committee

# IBER Committees



## SCIENTIFIC COMMITTEE

- **Jorge M. Sampaio** (LIP/FCUL – Univ. Lisboa), Chairman, DFAM – SPF
- **Alberto Lesarri** (Univ. Valladolid), Chairman, GEFAM – RSEF/RSEQ
- **Luis Bañares** (Univ. Complutense)
- **José A. Fernández** (Univ. País Vasco)
- **Joaquim Ferreira Santos** (LIBPhys. – Univ. Coimbra)
- **Francisco Gil** (CFIsUC – Univ. Coimbra)
- **Elena Jiménez** (Univ. Castilla-La Mancha)
- **Marta Manso** (LIBPhys/FCT – U. Nova Lisboa)
- **Sonia Marggi** (Univ. Complutense)
- **José P. Marques** (LIP/FCUL – Univ. Lisboa)
- **Ana L. Silva** (Univ. Aveiro)
- **Saulo Vázquez** (Univ. Santiago de Compostela)

## LOCAL COMMITTEE

- **José M. Vadillo** (Univ. Málaga), Chairman
- **Celina Bermúdez** (Univ. Valladolid)
- **Camilla Calabrese** (Univ. Valladolid)
- **Wenqin Li** (Univ. Valladolid)
- **Isabel Peña** (Univ. Valladolid)
- **Cristóbal Pérez** (Univ. Valladolid)
- **Amanda Steber** (Univ. Valladolid)





# IBER History

The IBER Conference series started in 1993 by initiative of the late Prof. Gerardo Delgado-Barrio, who served as first President (1988-95) of the Group of Atomic and Molecular Physics (GEFAM) of the Spanish Societies of Physics (RSEF) and Chemistry (RSEQ), and later as RSEF President in the period 1997-2005.

The IBER Conference extended the initial format of the Spanish GEFAM meetings to a larger biannual collaboration with the Portuguese Physics Society (SPF), establishing the first Iberian conference on Atomic and Molecular Physics. The IBER Conference has run uninterrupted for fifteen editions (except the 2021 Conference, which was postponed because of the COVID-19 pandemic). The Conference is organized sequentially in a Portuguese and a Spanish city.

The IBER Scientific Committee is formed by GEFAM-RSEF/RSEQ and SPF.

The previous IBER Conferences include:

- XV Conference (IBER 2019) – Évora, July 10-12, 2019
- XIV Conference (IBER 2017) – Barcelona, September 12-14, 2017
- XIII Conference (IBER 2015) – Aveiro, September 6-9, 2015
- XII Conference (IBER 2013) – Sevilla, September 9-11, 2013
- XI Conference (IBER 2011) – Coimbra, June 19-22, 2011
- X Conference (IBER 2009) – Santiago de Compostela, July 12-15, 2009
- IX Conference (IBER 2008) – Capuchos, September 7-9, 2008
- VIII Conference (IBER 2006) – Aranjuez, August 31 - September 4, 2006
- VII Conference (IBER 2005) – Lisboa, March 21-23, 2005
- VI Conference (IBER 2003) – Madrid, March 9-11, 2003
- V Conference (IBER 2002) – Lisboa, March 23-26, 2002
- IV Conference (IBER 2000) – El Escorial, May 30-June 2, 2000
- III Conference (IBER 1998) – Mira, May 4-7, 1998
- II Conference (IBER 1995) – Bilbao, July 10-12, 1995
- I Conference (IBER 1993) – Lisboa, July 5-7, 1993

# Venue



The IBER 2022 Conference venue is the **Faculty of Medicine** of the **University of Málaga**, located at the *Boulevard Louis Pasteur, 32* (29010 Málaga) of the **Teatinos University Campus**. The Faculty of Medicine is ca. 6 km away from the city center and is accessible by walk, subway (Metro Málaga, Line 1, Stop *Universidad*), urban bus (EMT Málaga, Lines 8, 11, 22, 25) or taxi. The Metro stop is just 170 m (2 min) from the Conference venue.

The scientific activities will take place at the **Aula Magna** (Main Hall) and **Aula IV** (Room IV). Registration, conference information and the poster session will be close to the conference rooms. Coffee breaks will be also provided next to the conference halls.

The lunch service will be served at the Restaurant of the Faculty of Medicine. On-site indications will be provided.

The social activities, including a two-hours touristic boat tour and the Gala Dinner will be organized downtown. The touristic activity (Thursday 22) will start at 19 h from Dock 1 of the Málaga Harbor (*Flye Blue Málaga*). The Gala Dinner, including the presentation of the Delgado-Barrio Award and the announcement of the next IBER meeting, will take place on Friday 23 (20 h) at the restaurant "*Los Patios de las Beatas*", located at *Calle Beatas, 43*, close to the Picasso Museum.

**EMERGENCIES:** For medical or police emergencies please call **112** (free number) or download the app **112 Andalucía**, which will transmit also your coordinates.

**CONFERENCE SERVICE:** For Conference problems please contact the organizers or email to [contact@iber2022.com](mailto:contact@iber2022.com). In case of urgent requests please phone to +34-983-185895.

**SOCIAL NETWORKS:** The IBER 2022 twitter account [@F\\_GEFAM\\_Q](https://twitter.com/F_GEFAM_Q) will inform about the progress of the Conference. Detailed Conference information will be maintained at the IBER 2022 web page [iber2022.com](http://iber2022.com).



Figure 1. The Faculty of Medicine building at the Teatinos University Campus.

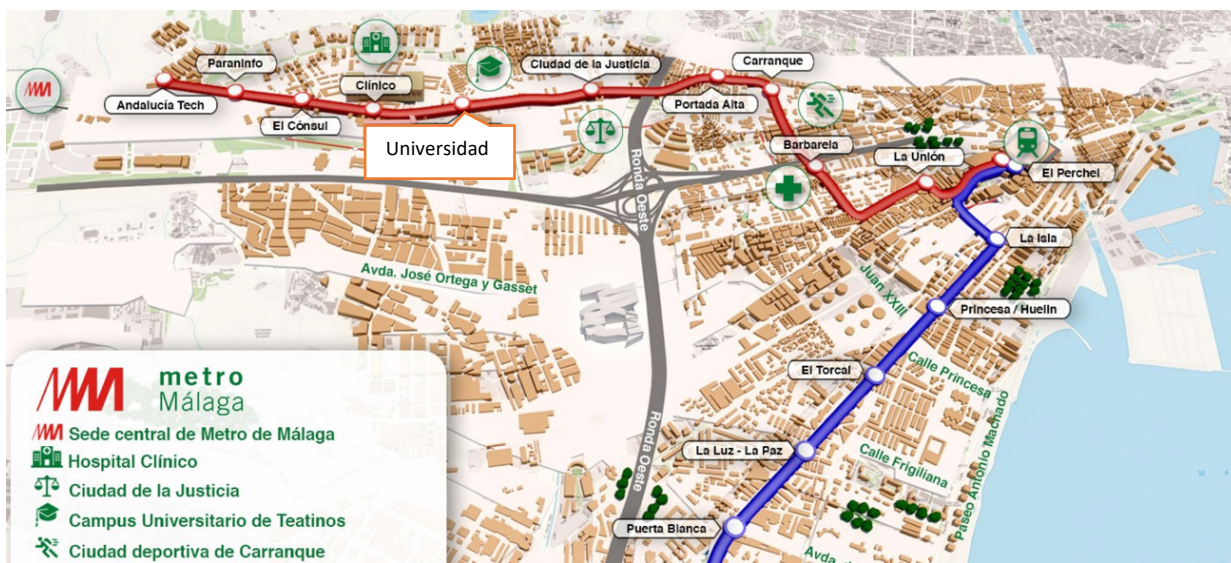


Figure 2. Metro access to the Faculty of Medicine (Line 1 in red, stop Universidad)



# IBER 2022 at a Glance



WEDNESDAY		SEPTEMBER 21		THURSDAY		SEPTEMBER 22		FRIDAY		SEPTEMBER 23	
8:00-9:00	REGISTRATION	Hall									
9:00-09:10	OPENING SESSION	Aula Magna									
<b>Session 1</b>											
09:10-09:50	PLENARY P1: MEYER	Aula Magna	Aula IV	09:10-09:50	PLENARY P5: LUCCHINI	Aula IV		09:10-09:50	PLENARY P9: GANS	Aula IV	
09:50-10:30	PLENARY P2: CRESPO	Aula Magna	Aula IV	09:50-10:30	PLENARY P6: ANTOGNINI	Aula IV		09:50-10:30	PLENARY P10: ARUNAN	Aula IV	
10:30-11:00	COFFE BREAK			10:30-11:00	COFFE BREAK			10:30-11:00	COFFE BREAK		
<b>Session 2</b>				<b>Session 6</b>				<b>Session 10</b>			
11:00-11:30	INVITED I1: AMARO	Room IV	Room IV	11:00-11:30	INVITED I4: HENRIQUES	Room IV		11:00-11:30	INVITED I7: VELOSO	Room IV	
11:30-12:00	INVITED I2: GARCIA-VELA	Room IV	Room IV	11:30-12:00	INVITED I5: MARTINEZ-HAYA	Room IV		11:30-12:00	INVITED I8: COGINERO	Room IV	
12:00-12:15	ORAL O1: SOLÁ	Room IV	Room IV	12:00-12:15	ORAL O10: PROSMITI	Room IV		12:00-12:15	ORAL O19: VILLARREAL	Room IV	
12:15-12:30	ORAL O2: FERNÁNDEZ	Room IV	Room IV	12:15-12:30	ORAL O11: MELLADO-ALCEDO	Room IV		12:15-12:30	ORAL O20: REVUELTA	Room IV	
12:30-12:45	ORAL O3: ALVAREZ	Room IV	Room IV	12:30-12:45	ORAL O12: FERREIRA DA SILVA	Room IV		12:30-12:45	ORAL O21: BELLO	Room IV	
12:45-13:00	ORAL O4: SILVA	Room IV	Room IV	12:45-13:00	ORAL O13: RECIO	Room IV		12:45-13:00	ORAL O22: TORRES	Room IV	
13:00-13:15	ORAL O5: MORCILLO	Room IV	Room IV	13:00-13:15	ORAL O14: MANDADO	Room IV		13:00-13:15	ORAL O23: ROQUE	Room IV	
13:15-14:30	LUNCH	Cafeteria		13:15-14:30	LUNCH	Cafeteria		13:15-14:30	LUNCH	Cafeteria	
<b>Session 3</b>				<b>Session 7</b>				<b>Session 11</b>			
14:30-15:10	PLENARY P3: GOMEZ-CADENAS	Aula Magna	Aula Magna	14:30-15:10	PLENARY P7: MATA	Aula Magna		14:30-15:00	INVITED I9: FRONTERA	Aula Magna	
15:10-15:50	PLENARY P4: GARCIA RUJZ	Aula Magna	Aula Magna	15:10-15:50	PLENARY P8: MARQUES	Aula Magna		15:00-15:30	INVITED I10: GUERRA	Aula Magna	
15:50-16:05	ORAL O6: FERRO-COSTAS	Aula Magna	Aula Magna	15:50-16:05	ORAL O15: MARTÍNEZ-NUÑEZ	Aula Magna		15:30-15:45	ORAL O24: ANGUIITA-ORTIZ	Aula Magna	
16:05-16:20	ORAL O7: GONZÁLEZ	Aula Magna	Aula Magna	16:05-16:20	ORAL O16: DOMINGOS	Aula Magna		16:00-16:30	COFFE BREAK		
16:20-16:50	COFFE BREAK			16:20-16:50	COFFE BREAK			<b>Session 12</b>			
<b>Session 4</b>				<b>Session 8</b>				<b>Session 12</b>			
16:50-17:20	INVITED I3: GAWELDA	Aula Magna	Aula Magna	16:50-17:20	INVITED I6: GLOWACKI	Aula Magna		16:30-16:45	CLOSING SESSION	Aula Magna	
17:20-17:35	ORAL O8: HERNANDEZ-ROJAS	Aula Magna	Aula Magna	17:20-17:35	ORAL O17: MONTERO	Aula Magna		16:45-17:30	GEFAM MEMBERS ASSEMBLY	Aula Magna	
17:35-17:50	ORAL O9: MATEO	Aula Magna	Aula Magna	17:35-17:50	ORAL O18: TEIXEIRA	Aula Magna		20:00-22:00	GALA DINNER and DELGADO-BARRIO AWARD	Restaurant downtown	
18:00-19:00	POSTER SESSION			19:00-21:00	TOURISTIC ACTIVITY	Harbor					



# IBER 2022 Program

WEDNESDAY		SEPTEMBER 21
8:00-9:00	<b>REGISTRATION</b>	Hall
9:00-9:10	<b>OPENING SESSION</b>	Aula Magna
<b>Session</b>	<b>1</b> <b>Chair: L. Bañares</b>	
9:10-9:50	<b>PLENARY P1: M. Meyer,</b> Multi-Photon Processes and Molecular Dynamics in the Soft X-Ray Regime: The Small Quantum Systems (SQS) Instrument at the European XFEL	Aula Magna
9:50-10:30	<b>PLENARY P2: J. R. Crespo López-Urrutia,</b> Highly Charged Ions from the Core of the Sun to Optical Clocks	Aula Magna
10:30-11:00	<b>COFFE BREAK</b>	
<b>Session</b>	<b>2</b> <b>Chair: B. Martínez Haya</b>	
11:00-11:30	<b>INVITED I1: F. D. Amaro</b> Gas Based Neutron Detectors: Recent Developments and Future Prospects	Room IV
11:30-12:00	<b>INVITED I2: A. García-Vela</b> The Role of Non-Adiabatic Couplings in the Photodissociation of the Methyl Radical	Room IV
12:00-12:15	<b>ORAL O1: I. Solá</b> Spatiotemporal Control of Trapped Rydberg Qubits	Room IV
12:15-12:30	<b>ORAL O2: J. M. Fernández</b> Raman Spectroscopy of High-Temperature Supersonic Jets of CO <sub>2</sub>	Room IV
12:30-12:45	<b>ORAL O3: C. Álvarez</b> Rotational and Vibrational Relaxation of CO <sub>2</sub> in Supersonic Jets	Room IV
12:45-13:00	<b>ORAL O4: P. A. O. C. Silva</b> A Different Concept for Gas Proportional Scintillation Counter: The Annular Anode	Room IV

13:00-13:15	<b>ORAL O5: M. F. Morcillo Arencibia</b> Does the Molecular Position Affect the Structure and Stability of the H <sub>2</sub> @ C <sub>60</sub> Complex?	Room IV
13:15-14:30	<b>LUNCH</b>	Cafeteria
<b>Session</b>	<b>3</b> <b>Chair: C. A. O. Henriques</b>	
14:30-15:10	<b>PLENARY P3: J. J. Gómez-Cadenas</b> Desperately Seeking for Majorana	Aula Magna
15:10-15:50	<b>PLENARY P4: R. F. García Ruíz</b> Exotic Atoms and Molecules for Nuclear Science	Aula Magna
15:50-16:05	<b>ORAL O6: D. Ferro-Costas</b> The Cathedral Package: User-Friendly Tools for Chemical Kinetics	Aula Magna
16:05-16:20	<b>ORAL O7: D. González</b> Simulating Gas-Phase Interstellar Chemistry Using the CRESU Technique	Aula Magna
16:20-16:50	<b>COFFE BREAK</b>	
<b>Session</b>	<b>4</b> <b>Chair: S. Vázquez</b>	
16:50-17:20	<b>INVITED I3: W. Gawelda</b> Observing Solute-Solvent Coupled Structural Dynamics in Solvated Cu Photosensitizer with Ultrashort X-rays	Aula Magna
17:20-17:35	<b>ORAL O8: J. Hernández-Rojas</b> Trihydrogen Cation Helium Clusters: A New Potential Energy Surface	Aula Magna
17:35-17:50	<b>ORAL O9: H. Mateo</b> Computational Characterization of the Emission of the Keto Derivative of Oxyluciferin within Luciferase	Aula Magna
18:00-19:00	<b>POSTER SESSION</b>	

THURSDAY		SEPTEMBER 22	
<b>Session</b>	<b>5</b> <b>Chair: A. Longarte</b>		
9:10-9:50	<b>PLENARY P5: M. Lucchini,</b> Few-fs Limit of The Floquet Theory	Room IV	
9:50-10:30	<b>PLENARY P6: A. Antognini,</b> From the Proton Radius to the Best Tests of Quantum Electrodynamics	Room IV	
10:30-11:00	<b>COFFE BREAK</b>		
<b>Session</b>	<b>6</b> <b>Chair: A. García-Vela</b>		
11:00-11:30	<b>INVITED I4: C. A. O. Henriques</b> Neutral Bremsstrahlung Emission in Xenon Unveiled	Room IV	
11:30-12:00	<b>INVITED I5: B. Martínez-Haya</b> Proton in the Ring: Wandering Protons Inside Molecular Cavities	Room IV	
12:00-12:15	<b>ORAL O10: R. Prosmi</b> Quantum Simulations of Halogen Anions Hydration: Data- Driven Potential Models from Aqueous Clusters to Solutions	Room IV	
12:15-12:30	<b>ORAL O11: D. Mellado-Alcedo</b> Electronic Structure of Triatomic Ultra-Long Rydberg Molecules	Room IV	
12:30-12:45	<b>ORAL O12: R. Ferreira da Silva</b> Calculation of Atomic Inputs for Probing r-Process in Kilonovae	Room IV	
12:45-13:00	<b>ORAL O13: P. Recio</b> Photodissociation dynamics of bromiodomethane in the B band, 193 nm	Room IV	
13:00-13:15	<b>ORAL O14: M. Mandado</b> Predicting Electron Transport in Molecular Electronic Devices from Electron Deformation Orbitals	Room IV	
13:15-14:30	<b>LUNCH</b>		Cafeteria

<b>Session</b>	<b>7</b> <b>Chair: J. M. Sampaio</b>	
14:30-15:10	<b>PLENARY P7: R. Mata</b> Coupling of Proton Dynamics to Reaction Pathways in Biomolecular Systems	Aula Magna
15:10-15:50	<b>PLENARY P8: J. P. Marques</b> Biomedical and Astrophysical Applications of Atomic Parameters	Aula Magna
15:50-16:05	<b>ORAL O15: E. Martínez-Núñez</b> Automated Reaction Discovery Through Reactive MD Simulations	Aula Magna
16:05-16:20	<b>ORAL O16: S. Domingos</b> Beyond Structure Solving with Microwave Spectroscopy	Aula Magna
16:20-16:50	<b>COFFE BREAK</b>	
<b>Session</b>	<b>8</b> <b>Chair: E. Martínez-Núñez</b>	
16:50-17:20	<b>INVITED I6: D. R. Glowacki</b> Virtual Reality for Molecular Simulation and Design: From Quantum Chemistry to Drug Binding	Aula Magna
17:20-17:35	<b>ORAL O17: R. Montero</b> Time-Resolved Photoionization of Simple Aromatic Molecules in Water	Aula Magna
17:35-17:50	<b>ORAL O18: J. M. R. Teixeira</b> Primary Scintillation Yield in Xenon for Electrons and Alpha Particles	Aula Magna
19:00-21:00	<b>TOURISTIC ACTIVITY</b>	Málaga Harbour



FRIDAY		SEPTEMBER 23	
<b>Session</b>	<b>9</b> <b>Chair: J. P. Marques</b>		
9:10-9:50	<b>PLENARY P9: B. Gans,</b> Photoionization Spectroscopy of Free Radicals Using Synchrotron- and Laser-based Experiments		Room IV
9:50-10:30	<b>PLENARY P10: E. Arunan,</b> Molecular Beam Microwave Spectroscopy: Structure, Bonding and Dynamics		Room IV
10:30-11:00	<b>COFFE BREAK</b>		
<b>Session</b>	<b>10</b> <b>Chair: I. Solá</b>		
11:00-11:30	<b>INVITED I7: J. Veloso</b> X-Ray Fluorescence Spectroscopy and Imaging Analysis Using Gaseous Detectors Based Neutron Detectors		Room IV
11:30-12:00	<b>INVITED I8: E. J. Cocinero</b> Carbohydrate Research by High Resolution Spectroscopy and Other Applications		Room IV
12:00-12:15	<b>ORAL O19: P. Villarreal</b> Electron Transfer Between Heliophobic and Heliophilic Species in Helium Nanodroplets		Room IV
12:15-12:30	<b>ORAL O20: F. Revuelta</b> Observation of Confinement-Induced Resonances in a 3D Lattice		Room IV
12:30-12:45	<b>ORAL O21: R. Y. Bello</b> Angle-resolved Phases in Photoemission: From Atomic to Molecular Systems		Room IV
12:45-13:00	<b>ORAL O22: F. Torres</b> Exploring Carvacrol Interactions by Laser Spectroscopy in Jets		Room IV
13:00-13:15	<b>ORAL O23: R. Roque</b> How do Hydrocarbons Affect the Electroluminescence of He-CF <sub>4</sub>		Room IV
13:15-14:30	<b>LUNCH</b>		Cafeteria

<b>Session</b>	<b>11</b> <b>Chair: M. Mandado</b>	
14:30-15:00	<b>INVITED I9: A. Frontera</b> Unconventional Electron Donors: Metals as $\sigma/\pi$ -Hole Acceptors	Aula Magna
15:00-15:30	<b>INVITED I10: M. Guerra</b> High-Resolution X-ray Metrology in the Search for Physics Beyond the Standard Model	Aula Magna
15:30-15:45	<b>ORAL O24: N. Anguita-Ortíz</b> Computational Study of Ion Conduction through Eukaryotic Ion Channels by Molecular Dynamics	Aula Magna
16:00-16:30	<b>COFFE BREAK</b>	
<b>Session</b>	<b>12</b> <b>Chair: Organizing Committee</b>	
16:30-16:45	<b>CLOSING SESSION</b>	Aula Magna
16:45-17:30	<b>GEFAM MEMBERS ASSEMBLY</b>	Aula Magna
20:00-22:00	<b>GALA DINNER AND DELGADO-BARRIO AWARD</b>	Restaurant Downtown



# Plenary Speakers



**Michael Meyer**

**European XFEL**



**José R. Crespo**

**Max-Planck-Inst. Kernphysik**



**Juan J. Gómez-Cadenas**

**Donostia Int. Physics Center**



**Ronald F. García Ruíz**

**Massachusetts Inst. Technology**



**Matteo Lucchini**

**Politecnico di Milano, IFN-CNR**



# Plenary Speakers



**Aldo Antognini**

**ETH – Paul Scherrer Inst.**



**Ricardo Mata**

**Georg-August-Univ. Göttingen**



**José P. Marques**

**LIP – Univ. Lisboa**



**Berénger Gans**

**ISMO – CNRS, Univ. Paris-Saclay**



**Elangannan Arunan**

**Indian Inst. Science**







# Plenary Lectures





## Multi-Photon Processes and Molecular Dynamics in the Soft X-Ray Regime: The Small Quantum Systems (SQS) Instrument at the European XFEL

Michael Meyer

European XFEL, Holzkoppel 4, 20869 Schenefeld, Germany, [michael.meyer@xfel.eu](mailto:michael.meyer@xfel.eu)

Keywords: free-electron laser • non-linear phenomena • molecular dynamics • Coulomb explosion imaging • coherent diffraction imaging

The Small Quantum Systems (SQS) scientific instrument at the European X-ray Free Electron Laser in Germany is dedicated to investigations on atoms, molecules, clusters and nanoparticles. The instrument is installed behind the SASE3 soft X-ray undulator, which produces intense X-ray pulses in the photon energy range between 250 eV and 3000 eV. During operation the accelerator is generally delivering up to 3500 pulses per second to the SQS experimental stations with pulse energies of up to 10 mJ. These characteristics in combination with pulse durations in the range of 10 to 30 fs provide an ideal basis for numerous investigations involving site-selective core excitations and with a special focus on non-linear phenomena and the dynamics of ultrafast processes.

Since November 2018, three experimental stations are opened to the international scientific user community. The AQS (Atomic-like Quantum Systems), NQS (Nano-size Quantum Systems) and REMI (REaction Microscope) end stations, which are optimized for different samples and different type of experiments, were successfully brought into operation. First scientific investigations were concentrating on studies of multi-photon processes<sup>1</sup> using high-resolution electron, ion and electron-ion coincidence spectroscopy as well as on studies of larger systems using coherent diffraction imaging<sup>2</sup>. The experiments covered processes of (resonant) multiple ionization, above threshold ionization (ATI), double core hole (DCH) formation and stimulated X-ray Raman scattering (SXRS)<sup>3</sup> in atoms as well as X-ray induced dissociation dynamics of small molecules monitored via Coulomb explosion imaging (CEI)<sup>4</sup>, and highlighted the excellent performances of the instrument.

In the talk, after the presentation of the SQS instrument, a few examples of the current scientific results will be discussed including the latest developments related to time-resolved pump-probe experiments combining the soft X-ray FEL pulses either with a synchronized optical laser<sup>5</sup> or with another X-ray pulse of different photon energy. Finally, future possibilities focusing on the use of variable polarization and applications in the attosecond time domain will be briefly described.

<sup>1</sup> G. Kastirke et al., *Phys. Rev. X*, **2020**, *10*, 021052 and T. Mazza et al., *Phys. Rev. X*, **2020**, *10*, 041056.

<sup>2</sup> A.F. Feinberg et al., *Phys. Res. Rev.*, **2022**, *4*, 013029.

<sup>3</sup> U. Eichmann et al., *Science*, **2020**, *369*, 1630.

<sup>4</sup> R. Boll et al., *Nature Physics*, 2022, *18*, 423.

<sup>5</sup> D. Rivas et al., *Optica*, **2022**, *9*, 429.

## Highly Charged Ions from the Core of the Sun to Optical Clocks

José R. Crespo López-Urrutia

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Keywords: X-ray absorption • spectroscopy • frequency metrology • optical clocks

Atoms present in the radiative core of the Sun and other stars lose most or all of their electrons and become highly charged ions (HCI). As an example, iron, a key astrophysical element, retains there usually only the K-shell, and appears as helium-like  $\text{Fe}^{24+}$ . It is important to emphasize that charged particles (protons, helium nuclei, and HCI from various elements) are the dominant form of baryonic matter in the galaxies and the warm-hot ionized gas filling the intergalactic space. Not only that: their electronic transitions govern the radiative energy transfer by X rays in stellar cores. HCI survive at very close distances to the event horizon of black holes, and emit the last spectroscopic features from those and other harsh plasma environments.

From a theoretical point of view, the very large relativistic, quantum electrodynamic, and nuclear size effects seen in inner-shell electrons of heavy atoms can be best studied in HCI. The overall electronic structure with few bound electrons becomes easier to describe. Studying HCI along an isoelectronic sequence delivers systematic insights into those fundamental effects.

Moreover, in recent proposals, the insensitivity of HCI to external perturbations, together with the existence of highly forbidden optical transitions in many isoelectronic sequences were found to make HCI ideal candidates for optical frequency metrology references in ultrastable clocks.<sup>1</sup> Several systems have been proposed for the investigation of the time variation of fundamental constants, e. g.,  $\text{Ir}^{17+}$  and  $\text{Pr}^{9+}$  ions,<sup>2</sup> where orbital level crossings are present. High-precision studies of isotopic shifts using extensions of the King-plot method could potentially yield evidence, or exclude, fifth forces of new physics. Experiments with cold HCI<sup>3</sup> using frequency-metrology techniques<sup>4</sup> are already underway or in preparation in the PTB-MPIK collaboration. A setup including an extreme ultraviolet (XUV) frequency comb<sup>5</sup> aims at utilizing the stability of HCI under XUV irradiation to enable atomic clocks beyond the optical. The talk will present a general introduction to HCI, and recent experimental results.<sup>6,7</sup>

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<sup>4</sup> P. Micke, *et al.*, *Nature*, **2020**, *578*, 60

<sup>5</sup> J. Nauta, *et al.*, *Opt. Express* **2021**, *29*, 2624

<sup>6</sup> S. A. King, *et al.*, *Phys. Rev. X*, **2021**, *11*, 041049

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## Desperately Seeking for Majorana

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Keywords: experimental particle physics • neutrino physics • nuclear instrumentation  
• Canfranc underground laboratory • NEXT experiment

Discovering that the neutrino is its own antiparticle is one of the most intriguing questions currently open in particle Physics. In this talk I will offer a glimpse of the field, with special emphasis in the NEXT experiment, which is being carried out at the Canfranc Underground Laboratory in Spain.

## Exotic Atoms and Molecules for Nuclear Science

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Keywords: nuclear phenomena • exotic species • laser spectroscopy

Atoms and molecules containing nuclei with extreme proton-to-neutron ratios can be artificially created to study particular nuclear phenomena. Precision measurements of these systems can offer unique insights into the properties of the atomic nucleus, nuclear matter, and the fundamental particles and forces of nature. In this talk, I will present recent results and perspectives from laser spectroscopy experiments of these exotic species.



## Few-fs Limit of the Floquet Theory

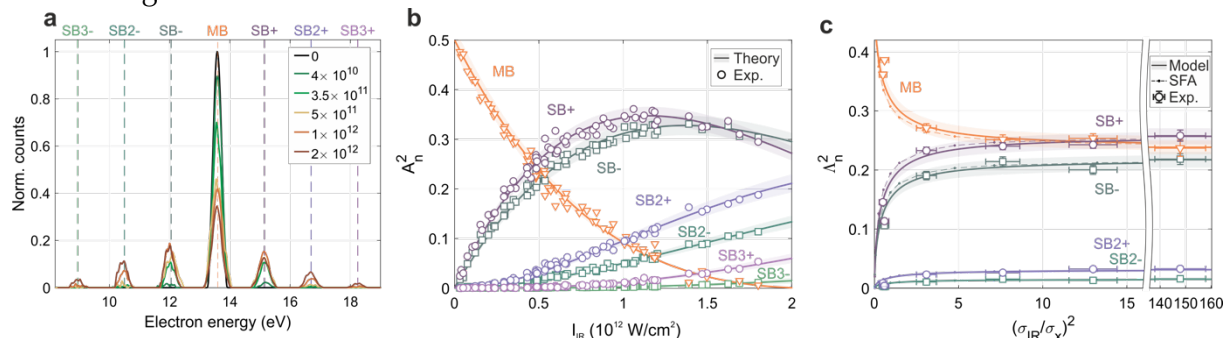
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Keywords: Floquet theory • ultrafast science

The capability to modify and control the properties of matter with optical pulses is a long-sought goal which has recently fostered intense research in many technological fields. In this framework, Floquet engineering proposes to drive matter with periodic external fields to induce new properties, absent in the equilibrium counterpart.<sup>1</sup> The recent advent of ultrafast science has offered the unique opportunity to combine Floquet engineering with extreme time resolution, providing us the fascinating possibility to switch the physical properties of quantum materials on unprecedented time scales. So far, the application of Floquet theory and its concepts has been limited to relatively long driving pulses (> 100s of fs). Therefore, what is the shortest driving pulse for which Floquet states can be realized remains an unsolved matter. We used few-fs infrared (IR) pulses of variable duration in combination with a femtosecond extreme-ultraviolet (XUV) pulse<sup>2</sup> to study the formation of Floquet states in a prototype system: the free electron. In combination with an analytical model, our results demonstrate that a Floquet-like approach can be still used to describe the light-induced state, if both the XUV and IR last for more than 2 cycles of the driving field.



**Figure 1.** **a**, Photoelectron spectra collected at selected IR intensities using the quasi-monochromatic pulse ( $\sim 146$  fs). Clear sideband (SB) peaks appear close to the main band (MB). **b**, Behavior of the Floquet ladder amplitude,  $A_n^2$ , as a function of the IR intensity. **c**, Behavior of the generalized Floquet ladder amplitudes,  $\Lambda_n^2$ , as a function of the IR duration (IR intensity  $\sim 10^{12}$  W/cm<sup>2</sup>).

Being able to follow the establishment of Floquet states on ultrashort time scales, our results give a new insight into the formation of light-dressed states, paving the way for the extension of Floquet engineering techniques to the petahertz domain.

### Acknowledgements

We acknowledge the people involved in the experiment, the attosecond research center in Milano, IFN-CNR in Padova.

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## From the Proton Radius to the Best Tests of Quantum Electrodynamics

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Keywords: muonic atoms • hydrogen • nuclear structure • laser spectroscopy

Laser spectroscopy of muonic atoms, hydrogen-like atoms formed by a negative muon and a nucleus, has recently provided the charge radii of the lightest nuclei (proton, deuteron,  $^4\text{He}$ ) with unprecedented accuracy. In this talk we present laser spectroscopy of these exotic atoms and their contribution to nuclear physics.

Moreover we will emphasize how these measurements are impacting the determination of fundamental constants leading to the best tests of atomic and molecular energy levels for few-body systems such as H, He,  $\text{H}_2^+$  and  $\text{H}_2$ , providing the best verification of Quantum Electrodynamics for bound systems

### Acknowledgements

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## Coupling of Proton Dynamics to Reaction Pathways in Biomolecular Systems

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Keywords: modelling • enzyme catalysis • QM/MM dynamics • pKa evaluation

In this talk, I will be reviewing some of our most recent works in modelling enzyme catalysis through hybrid quantum chemical approaches. The examples will include two decarboxylase enzymes<sup>1</sup> and the human transketolase.<sup>2</sup> The systems share a common trait. Their function/proficiency builds upon the use of protons to balance local (transient) electrostatic potentials. While for a large body of chemistry a protic medium is an added complication, enzymes have evolved over millennia to embrace protons and skillfully use their lability. By means of QM/MM dynamics and careful evaluation of  $pK_a$  values *in silico*, we are able to finally close decades-old discussions on some of these challenging biomolecular riddles. Future perspectives on the use of multicomponent methods and the coupling of the different timescales for these processes will be also discussed.

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## Biomedical and Astrophysical Applications of Atomic Parameters

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Keywords: X-rays • Auger rates • radiative transitions

The knowledge of accurate values of atomic inner-shell radiative and radiationless transition rates is essential in many fields of physics and technology such as spectroscopy, plasma physics, astrophysics, and more recently, in targeted cancer therapy.

Inner-shell transitions have been object of intense research, both theoretically and experimentally, since the second half of the 20th century, and several reviews can be found in the literature but, despite the increasing number of available theoretical and experimental works on this subject, available data are still scarce or outdated.

In this presentation I will review the current state of the theoretical determination of radiative and radiationless transitions for the inner shells of several elements, using the multi-configuration Dirac-Fock (MCDF)<sup>1</sup> method, outlining its importance in different fields with special emphasis in Auger targeted radiotherapy<sup>2</sup> and kilonovae emission modelling.<sup>3</sup>

### Acknowledgements

This work was partially supported by the *Fundação para Ciência e Tecnologia* (FCT), Portugal through the contract UIDP/50007/2020.

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## Photoionization Spectroscopy of Free Radicals Using Synchrotron- and Laser-Based Experiments

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Keywords: photoionization spectroscopy • PFI-ZEKE • synchrotron radiation

The photoionization spectroscopy of free radicals is a difficult task mainly because it implies the use of efficient radical sources and of tunable VUV radiations. In this talk, I will describe two different techniques employing either the threshold photoelectron spectroscopy (TPES) coupled with synchrotron radiation or the pulsed-field-ionization zero-kinetic-electron photoelectron spectroscopy (PFI ZEKE PES) coupled with a tunable VUV laser.

In the first part of the talk, I will briefly present a few results obtained on  $C_2$ ,<sup>1</sup>  $SiH$ ,<sup>2</sup> and  $SiC$  in collaborations (mainly with J.C. Loison, G. Garcia, *et al.*), using a flow tube reactor coupled with the DELICIOUS 3 spectrometer of the DESIRS beamline of the SOLEIL synchrotron.

In the second part, I will introduce a recent laser experiment that we built at ISMO to perform high-resolution PFI-ZEKE spectroscopy of free radicals. Preliminary results will be presented.<sup>3,4</sup>

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## Molecular Beam Microwave Spectroscopy: Structure, Bonding and Dynamics

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Keywords: hydrogen bond • van der Waals interactions • carbon bond • Coriolis interactions • tunneling

Microwave spectroscopy has proven to be the most accurate way of determining structure of molecules in the gas phase. What has not been as widely recognized is the application of microwave spectroscopy to infer about bonding, both within a molecule and between molecules. Our group has focused on weakly bound complexes of H<sub>2</sub>O and H<sub>2</sub>S, as the former is a text-book example for hydrogen bonding and the latter was thought to have van der Waals interactions. We have recently shown that both (H<sub>2</sub>O)<sub>2</sub> and (H<sub>2</sub>S)<sub>2</sub> have hydrogen bonds holding them together.<sup>1</sup> We defined a 'carbon bond' analogous to the hydrogen bond<sup>2</sup> and showed that CH<sub>3</sub>CN⋯CO<sub>2</sub> complex is bound by a carbon bond.<sup>3</sup> Though, (H<sub>2</sub>O)<sub>2</sub> is a classic example for hydrogen bond, three different large amplitude tunneling motions can break the hydrogen bond and enable each of the four H atoms to be involved in the hydrogen bond.<sup>4</sup> While the tunneling dynamics in (H<sub>2</sub>O)<sub>2</sub> has been investigated extensively, we showed recently how the presence of an argon atom affects this in Ar⋯(H<sub>2</sub>O)<sub>2</sub>.<sup>5</sup> The ground state microwave spectrum of C<sub>6</sub>H<sub>6</sub>⋯H<sub>2</sub>O was solved 3 decades ago, proving that water forms hydrogen bonds with water.<sup>6</sup> However, the excited state transitions could not be properly assigned and they were fitted to a free rotor Hamiltonian, with unacceptable residues. Microwave spectra of several similar complexes were fit with a free-rotor model leading to unacceptable residues. We have recently shown that a Hamiltonian including Coriolis interaction can explain the excited state transitions incorrectly assigned as a free rotor, for C<sub>6</sub>H<sub>6</sub>⋯H<sub>2</sub>O and similar complexes.<sup>7</sup> This talk will highlight how microwave spectroscopy has been used to infer structure, bonding and dynamics in molecules/molecular complexes.

### Acknowledgements

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# Invited Lectures



## Gas Based Neutron Detectors: Recent Developments and Future Prospects

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Keywords: neutron detectors (cold, thermal, fast neutrons) • gaseous radiation detectors

Neutron imaging techniques are a vital non-destructive tool, widely used in a range of industrial, medical and consumer applications. Direct imaging methods (neutron radiography) are used to probe objects in industry and indirect methods (diffraction, small-angle scattering) to determine the shapes of biological molecules, to name a few applications. It is such a key research field that the world is venturing into the construction of novel neutron sources, along with the upgrade of many in operation for decades. The flagship is the European Spallation Source, a multi-disciplinary research facility equipped with what will be the world's most powerful pulsed neutron source; foreseen to start its scientific program in 2025. The list of novel large-scale neutron facilities includes the US Spallation Neutron Source, the Life Science Experimental Facility in Japan and the China Spallation Neutron Source. Instruments at these facilities depend on the deployment of position sensitive neutron detectors (PSND) with high performance in aspects such as counting rate capability and spatial resolution. For decades that helium-3 filled gaseous detectors have been the workhorse in neutron detection, but the ongoing shortage of this material has led to the search for innovative alternatives, most of them using solid boron-10. I will present an update regarding some of the recent developments and novel insights in the field. Focus will be in the use of ultra-thin boron-10 layers, sharing some of the technical challenges and requirements encountered in their production and the impact in image quality and detection efficiency.

### Acknowledgements

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## The Role of Non-Adiabatic Couplings in the Photodissociation of the Methyl Radical

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Keywords: photodissociation dynamics • resonances • wave packet • alkyl radicals

The nonadiabatic photodissociation dynamics of the CH<sub>3</sub> (and CD<sub>3</sub>) radical from the 3p<sub>z</sub> and 3s Rydberg states is investigated by applying a one-dimensional (1D) wave packet model that uses recently calculated *ab initio* 1D electronic potential-energy curves and non-adiabatic couplings. Calculated predissociation lifetimes are found to be too long as compared to the experimental ones. The 1D dynamical model, however, is able to predict qualitatively and explain the fragmentation mechanisms that produce the hydrogen-fragment translational energy distributions (TED) measured experimentally for the ground vibrational resonance of the 3p<sub>z</sub> and 3s Rydberg states (CH<sub>3</sub>(v=0, 3p<sub>z</sub>) and CH<sub>3</sub>(v=0, 3s)). The CH<sub>3</sub>(v=0, 3p<sub>z</sub>) TED found experimentally displays a rather large energy spreading, while the experimental CH<sub>3</sub>(v=0, 3s) TED is remarkably more localized in energy. The present model also predicts a widely spread CH<sub>3</sub>(v=0, 3p<sub>z</sub>) TED, produced by a complex dissociation mechanism which involves predissociation to one dissociative valence state through a non-adiabatic coupling, as well as transfer of population to a second valence state through three conical intersections. Also, in agreement with experiment, the model predicts a rather localized CH<sub>3</sub>(v=0, 3s) TED because the conical intersections no longer operate in this photodissociation process, and predissociation occurs only into a single valence state. Another complex dissociation mechanism is predicted by the model for initial CH<sub>3</sub>(v>0, 3s) and CD<sub>3</sub>(v>0, 3s) resonances. Thus, the present 1D quantum model reveals a rich photodissociation dynamics of methyl, where a variety of complex fragmentation mechanisms is favored by the presence of different non-adiabatic couplings between the electronic states involved

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## Observing Solute-Solvent Coupled Structural Dynamics in Solvated Cu Photosensitizer with Ultrashort X-rays

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Keywords: X-ray free electron laser • structural dynamics • ultrafast electron transfer

Photochemical reactions in solution are governed by a complex interplay between transient intramolecular electronic and structural changes and accompanying solvent rearrangements. However, the mechanisms of the solute–solvent coupling remain largely unknown because conventional optical methods cannot disentangle solute and solvent motions with atomic spatiotemporal resolution. Here, we simultaneously measure femtosecond X-ray emission and X-ray scattering to track both the intramolecular and solvation structural dynamics initiated by a photoinduced metal-to-ligand-charge-transfer transition in a prototype Cu(I) photosensitizer.

Quantitative analysis assisted by molecular dynamics simulations reveals a two-step ligand flattening, which has long been indiscernible. The first step is a ballistic flattening, triggering coherent motions of surrounding acetonitrile molecules. This solvent response mediates the decay of intramolecular coherent vibrations. The second step is determined by the mutual interplay with acetonitrile molecules approaching the Cu atom. These results provide an atomic-scale view of how the solvent reorganization can remarkably influence photochemical reactions and demonstrate the ability of ultrafast X-ray techniques to overcome limitations of optical methods.



## Neutral Bremsstrahlung Emission in Xenon Unveiled

Carlos A.O. Henriques, *on behalf of the NEXT collaboration*

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Keywords: neutral bremsstrahlung • scintillation • neutrinos • dark matter • NEXT

The interaction of an electron with the dipole field of a neutral atom or molecule can lead to radiative photon emission by analogy with the familiar case of Nuclear Bremsstrahlung. This process is known as Neutral Bremsstrahlung (NBrS), and it can occur even in noble atoms by virtue of their induced dipole moment. Neutral Bremsstrahlung in noble gases has been neglected in favor of excimer-based Vacuum-Ultraviolet (VUV) emission, being only recently studied in argon.

In this study, we have found strong evidence of Neutral Bremsstrahlung emission in xenon, obtained using both the NEXT-White Time Projection Chamber (TPC), at present the largest optical Xe-TPC in operation, and a dedicated setup based on a Gas Proportional Scintillation Counter (GPSC). The secondary scintillation yield was measured over 5 orders of magnitude for a wide range of electric fields. A non-negligible light production signal was detected even for low electric fields, under which drifting electrons have not sufficient kinetic energy to excite Xe atoms. Comparison with first-principle calculations allows us to assign this effect to Neutral Bremsstrahlung, which is intrinsically broadband and, as confirmed by our measurements, immune to quenching, unlike excimer-based electroluminescence emission.

For photon wavelengths below 1000 nm, the NBrS yield increases from  $\sim 10^{-2}$  ph cm<sup>-1</sup> bar<sup>-1</sup> e<sup>-1</sup> at reduced electric fields of about 50 V cm<sup>-1</sup> bar<sup>-1</sup> to  $\sim 3 \times 10^{-1}$  ph cm<sup>-1</sup> bar<sup>-1</sup> e<sup>-1</sup> at 500 V cm<sup>-1</sup> bar<sup>-1</sup>. Above 1.5 kV cm<sup>-1</sup> bar<sup>-1</sup>, the NBrS intensity,  $\sim 1$  ph cm<sup>-1</sup> bar<sup>-1</sup> e<sup>-1</sup> is two orders of magnitude lower than conventional secondary scintillation.

Despite being fainter than its excimer-based counterpart, our calculations reveal that NBrS photons can interfere with the ability to measure low primary-scintillation signals in gaseous or liquid Xe TPCs, commonly employed in rare event searches. This new source of light emission opens a viable path towards the development of single-phase liquid Xe TPCs based on secondary scintillation amplification for neutrino and dark matter physics, avoiding the very high electric fields required by conventional electroluminescence (Ref. 1 and references therein).

### Acknowledgements

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## Proton in the Ring: Wandering Protons Inside Molecular Cavities

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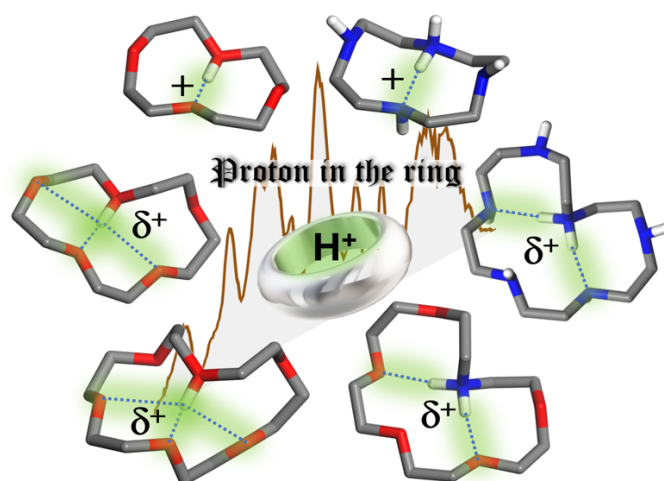
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Keywords: proton bond • crown ethers • inclusion complexes • spectroscopy

The proton bond is a paradigmatic quantum molecular interaction and a major driving force of supramolecular chemistry. The ring cavities of crown ethers provide an intriguing environment, promoting competitive proton sharing with multiple coordination anchors. This study shows that protons confined in crown ether cavities form dynamic bonds that migrate to varying pairs of coordinating atoms when allowed by the flexibility of the macrocycle backbone.<sup>1</sup> Prototypic native crown ethers (12-crown-4, 15-crown-5 and 18-crown-6) and aza-crown ethers (cyclen, 1-aza-18-crown-6 and hexacyclen) are investigated. For each system, Infrared action spectroscopy experiments and ab initio Molecular Dynamics computations are employed to elucidate the structural effects associated with proton diffusion and its entanglement with the conformational and vibrational dynamics of the protonated host. Results will as well be presented for cases in which the protonated crown ether is hydrated, hence incorporating a competitive binding of the proton with water and the ether moieties of the ring backbone.



**Figure 1.** Proton delocalization and intracavity proton bonding are investigated with infrared action vibrational spectroscopy, quantum-chemical computations and ab-initio Molecular Dynamics.

<sup>1</sup> F. Gámez, J.R. Avilés-Moreno, G. Berden, J. Oomens, B. Martínez-Haya, *Phys. Chem. Chem. Phys.*, **2021**, *23*, 21532.

## Virtual Reality for Molecular Simulation and Design: From Quantum Chemistry to Drug Binding

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Keywords: virtual reality • real-time simulation • immersive technologies

The mechanics of nanoscale molecular objects –which arise through electrostatic forces acting on particles in non-uniform fields– are relatively well characterized owing to decades of study. Nevertheless, because dynamics at this scale differ from the familiar mechanics of everyday objects, they are often non-intuitive, even for highly trained researchers. Moreover, because molecular systems have many of degrees of freedom, their motion involves a complicated, highly correlated, and 3D many-body dynamical choreography with few analogues in day-to-day experience. We have begun to explore the application of immersive technologies like virtual reality (VR) to enhance researchers' cognition of nanoscale domains, enabling the design and manipulation of real-time simulations of molecular structures in 3D.<sup>1-2</sup> In this talk, I will focus on our recent efforts designing a flexible, open-source, multi-person VR software framework which enables groups of researchers to simultaneously cohabit real-time simulation environments and interactively build, inspect, visualize, and manipulate the dynamics of complex molecular structures with atomic-level precision.<sup>3</sup> I will outline a range of application domains where we are using Narupa to obtain microscopic insight into 3D dynamical concepts and enable effective research and communication, including transport dynamics in materials,<sup>1</sup> reaction discovery using 'on-the-fly' quantum chemistry,<sup>4</sup> protein-ligand binding,<sup>5</sup> and machine learning potential energy surfaces.<sup>4</sup> I will also discuss future applications for immersive technologies like VR to facilitate more efficient research and communication across a wide range of scientific domains.

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<sup>2</sup> M. O'Connor *et al.*, Sampling molecular conformations and dynamics in a multiuser virtual reality framework. *Science Advances*, **2018**, *4*, eaat27731.

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<sup>5</sup> H. M. Deeks *et al.*, Sampling protein-ligand binding pathways to recover crystallographic binding poses using interactive molecular dynamics in virtual reality, arXiv: [1908.07395](https://arxiv.org/abs/1908.07395), **2019**.

## X-Ray Fluorescence Spectroscopy and Imaging Analysis Using Gaseous Detectors Based Neutron Detectors: Recent Developments and Future Prospects

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Keywords: EDXRF • X-ray Imaging • MPGD • gaseous detectors

Neutron EDXRF analysis techniques are known for its non-destructive and non-invasive character, which makes them suitable for the identification and quantification of elements in analytes with good detection efficiency and sensitivity. As such, EDXRF is widely used on a variety of areas, including biomedical research, industry, material science, art and cultural heritage studies. Most of these studies are conducted using conventional EDXRF systems, such as portable XRF spectrometers or imaging spectrometers, either scanning systems or full-field of view systems, usually based on solid state detectors, that either allow elemental identification/quantification and/or elemental distribution mapping of small regions of interest.

During the last years, gaseous detectors, such as the Micropattern Gaseous Detectors (MPGDs), have received increasing attention in the scientific community by showing a good potential as full-field detectors for EDXRF imaging systems. MPGDs provide accurate determination of the interaction position of each X-ray photon in the sensitive volume of the detector, as well as energy information, making possible to map the distribution of elements in large area samples with fair energy resolution and detection efficiency, at a reasonable cost. This type of systems has already been used for the elemental mapping of different samples, ranging from applications in the cultural heritage field,<sup>1,2,3</sup> to the biomedical field.<sup>4,5</sup>

In this talk, a complete overview of the EDXRF imaging systems based on gaseous detectors, both apparatus and applications, will be presented.

### Acknowledgements

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<sup>5</sup> F.D. Leite, *et al.*, *Spectrochimica Acta Part B*, **2022**, in press

## Carbohydrate Research by High Resolution Spectroscopy and Other Applications

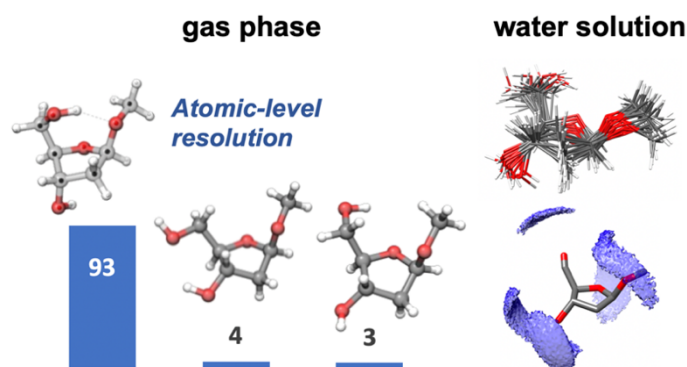
Aran Insausti,<sup>1</sup> Camilla Calabrese,<sup>1,2</sup> Elena Alonso,<sup>1,2</sup> Maider Parra,<sup>1</sup> Otger Crehuet,<sup>1</sup> Emilio J. Cocinero<sup>1</sup>

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Keywords: carbohydrate • gas phase • microwave spectroscopy • laser spectroscopy • conformational analysis

I present several studies on biomolecules (carbohydrates and glycopeptides) and several applications, exploiting an experimental strategy which combines microwave and laser spectroscopies in high resolution, NMR, computation and synthesis. Laser spectroscopy offers high sensitivity and selectivity, making it ideal for studying biochemical systems of medium-large size.<sup>1-2</sup> Moreover, microwave spectroscopy provides higher resolution and direct access to molecular structure.<sup>3</sup> This combined approach provides not only accurate chemical insight on conformation, structure and molecular properties, but also benchmarking standards guiding the development of theoretical calculations. In order to illustrate these possibilities, we present the results on the conformational landscape of several carbohydrates and glycopeptides<sup>2,3</sup> with different biological roles. In addition, other applications of high resolution spectroscopies are showed.<sup>4</sup>



**Figure 1.** Conformations and populations in gas and solution phases of 2-deoxyribose.

<sup>1</sup> E. J. Cocinero, P. Çarcabal, T. D. Vaden, J. P. Simons, B. G. Davis, *Nature*, **2011**, 469, 76.

<sup>2</sup> I. A. Bermejo, I. Usabiaga, I. Compañón, J. Castro-López, A. Insausti, J. A. Fernández, A. Avenzoza, J. H. Busto, J. Jiménez-Barbero, J. L. Asensio, J. M. Peregrina, G. Jiménez-Osés, R. Hurtado-Guerrero, E. J. Cocinero and F. Corzana *J. Am. Chem. Soc.*, **2018**, 140, 9952.

<sup>3</sup> C. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-López, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, F. Corzana, E. J. Cocinero, *ACS Cent. Sci.*, **2020**, 6, 293.

<sup>4</sup> C. Calabrese, B. Temelso, I. Usabiaga, N. A. Seifert, F. J. Basterretxea, G. Prampolini, G. C. Shields, B. H. Pate, L. Evangelisti and E. J. Cocinero, *Angew. Chem. Int. Ed.*, **2021**, 60, 16895.



## Unconventional Electron Donors: Metals as $\sigma/\pi$ -Hole Acceptors

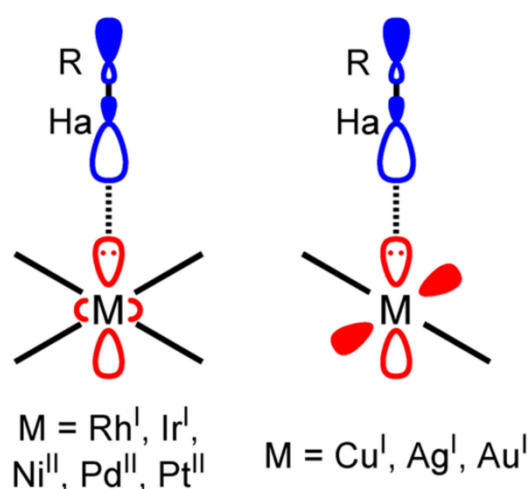
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Keywords:  $\sigma$ ,  $\pi$ -hole interactions • metal centers • supramolecular chemistry • halogen bonds • DFT calculations

In this communication, the role of metal centers as electron donors is analyzed from two perspectives. Firstly, it highlights recent studies discovering unconventional halogen and chalcogen bonding (HaB and ChB, respectively) that involves positively charged metal centers. These centers provide their filled d-orbitals for HaB/ChB, and thus behave as nucleophilic components toward the  $\sigma$ -holes at the halogen or chalcogen atoms (see Figure 1a). This role of some electron-rich transition metal centers can be regarded as an oxymoron in the sense that the metal is, in most cases, formally cationic; consequently, its nucleophilic function is surprising. The importance of Ha $\cdots$ d-[M] (Ha=halogen; M is Group 9 (Rh, Ir), 10 (Ni, Pd, Pt), or 11 (Cu, Au) interactions in crystal engineering is emphasized by showing remarkable examples reported and uncovered by processing of the Cambridge Structural Database (CSD),<sup>1</sup> where this Ha $\cdots$ d-[M] directional interaction guides the formation of solid supramolecular assemblies of different dimensionalities. Secondly,  $\pi$ -hole $\cdots$ d-[M] interactions are described as well as their application in the construction of unprecedented supramolecular assemblies.

The results derived from this study might be useful to those scientists working in the fields of supramolecular chemistry and crystal engineering as well as to inspire chemists working in supramolecular catalysis.



**Figure 1.** Metal centers as electron donors in halogen bonding interactions (Ha = halogen).

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## High-Resolution X-ray Metrology in the Search for Physics Beyond the Standard Model

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Keywords: X-ray spectrometry • double crystal spectrometer • bound state QED • atomic structure • highly charged ions

In the last decades, high-precision spectroscopy has been used to investigate subtle effects in simple and complex systems in order to find possible mismatches between theory and experiments. This research avenue is complementary to high energy physics where one tries to find new physics by searching at smaller scales and higher energies. In this work we focus on the use of metrology grade instruments to look for very subtle effects that might hint onto hidden physics such as the recent claims of discrepancies in bound-state quantum electrodynamics contributions in 2 electron atoms,<sup>1</sup> the proton radius puzzle<sup>2</sup> and even the search for dark matter.<sup>3</sup>

The use of metrology grade instruments can also solve a metrological problem regarding to the transfer of standards for calibration, which become important when looking for these subtle effects. The Double Crystal Spectrometer (DCS) that is being built in Lisbon can shed light on some of these problems. Coupled to high-accuracy atomic structure calculations, some inconsistencies between experiments and theory in X-ray emission could be investigated.

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<sup>3</sup> S. Friedrich, G.B. Kim, C. Bray, R. Cantor, J. Dilling, S. Fretwell, J. A. Hall, A. Lennarz, V. Lordi, P. Machule, D. McKeen, X. Mougeot, F. Ponce, C. Ruiz, A. Samanta, W. K. Warburton, K. G. Leach, *Phys. Rev. Lett.*, **2021**, *126*, 021803.



# Oral Communications



## Spatiotemporal Control of Trapped Rydberg Qubits

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Keywords: quantum control • quantum Computing • Rydberg atoms

Atoms trapped by optical tweezers, interacting through Rydberg blockade, can be used to generate few multi-particle entanglement and simple quantum circuits.<sup>1</sup> To further the quest of the quantum computer, we need to improve the system addressability and controllability. One of the problems in the usual designs with ordered arrays of atoms largely separated in optical traps, is the long duration of the two-qubit gates, which must operate in the micro- or sub-microsecond regime to avoid exciting more than one atom in a Rydberg state using the dipole blockade mechanism.<sup>2</sup> Optimal control theory can be used to find efficient and robust pulse sequences,<sup>3</sup> but it remains very challenging to accelerate the processes without changing the set-up. In this work we speed up the gate operation times by using denser arrays that allow to boost the dipole-blockade. The price to pay is that the qubits can no longer be regarded as independent, as the pulse profiles may overlap significantly with more than one qubit site. This problem can be addressed by controlling the position of the atoms with respect to the different laser beams, adding a spatial control knob into the problem, or with finer technology, using structured light. To optimize the gate performance in this set-up, we need to apply optimization techniques that deal not only with the temporal parameters of the laser, but also with the spatial position of the qubits or the field structure. As a first application attempting a spatiotemporal control of trapped atoms to address quantum computation processes, in this work we show how to prepare a C-PHASE in two-qubit and three-qubit systems. Our results suggest that quantum control might be possible in multiple-qubit systems, where maximal addressability and fast and reasonably robust solutions will be achieved by controlling the pulse shapes and the structure of irregular arrays of two- and three-dimensional assemblies of trapped atoms.

### Acknowledgements

Financial support from the Quantum Computing Technology Development Program (NRF--2020M3E4A1079793) is gratefully acknowledged.

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## Raman Spectroscopy of High-Temperature Supersonic Jets of CO<sub>2</sub>

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Keywords: Raman spectroscopy • CO<sub>2</sub> • supersonic jets • high-temperature

Supersonic jets in the laboratory provide an ideal medium to investigate the gas behaviour under non equilibrium conditions.<sup>1,2,3</sup> Raman spectroscopy is a powerful, non-intrusive, technique to probe gas jets at molecular level with high spatial resolution, as we have demonstrated in the Laboratory of Molecular Fluid Dynamics of the IEM.

CO<sub>2</sub> is the main component of the atmospheres of Mars and Venus and plays an important role in the energy budget of the Earth's atmosphere and its global warming. In the upper layers of our atmosphere, CO<sub>2</sub> can be far from thermodynamic equilibrium. Despite these important implications, there is a lack of reliable experimental data on the many processes involving CO<sub>2</sub> internal relaxation in such environments.<sup>4</sup>

For this work, we have designed and built a new high-temperature nozzle, with resistive heating cartridges, able to reach up to 1100 K. With this new set-up we have generated several jets of CO<sub>2</sub> at stagnation temperatures between 300 and 800 K and probed them at different points along the jet axes by means of Raman spectroscopy.

We will present first a detailed description of the experimental set-up, the Raman technique, and its capabilities, illustrated by some examples of rotational and vibrational Raman spectra of hot CO<sub>2</sub> in supersonic jets. Then, the evolution of the rotational and vibrational temperatures along the jets and through their shock wave will be shown.

### Acknowledgements

This research is funded by the Spanish *Ministerio de Ciencia, Innovación y Universidades*, through grants No. PRE2018-085960 and FIS2017-84391-C2-1-P.

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## Rotational and Vibrational Relaxation of CO<sub>2</sub> in Supersonic Jets

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Keywords: Raman spectroscopy • CO<sub>2</sub> • supersonic jets • non-equilibrium thermodynamics • kinetics

CO<sub>2</sub> is the main component of the atmospheres of Mars and Venus and plays an important role in the energy budget of the Earth's atmosphere and its global warming. In the upper layers of our atmosphere, CO<sub>2</sub> can be far from thermodynamic equilibrium. Despite these important implications, there is a lack of reliable experimental data on the many processes involving CO<sub>2</sub> internal relaxation in such environments.<sup>1</sup>

In the laboratory, supersonic gas jets are a well-suited medium to study the inelastic collisions between molecules under non-local thermodynamic equilibrium (n-LTE) conditions. Inelastic collisions are the main mechanism involved in the relaxation of the internal motions of these molecules.<sup>2</sup>

We present an original approach to the CO<sub>2</sub> relaxation problem. We probed several supersonic jets from hot nozzles by Raman spectroscopy with high-spatial resolution. The intensity of the observed Raman signal allows us to measure both the individual populations of the rotational and vibrational energy levels of the molecules, as well as their total number density at different points along the jet axis.

From these measured quantities, vibrational, rotational, and translational temperatures were retrieved at each point, illustrating the breakdown of equilibrium between these degrees of freedom, and the corresponding increment of entropy. Finally, from the time evolution of the rotational and vibrational populations, a first set of rate coefficients for the dominant inelastic collisions have been obtained.

### Acknowledgements

This research is funded by the Spanish *Ministerio de Ciencia, Innovación y Universidades*, through grants No. PRE2018-085960 and FIS2017-84391-C2-1-P.

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## A Different Concept for Gas Proportional Scintillation Counter: The Annular Anode

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Keywords: electroluminescence • gas detectors • scintillation counters • X-ray detectors

The Gas Proportional Scintillation Counters (GPSC) exploit the photon emission from the de-excitation of noble gas atoms as a detection mechanism. The size of the detector radiation window relative to the photosensor active area has always been a limitation in this type of detectors, since the amount of light collected by the photosensor may vary according to the axial distance of the incident x-ray interaction due to solid angle effects. An annular geometry for the detector anode defines a scintillation region for which the solid angle subtended by the photosensor remains constant, independent from the radiation interaction position, thus enabling to obtain a GPSC design with a large radiation window. Along with this advantage, the simplicity and robustness of this novel geometry could provide a step forward into the design of a portable GPSC, coupled to low power electronics, e.g., using SiPM or Large Area APDs instead of PMTs. We report on the simulation studies of the electric field in the detector volume for several parameters, like anode diameter, shape, and applied voltage in order to maximize the annular anode GPSC detection efficiency. Simulation results also show the expected scintillation yield and energy resolution for 5.9 keV x-rays. Experimental studies for 5.9 keV x-rays are presented for an annular anode GPSC with a radiation window area of 50 cm<sup>2</sup> and a photosensor sensitive area of 18 cm<sup>2</sup>. This type of portable, room-temperature detector, with large-detection-area and/ large-detection-volume can be an interesting choice for x-ray astronomy, competing with solid-state detectors.

### Acknowledgements

This work is funded by national funds through FCT – *Fundação para a Ciência e a Tecnologia*, I.P., in the framework of project UIDB/FIS/04559/2020 and UIDP/FIS/04559/2020.

## Does the Molecular Position Affect the Structure and Stability of the $H_2 @ C_{60}$ Complex?

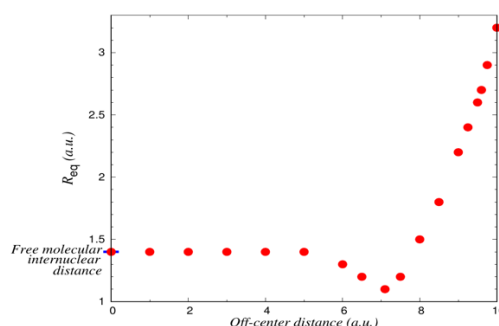
Milagros F. Morcillo Arencibia,<sup>1</sup> José M. Alcaraz Pelegrina,<sup>1</sup> Antonio J. Sarsa Rubio,<sup>1</sup> Juan M. Randazzo<sup>2</sup>

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Keywords: quantum confinement • molecular structure • configuration interaction

The study of confined systems has been a subject of considerable interest in recent years owing to their promising applications in different fields because of the changes in their physical and chemical properties due to the confinement.<sup>1</sup> In this work we address the problem of how the position of  $H_2$  inside the confining cage affects the energy and size of the molecule. Therefore, we consider it not located at the center of the cavity and a partial wave expansion for the potential is required. We use an off-center coordinate system centered at one of the H atoms.<sup>2</sup> A model based on two Woods-Saxon potentials is employed for the fullerene cage. In Figure 1 we plot the equilibrium bond length,  $R_{eq}$ , as a function of the off-center position of the confining potential. It is seen that  $R_{eq}$  is not modified until the off-center distance is 5 a.u., when the molecule shrinks since it is closer to the inner surface of the fullerene, reaching the minimum inter-atomic distance for both nuclei trapped within its surface. For larger off-center distances, one of the nuclei is out of the cavity and the other one is still trapped, therefore they tend to be separated.



**Figure 1** Equilibrium inter-atomic distance,  $R_{eq}$ , of  $H_2$  for different positions of the center of the confining cavity. The inter-atomic distance for the free molecule is also shown.

### Acknowledgements

This work was partially supported by the *Junta de Andalucía* Grant P20\_00146 from the program PAIDI (2020) under FEDER funds. M.F. M.-A. acknowledges partial support from a Ph.D fellowship from the Spanish *Ministerio de Universidades*, Grant FPU16/05950.

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## The Cathedral Package: User-Friendly Tools for Chemical Kinetics

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Keywords: chemical kinetics • cathedral package • rate constants • conformers

A new era of ab initio kinetics has emerged thanks to the improvements in hardware capabilities. Nowadays, it is possible to simultaneously include most of the elementary reactions involved in complex mechanisms. Unfortunately, an accurate rate constant determination remains a key challenge (even for gas-phase processes), not just due to the approximations involved in their calculation, but also due to the steps required to achieve them. In fact, manual actions and deep knowledge of chemical dynamics are required for such tasks, restricting them to advanced users. As a consequence, there is a great demand for automated codes and user-friendly interfaces.

We have been working on integrated computational codes able to bring theoretical studies of chemical kinetics closer to non-expert users. Specifically, we have developed The Cathedral package consisting on the following programs:

- Pilgrim,<sup>1</sup> employs direct-dynamics to calculate thermal rate constants of chemical reactions and to simulate chemical kinetics mechanisms;
- Torsiflex,<sup>2,3</sup> locates all the conformational isomers of flexible molecules;
- Q2DTor,<sup>4</sup> treats torsional anharmonicity in flexible molecules with two coupled torsions by means of the extended two-dimensional torsional (E2DT) method.<sup>5</sup>

These codes are available, free of charge, at the GitHub webpage<sup>6</sup> and they can be applied to different fields, as organometallic catalysis, gas-phase mass spectrometry, the simulation of microwave spectra, the calculation of thermodynamic properties, the study of many chemical reactions occurring in the gas phase, *et cetera*. At the moment, we are concentrating our efforts in applying them to combustion chemistry and to processes taking place at ultra-low temperatures.

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<sup>6</sup> GitHub: The Cathedral Package, <https://github.com/cathedralpkg>



## Simulating Gas-Phase Interstellar Chemistry Using the CRESU Technique

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Keywords: prebiotic Chemistry • reaction kinetics • bimolecular reactions • low-temperature kinetics

Astrochemistry is a field that has experienced an enormous increase in the last decades due to the development of the radioastronomy, making possible the detection of more than 270 molecules in the interstellar medium (ISM) or circumstellar shells.<sup>1</sup> The discovery of this chemical richness has strengthened the exogenous hypothesis, in which the prebiotic molecules were synthesized in space and then delivered to the Earth by meteorites, comets or asteroids.<sup>2</sup> The chemistry of N-bearing species in the coldest regions (~10-100 K) of the ISM is thought to be closely linked to the formation of the simplest amino acid, glycine, observed in several comets but undetected in the ISM so far.<sup>3</sup> Astrochemical networks model the abundances of the IS species using hundreds of reactions. Thus, they are constantly being improved with the inclusion of the rate coefficients ( $k$ ) for the different processes, such as radical-molecule reactions in the gas-phase. However,  $k$  must be characterized under the appropriate temperature range (10-100 K) in laboratory experiments. For this reason, we have studied the gas-phase reactivity of two species found in the ISM, methylamine ( $\text{CH}_3\text{NH}_2$ ) and ammonia ( $\text{NH}_3$ ), towards the abundant IS hydroxyl (OH) radical between 11.7 and 177.5 K using the most powerful CRESU technique (French acronym for *Reactions Kinetics in a Uniform Supersonic Flow*). This technique, based on supersonic expansions through a Laval nozzle,<sup>4</sup> is capable of reproduce the IS temperatures in the gas-phase without condensation problems. The OH radicals are generated by pulsed laser photolysis of  $\text{H}_2\text{O}_2$  and the OH temporal profile is monitored by laser induced fluorescence. The results revealed an increase in  $k$  for both reactions as temperature is decreased in the whole temperature range investigated.

<sup>1</sup> A continuously updated list of the observed molecules is available online: <http://www.astrochymist.org>.

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## Trihydrogen Cation Helium Clusters: A New Potential Energy Surface

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Keywords: *ab initio* calculations • global optimization

We present a new analytical potential energy surface (PES) for the interaction between the trihydrogen cation and the He atom in its electronic ground state. The proposed PES for the interaction  $H_3^+$ -He has been built as a sum of two contributions: a polarization energy term due to the electric field generated by the molecular cation in the position of the polarizable He atom, and an exchange-repulsion and dispersion interactions represented by a sum of "atom-bond" potentials between the three bonds of  $H_3^+$  and the He atom. The analytical representation of this second contribution has been done with the Pirani formalism and with "Improved Lennard-Jones" potentials.<sup>1</sup>

All parameters of this new PES have been chosen and fitted from data obtained from high-level *ab initio* calculations performed for a relatively small set of points with the NWChem Quantum Chemistry software package.<sup>2</sup>

Using this new PES, assuming pair-wise interactions and performing the classical Basin-Hopping optimization algorithm,<sup>3</sup> we have found the minimum energy configurations of small He clusters doped with  $H_3^+$ ,  $H_3^+(He)_N$ , with  $N = 1, 2, \dots, 16$ . The energetic study of these aggregates allows us to find magic numbers related to the greater relative stability of some aggregates in agreement with those found experimentally by the Group of Prof. Scheier in Innsbruck.<sup>4</sup> Our simulation gives the geometric structure of this magic clusters.

### Acknowledgements

We acknowledge financial support from the Spanish *Ministerio de Ciencia e Innovación* through Grant PID2019-105225GB-I00 (MICINN / FEDER, UE).

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## Computational Characterization of the Emission of the Keto Derivative of Oxyluciferin within Luciferase

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Keywords: bioluminescence • oxyluciferin • molecular dynamics

Bioluminescence is a natural process in which an enzymatic reaction of a luciferin/luciferase complex leads to an electronically excited chromophore that, upon relaxation, emits light in the visible region.<sup>1</sup> These systems present a wide range of applications in medicine,<sup>2,3</sup> which can be enhanced when the photophysical properties of the chromophore are improved. A theoretical approach to this problem can provide a deep understanding of the photophysics of the system and, thus, guide an efficient design of the luciferin/luciferase complex.

Different computational factors on the emission spectrum of the D-luciferin/luciferase system present in fireflies as well as the characteristics of the electronic transition have been analyzed. First, the impact of the sampling process on the spectrum has been investigated by means of three different criteria for choosing the chromophore/enzyme configurations from a molecular dynamics trajectory, which are subsequently employed in the excited-state computations: random selection, equidistant selection, and selection based on the Metropolis criterium. Additionally, classical and QM/MM molecular dynamics simulations have been evolved to investigate the effect of the potential energy model used during the sampling of the first electronically excited state potential energy surface. Finally, the sampled space has been analyzed to determine the geometrical features that affect the properties of the transition.

### Acknowledgements

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## Quantum Simulations of Halogen Anions Hydration: Data-Driven Potential Models from Aqueous Clusters to Bulk Solutions

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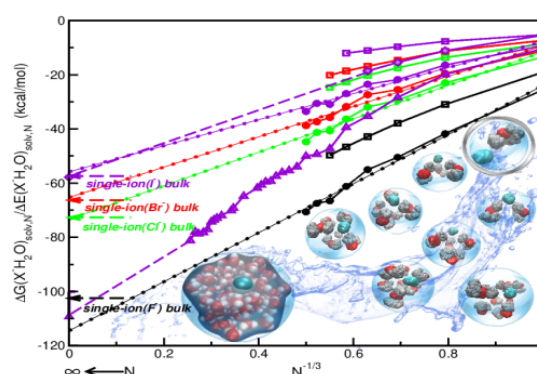
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Keywords: electronic structure calculations • benchmark dataset • data-driven modelling • ion hydration • quantum computer simulations

Dissolved ions in aqueous media are ubiquitous in many physicochemical processes, playing a crucial role in the structure of the water molecules network. A thorough understanding of the underlying forces from small clusters to bulk solutions still remains elusive. Thus, we introduced a systematic analysis of the interaction energies obtained from high-level electronic structure methodologies, to assess various dispersion-corrected density functional approaches, as well as ab initio-based data-driven potential models for halide ion–water clusters.<sup>1</sup> Following a bottom-up data-driven potential approach, we have then looked into both classical and quantum behavior of poly-hydrated halides, employing an evolutionary programming procedure and classical / quantum path-integral molecular dynamics simulations.<sup>2</sup> Our results on the ongoing conflicting distribution of different ions in aqueous environments, as well as the transition from nanoscale clusters to macroscopic condensed phases will be discussed (see Figure 1).



**Figure 1.** Computed single-ion solvation energetics of halide-water systems as a function of  $N$  solvating water molecules. Linear trends in the large cluster size regime and comparison with experimentally determined single-ion bulk solvation free energies are also shown.

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## Electronic Structure of Triatomic Ultra-Long Rydberg Molecules

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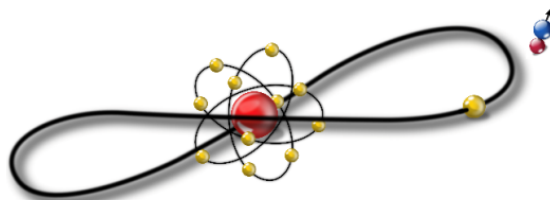
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Keywords: Rydberg molecule • kinetic coupling • avoided crossing • decay rate • ultracold chemistry

Triatomic ultra-long Rydberg molecules are formed by a Rydberg atom, an excited atom with an electron with high principal quantum number, and a polar molecule, see Fig.1. The creation of Rydberg molecules is motivated by its interesting properties.<sup>1,2,3</sup> They present strong permanent dipole moment, sensitivity to small external electric field, and possible applications in ultracold chemical reactions<sup>4</sup> or quantum simulations.<sup>5</sup> In this work, we investigate the electronic structure and properties of the Rydberg molecule Cs-RbCs.

A complete study of the rovibrational states bounded by the adiabatic electronic potentials have been performed. A special treatment has been developed for the close-energy adiabatic potential curves. The system is described beyond the Born-Oppenheimer approximation, and the coupled Schrödinger equation is solved by including the kinetic coupling terms of two neighbouring electronic potential curves. For each vibrational bound state, we obtain the weight of the Rydberg partial waves into the Rydberg molecule and the Franck-Condon factors which guide the required experimental conditions to create these Rydberg molecules. We determine the electric dipole moment and orientation of the diatomic molecule with the Rydberg trimer and study the coupling. In addition, we provide transition probabilities for the avoided crossing of the adiabatic potential curves, which might characterize the ultracold chemical reaction of the Rydberg atom with the diatomic molecule.



**Figure 1.** A sketch (not to scale) of the triatomic molecule formed by the Rydberg atom and a polar molecule.

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## Calculation of Atomic Inputs for Probing $r$ -Process in Kilonovae

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Keywords: opacity • atomic data • kilonovae • oscillator strengths • neutron stars

The observation of a kilonova electromagnetic transient linked to the gravitational wave signal GW170817 offered the first direct evidence that  $r$ -process elements are created in neutron-star mergers. To capitalize on such an opportunity, it is critical to combine an improved description of nuclear and atomic parameters with sophisticated astrophysical simulations in order to provide accurate predictions of  $r$ -process nucleosynthesis yields and their electromagnetic signals when confronted with observational data.

A sample of results for a few-weakly ionized ions of relevant  $r$ -process elements is presented. Our primary focus is on lanthanides and actinides, for which lists of atomic properties are either incomplete or nonexistent. The atomic data was computed using the Flexible Atomic Code (FAC),<sup>1</sup> which performs structure calculations using an RCI method with a central potential determined by minimizing the energy of a mean configuration. We discuss the impact in our calculations of using this central potential approximation and how it can be improved, systematically, in order to improve the accuracy of the calculations. Furthermore, we investigate the effect of the accuracy of low-lying levels and the influence of level and line density on the opacity, for which convergence studies were performed.<sup>2</sup>

### Acknowledgements

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## Photodissociation Dynamics of Bromiodomethane in the B Band, 193 nm

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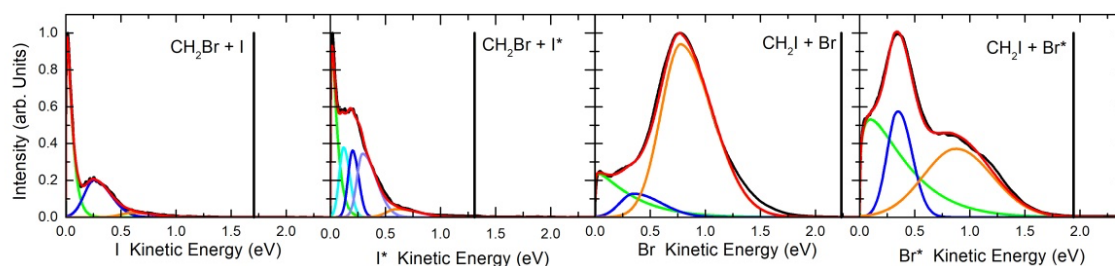
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Keywords: photodissociation • bromiodomethane • slicing • *ab initio*

The photodissociation of Bromiodomethane ( $\text{CH}_2\text{BrI}$ ) has received significant attention due to its role in producing pollutant species<sup>1,2</sup> and ozone depletion.<sup>3</sup> It presents an intricate structure of the excited states and a high bond selectivity.<sup>4</sup> The A absorption band was attributed to C-I dissociation, while the A' band to C-Br bond fission. However, the B band (around 193 nm) has not been deeply investigated.

Through detection of atomic I ( $^2\text{P}_{3/2}$ ), I\* ( $^2\text{P}_{1/2}$ ), Br ( $^2\text{P}_{3/2}$ ), and Br\* ( $^2\text{P}_{1/2}$ ) by using a combination of laser pump-and-probe and slicing imagine techniques coupled with (2+1) REMPI and high *ab initio* calculations show three contributions. The first contribution corresponds to a statistical process, while the other two are different dissociation pathways. The faster has been assigned to a predissociation through the  $9\text{A}'$  state. The latter and most energetic contribution observed could be a secondary dissociation after absorbing a second 193 nm photon, favoured through the C-Br dissociation rather than through the C-I bond cleavage due to geometrical restrictions. The calculated anisotropy parameter supports the proposed mechanism.



**Figure 1.** Kinetic energy distribution of the four detected fragments (I  $^2\text{P}_{3/2}$ , I\*  $^2\text{P}_{1/2}$ , Br  $^2\text{P}_{3/2}$ , and Br\*  $^2\text{P}_{1/2}$ , from left to right) after excitation at 193 nm.

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<sup>4</sup> L. J. Butler, *et al.*, *J. Chem. Phys.*, **1987**, 86, 2051.

## Predicting Electron Transport in Molecular Electronic Devices from Electron Deformation Orbitals

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Keywords: computational chemistry • molecular electronics • molecular wires • molecular rectifiers • molecular capacitors • molecular junction

The response of an electron system to an electric voltage can be quantified by means of the electron deformation density and its associated matrix. The eigenvectors of this matrix are called electron deformation orbitals (EDOs).<sup>1</sup> When the EDOs are constructed on the basis of molecular orbitals, they come in electron-hole pairs, each pair containing a positive and a negative function sharing the same absolute eigenvalue. Recently, it was shown that, within the time-energy uncertainty framework, the electric conductance can be explicitly obtained from coupled electron transmission channels represented by EDOs pairs.<sup>2</sup> The formation of these channels is ruled by symmetry relations between occupied molecular orbitals (MOs) and energetically accessible unoccupied ones, which allows understanding and predicting differences among the electric conductivity of structurally similar molecular chains. This MO picture also connects the electron transport in molecular systems with the underlying ideas behind the band theory in mesoscopic systems.

As virtues of the EDOs analysis of the electron transport, it can be mentioned that: the method provides a direct connection between polarization and conductance, the strong mixing between molecular and metal electronic levels in a covalent molecular junction is properly accounted for, the effect of the bias voltage on the electronic levels is included explicitly in the calculations, and the method can be applied in combination with SCF or post-SCF electronic structure theories at the same computational cost for the electron transport calculations.

In this communication, the electron transport approach based on EDOs is first introduced to then present some applications to the study of different molecular electronic devices, including molecular wires,<sup>3</sup> molecular rectifiers<sup>4</sup> and molecular capacitors.

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## Automated Reaction Discovery Through Reactive MD Simulation

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Keywords: MD simulations • graph theory • automated methods

A computational protocol is proposed in this talk for use in discovering reaction mechanisms. The method does not rely on either chemical intuition or assumed *a priori* mechanisms, working in a fully automated fashion.

The pipeline consists of three steps: i) exploration of reaction mechanisms through MD simulations or chemical knowledge-based algorithms, ii) use of Graph Theory to build the reaction network, and iii) kinetics simulations. The method has been successfully employed to study combustion chemistry, cycloaddition reactions, photodissociations, organometallic catalysis, radiation damage of biological systems, simulation of mass spectrometry experiments, and astrochemistry, and a few examples will be given in this talk.

This methodology has been implemented in the open-source program AutoMeKin.<sup>1</sup>

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<sup>1</sup> E. Martínez-Núñez, G.L. Barnes, D.R. Glowacki, S. Kopec, D. Peláez, A. Rodríguez, R. Rodríguez-Fernández, R.J. Shannon, J.J.P. Stewart, P.G. Tahoces, S.A. Vazquez, *J. Comput. Chem.*, **2021**, 42, 203.

## Beyond Structure Solving with Microwave Spectroscopy

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Keywords: microwave spectroscopy • functional molecules • molecular structure

Since the dawn of the chirped-pulse era,<sup>1</sup> broadband rotational spectroscopy has become a foundation for new methods to explore beyond conventional spectroscopy and attain next-level tracing and even acquire control over molecular properties.<sup>2</sup> The improved sensitivity of the technique has unlocked studies of increasingly more complex molecular species,<sup>3</sup> including classes of large functional molecules such as artificial molecular motors.<sup>4</sup> With the intrinsically narrow line widths of rotational transitions, microwave spectra are molecular fingerprints that grant unambiguous assignment of exact three-dimensional structures, and even allow identification and quantification of enantiomers using recently developed strategies.<sup>5,6</sup> In this contribution, we will present recent results that showcase the reach of rotationally resolved spectroscopy in and beyond the realms of molecular structure-solving.

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## Time-Resolved Photoionization of Simple Aromatic Molecules in Water

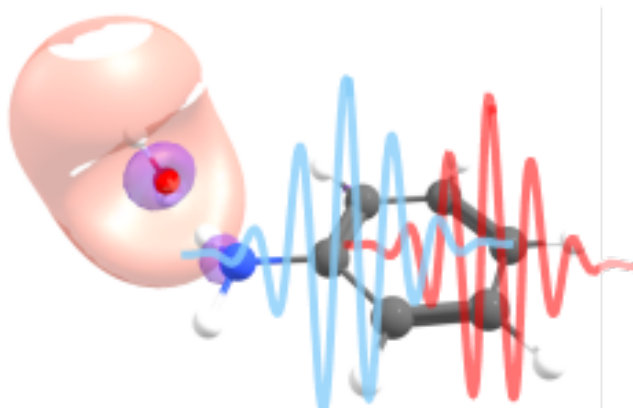
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Keywords: aniline • transient absorption • ionization • dynamics

The ability to photoionize after excitation along the nearest absorption of their UV spectra, well below the measured gas phase ionization potential, has been observed for different simple aromatic molecules solved in water. In this contribution, we will describe the case of aniline, whose dynamics, after excitation at 267 nm, has been tracked from the femto (fs) to the nanoseconds (ns) scale, by pump-probe broadband transient absorption (TA) methods. The complex TA spectrum recorded at the earliest delay times is analyzed by using a pump-repump-probe scheme that permits to interrogate the nature of the contributing species. The collected data indicate that in parallel to the long-living  $\pi\pi^*$  state responsible of the fluorescence, a charge transfer to solvent state (CTTS) is formed shortly after the excitation. The photoionization of the molecule will be discussed in terms of the electronic nature of this charge-transfer character state, and the influence of the water-solute interactions on it.



**Figure 1.** Cartoon of UV and IR laser pulses interacting with the aniline molecule and giving rise to the CTTS state.

## Primary Scintillation Yield in Xenon for Electrons and Alpha Particles

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Keywords: particle physics experiments • gaseous radiation detector • gas Proportional scintillation counter • xenon scintillation • primary scintillation yield

Xenon scintillation plays an increasingly significant role in particle physics experiments, such as double beta decay and double electron capture detection, with or without neutrino emission, and dark matter search. However, information on primary scintillation yield in the absence of recombination is still limited and dispersed. The mean energy required to produce a vacuum ultraviolet scintillation photon ( $W_{sc}$ ) in gaseous Xe has been measured in the range of 30-120 eV. Lower  $W_{sc}$ -values are often reported for alpha particles when compared to electrons produced by gamma or x-rays, being this difference not yet understood.

For detailed studies of the absolute primary scintillation yield in gaseous Xe at 1.2 bar, we employed a dedicated setup consisting in a Gas Scintillation Proportional Counter (GPSC) with photomultiplier (PMT) readout (Figure 1). The simulation model for accessing the geometric efficiency of the detector was developed and benchmarked through waveform-shape analysis of primary and secondary scintillation signals produced at different distances from the photosensor. We performed a systematic study using gamma and x-rays with energies in the range of 5.9-60 keV, and ~2-MeV alpha particles.  $W_{sc}$ -values between 30 and 50 eV were obtained for different energies without significant differences between alpha particles and electrons.

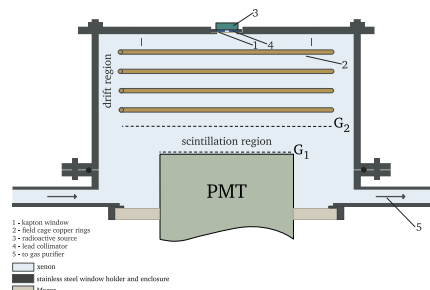


Figure 1. Schematic of the GPSC used in this work.

### Acknowledgements

This work is funded by national funds through FCT– *Fundação para a Ciência e a Tecnologia*, I.P., in the framework of projects UIDB/FIS/04559/2020 and UIDP/FIS/04559/2020 and PTDC/FIS-NUC/3993/2021.

## Electron Transfer Between Heliophobic and Heliophilic Species in Helium Nanodroplets: A Path Integral Molecular Dynamics study

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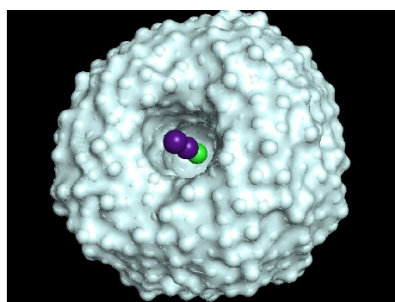
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Keywords: helium nanodroplets • charge transfer process • PIMD simulations

Electron transfer from a heliophobic  $\text{Cs}_2(^3\Sigma_u)$  dimer, located on the surface of a He droplet, to a heliophilic, fully immersed  $\text{C}_{60}$  molecule is studied through PIMD simulations in the NVT (2K) and NVE ensembles to provide real-time dynamics. After electron ionization mass spectroscopy measurements<sup>1</sup> this spatially quenched reaction was characterized as a long-range electron transfer in a high-level *ab initio* study.<sup>2</sup> A droplet size of 2090 atoms is assumed to account for spatial hindrance on reactivity. By increasing the number of beads in the simulations, the relevance of quantization is studied without an implicit assumption of superfluidity. Reaction probability increases with the level of quantization, and proceeds showing a rotational motion of cesium dimer which involves a substantial displacement of helium, as shown in figure below. It raises the issue of whether the interacting species are driven out-of-equilibrium after impurity uptake, since reactivity is strongly quenched if a full thermal equilibration is assumed. The results of this study have been recently published.<sup>3</sup>



### Acknowledgements

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## Observation of Confinement-Induced Resonances in a 3D Lattice

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Keywords: quantum gas • optical lattice • inelastic confinement-induced resonance

We report on the observation of confinement-induced resonances for strong three-dimensional (3D) confinement in a lattice potential. Starting from a Mott-insulator state with single-site occupancy, we detect loss and heating features at specific values for the confinement-length scale and the 3D scattering length. Two independent models, based on the coupling between the center-of-mass and the relative motion of the particles as mediated by the lattice, predict the resonance positions to a good approximation, suggesting a universal behavior. Our results extend confinement-induced resonances to any dimensionality and open up a new method for interaction tuning and controlled molecule formation under strong 3D confinement.

### Acknowledgements

We thank E. Dobler for help with the experiment and discussions. The Innsbruck team gratefully acknowledges funding by the DFG-FWF Forschergruppe FOR2247 under the FWF project number I4343-N36, via a Wittgenstein prize grant under project number Z336-N36, and by the European Research Council (ERC) under project number 789017. AS thanks that part of the research was supported by the National Science Foundation under Grant No. NSF PHY-1748958. FR acknowledges support by PGC2018-093854-BI00 and PID2021-122711NB-C21 funded by MCIN/AEI/10.13039/501100011033, and by the Comunidad de Madrid under the Grant APOYO-JOVENES-4L2UB6-53-29443N (GeoCoSiM)

## Angle-Resolved Phases in Photoemission: From Atomic to Molecular Systems

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Keywords: attosecond • photoionization • photoelectron angular distribution • coherent control • autoionization

Attosecond science has paved the way for studying electron dynamics in real time, from atomic to molecular systems. In particular, attosecond interferometric techniques have been used to access not only the ionization amplitudes but also the phases associated with the scattering states describing the ejected photoelectron.<sup>1</sup> Thus, opening up the prospect of steering molecular dynamics, extracting photoionization time delays and more importantly reconstruct electronic wave-packets. Currently, two methods are mainly used to retrieve the phases and amplitudes, the streaking technique which combines a single attosecond pump pulse with an infrared probe pulse and the RABBITT technique which combines a train of attosecond pulses with the infrared pulse used to generate them. Recently an alternative method for measuring the phases in photoemission has been put forward.<sup>2,3</sup> This method combines two phase locked extreme ultraviolet pulses of frequency  $\omega$  and  $2\omega$ , from a free electron laser. By varying the relative optical-phase between the two pulses the phase difference between the two ionization channels can be measured. In the present work, we apply this technique to theoretically obtain the phase difference, as a function of the electron emission angle, between the two ionization channels. First, we consider atomic systems such as Argon over a large range of frequencies, paying special attention where one or both of the two-colors ( $\omega$  or  $2\omega$ ) is in resonance with a bound electronic state or with an autoionizing Rydberg state. Second, in a molecular system, we investigate the role played by the nuclear degrees of freedom in such interferences. As in the atomic case, we consider the region where the frequencies are in resonance with a vibrationally bound intermediate state.<sup>4</sup>

<sup>1</sup> L. Cattaneo *et al.*, *Nat. Physics*, **2018**, *14*, 733.

<sup>2</sup> D. You *et al.*, *Phys. Rev. X*, **2020**, *10*, 031070.

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## Exploring Carvacrol interactions by laser spectroscopy in jets

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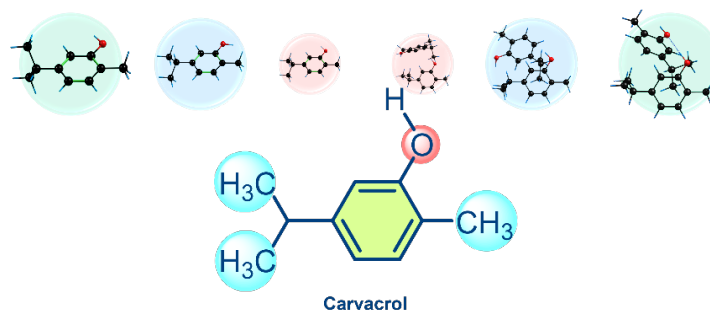
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Keywords: conformational study • alcohols • laser spectroscopy • gas phase • non-covalent interactions

Carvacrol is a phenol monoterpene that represents one of the major phytochemicals of essential oils extracted from numerous aromatic plants and has been reported to display a wide array of biological activities such as antioxidant, analgesic, anti-inflammatory, anticarcinogenic and antibiotic.<sup>1</sup> Due to the pharmacological importance of carvacrol, several biological studies have been carried out. However, regarding to conformational structure of this compound there are only few reports using microwave spectroscopy<sup>2</sup> and cryogenic argon matrices.<sup>3</sup> In this context, the mass-resolved laser spectroscopy in combination with computational methods, represent an efficient technique to determine the molecular conformation and non-covalent interactions in molecular aggregates.

In this work, we study the conformational landscape of carvacrol and its aggregates (Figure 1), using mass-resolved excitation spectroscopy and quantum chemical calculations. Experimental setup consists of a pulsed valve that injects the sample into a high-vacuum chamber, forming a supersonic expansion. Molecular aggregates present in the generated beam, are excited and ionized using resonance enhanced multiphoton ionization (REMPI) and sent to a time-of-flight (TOF) mass spectrometer. REMPI technique can be combined with IR and other UV laser (double resonance techniques), to obtain more detailed structural information. Our goal is to characterize carvacrol aggregates conformations and their non-covalent interactions.



**Figure 1.** Carvacrol and its aggregates.

<sup>1</sup> M. Sharifi-Rad, E. M. Varoni, M. Iriti, M. Martorel, W. N. Setzer M. M. Contreras, B. Salehi, A. Soltani-Nejad, S. Rajabi, M. Tajbakhsh, J. Sharifi-Rad, *Phytother. Res.*, **2018**, *32*, 1675.

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<sup>3</sup> A. J. Lopes-Jesus, R. Fausto, I. Reva, *J. Phys. Chem. A*, **2021**, *125*, 8215.

## How do Hydrocarbons Affect the Electroluminescence of He-CF<sub>4</sub>?

R. J. C. Roque, R. D. P. Mano, F. D. Amaro, J. M. F. dos Santos, C. M. B. Monteiro

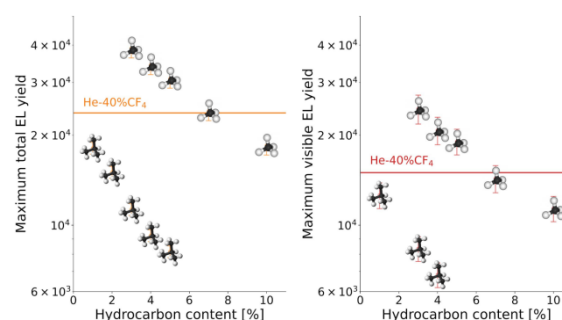
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Keywords: electroluminescence • optical gaseous detectors • gas electron multiplier

He-CF<sub>4</sub> is a very attractive gas mixture for optical tracking detectors for Dark Matter Search. Whereas He assures a low target mass (relevant for track reconstruction and low WIMP mass sensitivity), CF<sub>4</sub> is a fast and efficient scintillator in the UV and visible wavelengths, also providing sensitivity to spin-dependent WIMP-nucleon interactions. The addition of hydrocarbons to He-CF<sub>4</sub> could further improve the low WIMP mass sensitivity.<sup>1</sup> Nevertheless, hydrocarbons are known to quench the electroluminescence (EL) produced by some scintillators. Therefore, it is necessary to find the best hydrocarbon admixture to He-CF<sub>4</sub> (species and concentration); one that improves the gas tracking capabilities without compromising the optical readout.

We studied how isobutane and methane admixtures affect the EL yield of He-CF<sub>4</sub> mixtures. The detector, operated in flow-mode, was irradiated with <sup>55</sup>Fe x-rays and a Large Area Avalanche Photodiode (LAAPD) was used to readout the EL produced in the avalanches of a single Gas Electron Multiplier (GEM). Besides the total EL, the visible component of the He-CF<sub>4</sub> emission was also quantified by placing a borosilicate glass window on top of the LAAPD window to cut-off the UV photons.

Our results show that using up to 7% methane to increase the WIMP sensitivity of Dark Matter Detectors filled with He-40%CF<sub>4</sub> will also improve their optical readout.



**Figure 1.** Maximum total and visible EL yield obtained for different methane and isobutane admixtures to He-40%CF<sub>4</sub>.

### Acknowledgements

The author is supported by FCT PhD studentship (ref. SFRH/BD/143355/2019).

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## Computational Study of Ion Conduction through Eukaryotic Ion Channels by Molecular Dynamics

Nuria Anguita-Ortiz,<sup>1</sup> Juan J. Nogueira<sup>1,2</sup>

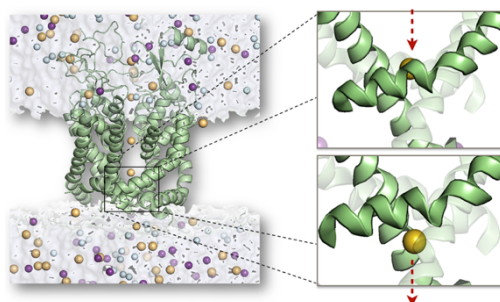
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Keywords: molecular dynamics • ion channel • ion conduction

Among transmembrane proteins, voltage-gated ion channels are those that produce electrical signals in excitable cells in order to regulate various biological processes, such as signal transduction or muscle contraction.<sup>1,2,3</sup> They open in response to the change in the transmembrane electrical potential, allowing the ions to pass through and cross the membrane.<sup>2</sup> Thus, it is essential to study the mechanism of permeability and selectivity of ion channels for understanding the function of cells and for the discovery of new drugs targeted to these membrane proteins.

In this project, the conduction mechanism of eukaryotic voltage-gated sodium channels, which is still under discussion, is investigated using conventional and electric-field biased classical molecular dynamics simulations, the last approach aimed to increase the number of permeation events. The key factors involved in the ion conduction events, such as ion desolvation at the pore entrance, the presence of an electric field, and interactions between ions and the selectivity filter, among others, are discussed. In addition, the ability of classical force fields to describe ion selectivity is addressed.<sup>4</sup>



**Figure 1.** Schematic of ion conduction through a eukaryotic voltage-gated sodium channel.

### Acknowledgements

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# Posters





## Unveiling the Permeation Mechanism by Using Energy Decomposition Analysis

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Keywords: EDA • QM/MM • membrane • drug • pollutant

The simulation of biological processes is a complex task which requires the combination of different quantum and classical mechanical techniques. Moreover, these hybrid calculations are often performed within a dynamic framework to account for vibrational and conformational sampling. In particular, the study of interaction energies at the quantum mechanics/molecular mechanics (QM/MM) level of theory in biological systems such as lipid membranes have demonstrated to be very important to understand the mode of action of substances (drugs or pollutants) once they are in our organism. In this contribution, the characterization of those interactions was performed by combining QM/MM calculations and energy decomposition analysis (EDA).<sup>1</sup> EDA-QM/MM provides not only the magnitude of the non-covalent interactions formed between the substances and the membrane but also the relative weight of the different contributions: electrostatic, repulsion and polarization, an information crucial to better understand the permeation mechanisms.<sup>2,3</sup>

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## Photochemistry of 2-Methylpentanal in the Troposphere

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Keywords: kinetics • gas-phase • atmosphere • pollutants

Aldehydes are very important trace gases for the physical chemistry of the troposphere mainly because they are directly emitted into the atmosphere or formed *in situ* from the photooxidation of organic compounds. Particularly, 2-methylpentanal (2MP,  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\text{H}$ ) is emitted into the troposphere from forest areas of Himalaya and from the production of food as a flavoring ingredient. During daytime, the oxidation of 2MP can be initiated by sunlight, hydroxyl radicals (OH), or chlorine atoms (Cl).

The aim of this work is, therefore, to study the atmospheric chemistry of 2MP, determining the photolysis quantum yield, the UV absorption cross sections and rate coefficients for the photolysis ( $J$ ) of 2MP in the actinic solar region ( $\lambda \geq 290$  nm) and the rate coefficients of the reaction with Cl atoms ( $k_{\text{Cl}}$ ) and OH radicals ( $k_{\text{OH}}$ ).  $k_{\text{Cl}}$  was determined at 298 K and 760 Torr of air in a smog chamber coupled to a Fourier Transform Infrared spectrometer to monitor the loss of 2MP, whereas  $k_{\text{OH}}$  was determined as a function of temperature (263-353 K) and pressure (50-600 Torr of helium) by using a pulsed laser photolysis-laser induced fluorescence system. Finally, the atmospheric implications of the 2MP reactivity will be discussed in terms of its lifetime due to the homogeneous reaction with Cl and OH, and photolysis by sunlight.

### Acknowledgements

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## Impact of $\text{CF}_3\text{CHF}_2\text{OCH}_3$ and $\text{CHF}_2\text{CHFOCF}_3$ on the Global Warming of the Atmosphere

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Keywords: greenhouse gas replacements • kinetics • global warming potential

Many efforts are currently being made to find alternatives to greenhouse gases. Particularly, hydrofluoroethers (HFEs) have been recognized as acceptable replacements, because of their relatively low global warming potential (GWP). The primary applications in which HFEs have replaced materials with higher GWPs include solvent applications such as precision cleaning and coating deposition, re-circulating chillers and secondary refrigerants.

To assess the suitability of HFEs as potential candidates for replacing high GWP species, it is essential to evaluate their expected impact on local air quality and climate change prior to their widespread use. For that purpose, we present the experimental determination of the rate coefficient for the gas-phase reaction of OH radicals ( $k_{\text{OH}}$ ) with  $\text{CF}_3\text{CHF}_2\text{OCH}_3$  (HFE-356mec3) and  $\text{CHF}_2\text{CHFOCF}_3$  (HFE-236ea1) at 298 K. To determine  $k_{\text{OH}}$  the pulsed laser photolysis-laser induced fluorescence technique was used.<sup>1,2</sup> From the kinetic results, the atmospheric lifetimes ( $\tau$ ) due to OH-reaction will be estimated to assess the permanence of these species in the atmosphere after emission and their impact on air quality. The Fourier Transform Infrared (FTIR) spectroscopy was employed to determine the IR absorption cross sections<sup>3</sup> needed to calculate the radiative efficiency (RE) of these HFEs. The estimated  $\tau$  and REs will allow to evaluate the impact of these HFEs on the global warming of our atmosphere, concluding if they are (or not) good candidates for substituting currently used high-GWP HFCs.

### Acknowledgements

Authors would like to thank the regional government of Castilla-La Mancha (CINEMOL project Ref.: SBPLY/19/180501/000052) and the University of Castilla-La Mancha (2021-GRIN-31279) for supporting this research.

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## Photodynamics of Azaindoles in the Gas Phase and Polar Media: The Influence of the Environment

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Keywords: azaindoles • photodynamics • ultrafast • relaxation • internal conversion

Azaindoles (AIs) can be considered prototype molecules to understand the deactivation channels operative, after near UV excitation, in the more complex purine DNA bases. We have tracked the relaxation dynamics of a family of AIs structural isomers, by fs pump-probe methods, in the gas phase (transient ionization) and in solvents of different polarity and chemical nature (fs-transient absorption and fluorescence up-conversion). In both environments, the observed excitation/relaxation phenomena involve two bright  $\pi\pi^*$  and a dark  $n\pi^*$  excitation. The collected experimental data, guided by theoretical calculations, evidence that the  $n\pi^*$  state functions as a gate state to access an internal conversion channel mediated by a conical intersection. The polarity of the medium tunes the energy of this  $n\pi^*$  state, modulating the behavior observed in solution. The study also permits to rationalize the distinctive radiative properties of the studied isomers in terms of their chemical structure.

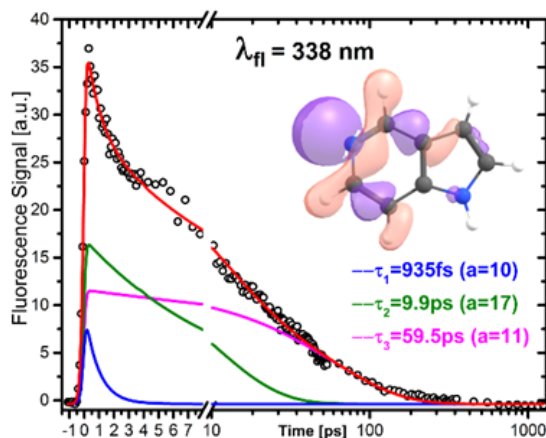


Figure 1. Fluorescence up-conversion transient of 5-AI in acetonitrile.

## Analysis of the Contribution of Ion Collisions to the Stark Profile in the $H_{\alpha}$ Line

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Keywords: Plasma spectroscopy • Stark effect • Ion contribution •  $H_{\alpha}$  line • Lorentzian functions

Laboratory plasmas can be characterized by Optical Emission Spectroscopy techniques by using Hydrogen Balmer series lines. The line shape is the result of the convolution of the several internal processes occurring in plasma, so a good plasma diagnosis is indispensable to have controlled all the plasma parameters, such as the electron density ( $n_e$ ), the electron temperature ( $T_e$ ) and the gas temperature ( $T_g$ ).

Previously, these spectroscopic lines were fitted by Voigt functions.<sup>1</sup> However, under some plasma conditions not all plasma processes leading to line broadening can be approximated accurately by a Lorentzian or a Gaussian profile. In particular, the Stark broadening contribution, resulting from the collisions of the emitter hydrogen atom with the charged particles, cannot be fitted by a single Lorentzian function.<sup>2</sup>

The main aim of this work is to obtain accurate analytical expressions for the  $H_{\alpha}$  line in the full range of plasma parameters as a sum of Lorentzian functions. This idea is based on the different features of the electric field induced by ions (low mobility) and electrons (high mobility).<sup>3</sup> Thus, the ionic electric field varies slowly with time as compared to emission processes, giving rise to “a typical Stark shift of the spectral line”. However, electrons generate “fast collisions” with the emitter H atom, leading to a broadening of the lines characterized by Lorentzian profiles. Therefore, the net effect can be described as a non-coherent superposition of Lorentzian profiles shifted by the ionic Stark effect.

### Acknowledgements

This work has been partially supported by the funds FEDER under contract 1380869-F.

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## Influence of the Geometrical Arrangement in the Donor-Acceptor Gap of Organic Photovoltaics

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Keywords: renewable energy • organic solar cells • HOMO-LUMO gap • DFT calculations

The need to find easily renewable and environmentally friendly energy sources is nowadays a global quest and solution-processed organic solar cells have attracted attention.<sup>1</sup> They are formed by mixed donor and acceptor molecules, and one of the most important parameters to study is the difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, which is commonly known as the HOMO-LUMO band gap, or simply, gap. In this work, the polymer 4mod-BT<sup>2</sup> has been considered as donor, while the 4TIC molecule<sup>3</sup> has been selected as acceptor. We have explored their gas-phase packing problem through an *ab initio* random structure search,<sup>4</sup> in which each single calculation has been performed within the DFT framework implemented in the SIESTA code.<sup>5</sup>

The conclusion we arrive to is that the gap varies within 0.3 eV, which is a significant value considering that gaps in this context are not much larger than 1 eV. Moreover, the gap is not found to correlate with the binding energy of the pair (for details, see Ref. 6).

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## Computational Quantum Chemistry Approaches in CO<sub>2</sub> Clathrate-Hydrates: from Finite-size Molecular Clusters to Extended Lattice Systems

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Keywords: CO<sub>2</sub> clathrate hydrates • CO<sub>2</sub> storage • DFT calculations • guest-host interactions

Clathrate hydrates are crystalline compounds formed by guest molecules within a three-dimensional host lattice of water cages. These structures have been involved in current technological and industrial applications. Specifically, the CO<sub>2</sub> clathrate has been proposed as a potential molecular material in the fight against environmental problems related to greenhouse gases capture and storage.<sup>1</sup>

The objective of this work is to understand of formation, energetics and structural stability of sI, sII and sH clathrate hydrates to describe the underlying processes at molecular level and determine the guest-host/host-host interactions dominated by hydrogen bonds and van der Waals forces. In particular, we consider two approaches: bottom-up and top-down. The first approach proposes to study the intermolecular interactions in finite-size systems of individual aperiodic cages, such as guest-free and guest-host CO<sub>2</sub> clathrates, and then extrapolate to their entire periodic unit cells. The second approach considers the unit cell that reproduces a periodic crystalline structure, and thus, guest-lattice effects are studied by a systematic evaluation of different density functionals. We consider functionals, including local and non-local dispersion corrections such as the exchange-hole dipole moment (XDM) and the semi-empirical model (DFT-D), as well as vdW-DF and vdW-DF2, respectively.

Our findings show that DFT-D approaches are able to describe properly the underlying interactions, once dispersion corrections are applied.<sup>2</sup> Further, the results obtained allow to generate reference interaction energies from accurate quantum-mechanical calculations by testing different approaches on CO<sub>2</sub>@sI/sII/sH systems. Such studies provide high-quality information with new insights that allow the construction of new reliable data-driven models and in turn have greater control of the properties of this promising material.<sup>3</sup>

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<sup>3</sup> J. Behler, *J. Chem. Phys.*, **2016**, 145. T. Mueller *et al.*, *J. Chem. Phys.*, **2020**, 152.

## Rovibrational Dynamics of a Diatomic Molecule in an Optical Centrifuge Molecule

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Keywords: rotational dynamics • vibrational dynamics • centrifuge pulse • transference to continuum • laser intensity

We present a theoretical study of the rotational and vibrational dynamics of a diatomic molecule in the electric field produced by an optical centrifuge. The time-dependent Schrödinger equation is solved by including a time profile of the optical centrifuge similar to the experimental laser pulse used by the experimental group of V. Milner.<sup>1</sup> Taking as prototype the Rb<sub>2</sub> molecule, we investigate the field-dressed dynamics of rovibrational states within the electronic state a<sup>3</sup>Σ considering peak intensities of the order of 10<sup>11</sup> W/cm<sup>2</sup>.

After the laser pulse, a significant population from the initial wave packet is transferred to other vibrational bands, which indicates that the rigid rotor approximation is no longer valid for this laser field regime. Moreover, in some cases, there is a large fraction of population going into the continuum, which might be greater than 30%, indicating the dissociation of the molecule. By decreasing the laser intensity, transitions to other vibrational states as well as to the continuum are reduced. We find a rather small population transferred (0.02%) to the continuum with  $I_0 \leq 1 \cdot 10^9$  W/cm<sup>2</sup>,  $\beta = 0.3$  fs<sup>-2</sup> and the initial states  $v_0 = 30$ ,  $J_0 = 0$  and  $v_0 = 35$ ,  $J_0 = 0$ .

These results are compared with those obtained from a laser pulse having the same turning-on and turning-off profiles, but constant intensity between them. For this pulse, a similar set of vibrational bands, but with a different weight, are populated. However, the population transferred into continuum is even larger for the same peak intensity. This can be explained in terms of the energy absorbed by the molecule, which is larger than with the centrifuge pulse.

<sup>1</sup> A. Korobenko, A. A. Milner, V. Milner, *Phys. Rev. Lett.*, **2014**, *112*, 113004.

## Rotational Spectroscopy of an Imine-Based Molecular Switch

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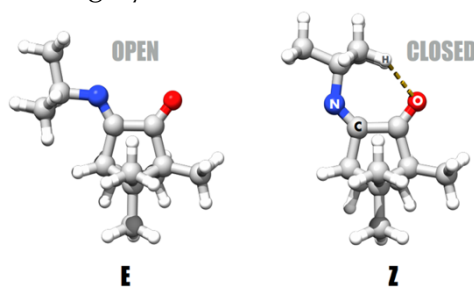
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Keywords: rotational spectroscopy • structure determination • molecular clusters

Imine-based molecular switches have been recently developed, but many of their properties remain largely unexplored.<sup>1</sup> The potential of these to perform multi-step unidirectional rotations make them an important addition to the existing nanomotor toolbox.<sup>2</sup> The photochemically-induced switching processes have possible applications in the regulation of chemical reactions, as well as performing mechanical functions. Microwave rotational spectroscopy allows us to study the 3D structure of these molecules with great precision since we can relate the pattern of rotational frequencies to the structure through the moments of inertia.<sup>3</sup> The various conformers of these switches generally have different energies, and when in equilibrium, they coexist with a given distribution. However, in solution the interactions with the solvent molecules can alter the energetic balance of these conformers.<sup>4</sup> In this contribution, we present rotational spectra of an imine-based molecular switch, prepared using supersonic molecular jets. Our analysis uncovered the structures of two monomeric entities, the *E* (open) and *Z* (closed) conformers, and of several other micro-solvated species. We used quantum chemistry calculations to interpret the change in stability of each species in isolated and solvated environments. We will discuss the suitability of rotational spectroscopy to engage in structural studies of highly functional micro-solvated molecular systems.



**Figure 1.** The two conformers of the camphorquinone imine studied in this contribution.

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## Electronic Structure of the Off-Center Helium Atom in a Multi-Layer Spherical Quantum Dot

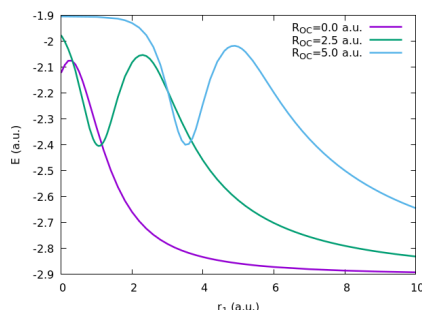
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Keywords: electronic structure • confinement • quantum dot

Modern technology advancements have allowed the production of quantum nano-crystals with unique optic magnetic and electronic properties, such as quantum dots (QDs), which present interesting technological applications.<sup>1,2</sup> Recently, it has been possible the fabrication of multilayer QDs (MLQDs), which has motivated many theoretical works focused on this topic.<sup>3,4</sup> Most of these works analyze a hydrogenic impurity located at the center of the MLQD, but a more detailed study considering other positions of the impurity inside the structure or more complex atoms are in order. In this work we address the problem of an off-center Helium atom in a multi-layer spherical quantum dot. The MLQD is defined as a core/shell/well/shell structure modelled by a parabolic confinement.<sup>4</sup> In Figure 1 we plot the ground state energy of He as a function of the radius of the spherical core of the MLQD,  $r_1$ , for different distances,  $R_{OC}$ , from the center of the structure to the atomic nucleus. The energy presents a series of minima and maxima as a function of the core radius which depend on the position of the atom: the energy is minimum when the nucleus is inside the well, while the maxima are reached when the atom is in one of the shells. The absolute maximum is found for  $R_{OC} = 5.0$  a.u. and  $r_1 = 0.0$ , i.e., there is not a core and the nucleus and the electronic cloud lie in the second shell. Furthermore, it is seen that an on-center atom configuration does not present a minimum in the energy for all the  $r_1$  values, indicating that the off-center atom will provide the most stable configuration depending on the MLQD parameters.



**Figure 1.** Ground state energy of the He atom inside a multi-layer quantum.

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## Studies of Primary and Secondary Scintillation Yield in Krypton

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Keywords: gaseous detectors • X-ray detectors • secondary scintillation • primary scintillation • krypton scintillation

The krypton electroluminescence yield was studied, at room temperature, as a function of the electric field in the gas scintillation gap. A large area avalanche photodiode has been used to allow the simultaneous detection of the electroluminescence pulses as well as the direct interaction of X-rays, the latter being used as a reference for the calculation of the number of charge carriers produced by the electroluminescence pulses and, thus, the determination of the number of photons impinging the photodiode. An amplification parameter of 113 photons per kV per drifting electron and a scintillation threshold of 2.7 Td ( $0.7 \text{ kV cm}^{-1} \text{ bar}^{-1}$  at 293 K) was obtained, in good agreement with the simulation data reported in the literature. On the other hand, the ionisation threshold in krypton was found to be around 13.5 Td ( $3.4 \text{ kV cm}^{-1} \text{ bar}^{-1}$ ), less than what had been obtained by the most recent simulation work-package. The krypton amplification parameter is about 80% and 140% of those measured for xenon and argon, respectively. The electroluminescence yield in krypton is of great importance for modeling krypton-based double-phase or high-pressure gas detectors, which may be used in future rare event detection experiments. Preliminary results for the primary scintillation yield in gaseous krypton will also be presented.

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## Laboratory Rotational Spectroscopy and Astronomical Search of Ethynyl-Substituted Naphthalene

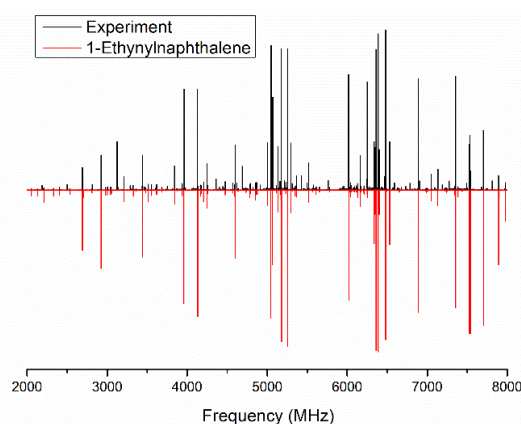
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Keywords: astrochemistry • polycyclic aromatic hydrocarbons • structural determination • computational chemistry • ISM

Polycyclic aromatic hydrocarbons (PAHs) constitute one of the most abundant forms of interstellar carbon in the universe. They are proposed as carriers of the infrared emission features that dominate the spectra of most galactic and extragalactic sources. However, the formation processes of these species have been poorly understood due to the inability to detect individual PAH molecules. The recent interstellar detections of the first pure PAH indene<sup>1</sup> and the two isomers of the PAH cyanonaphthalene<sup>2</sup> bring interest in related molecular species that could be present in similar astronomical environments. In this context, 1- and 2-ethynyl-naphthalene are promising candidates to be observed in the Taurus molecular cloud (TMC-1), where 1- and 2-cyanonaphthalene have been detected. To enable the interstellar search of these species, their pure rotational spectra need to be investigated in the laboratory. We report the rotational spectra of 1- and 2-ethynyl-naphthalene using a broadband Fourier-transform microwave spectrometer in the 2-8 GHz frequency range (Figure 1). The experimental investigation has been supported by quantum chemical calculations. Accurate spectroscopic parameters have been derived from the analysis of the experimental spectra, allowing for reliable predictions for astronomical searches. Our searches in TMC-1 for both isomers provide upper limits for the abundances of these species.



**Figure 1.** Rotational spectrum of 1-ethynyl-naphthalene.

<sup>1</sup> J. Cernicharo, M. Agúndez, C. Cabezas, *et al.*, *A&A*, **2021**, 649, L15; A. M. Burkhardt, L. K. Lee, P. B. Changala *et al.*, *Apl*, **2021**, 913, L18.

<sup>2</sup> B. A. McGuire, R. A. Loomis, A. M. Burkhardt *et al.*, *Science*, **2021**, 371, 1265.

## Non-covalent Interactions in the Alcohol-Thiol Heterodimer Formed Between 2-Phenylethanethiol and 2-Phenylethanol Using Microwave Spectroscopy

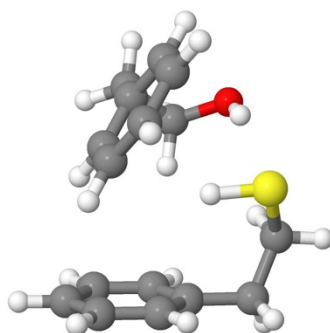
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Keywords: molecular recognition • non-covalent interactions • hydrogen bonding • rotational spectroscopy

Non-covalent interactions between molecules containing thiol (—SH) or alcohol (—OH) groups play an important role in organic and organometallic synthesis, protein structure and supramolecular Chemistry. Previous investigations in the gas phase have included rotational or vibrational spectroscopy of thiol<sup>1</sup> or alcohol<sup>2</sup> homodimers. However, the observations of mixed heterodimers involving —SH and —OH groups are rare. In this work, we used rotational spectroscopy to detect the non-covalent interactions in the heterodimer formed between 2-phenylethanethiol and 2-phenylethanol (2PET-2PEA). Only one isomer was observed for the heterodimer (Figure 1), with a primary O-H...S hydrogen bond and a cooperative S-H... $\pi$  interaction. The observed structure is similar to the dimers of 2-phenylethanethiol or 2-phenylethanol.<sup>3</sup> During the conference supporting experimental and computational results on this problem will be offered.



**Figure 1.** The structure of the observed heterodimer of 2PET-2PEA.

<sup>1</sup> a) R. T. Saragi *et al.*, *J. Phys. Chem. Lett.* **2021**, *12*, 1367. b) R. T. Saragi *et al.*, *Symmetry* **2021**, *13*, 2022.

<sup>2</sup> a) M. Juanes *et al.*, *Phys. Chem. Chem. Phys.*, **2022**, *24*, 8999. b) M. Juanes *et al.*, *Molecules*, **2022**, *27*, 2584

<sup>3</sup> A. Camiruaga, R. T. Saragi *et al.*, *submitted*, **2022**.

## The Hydration of Polycyclic Aromatic Compounds: The Case of $\alpha$ -Naphthaldehyde

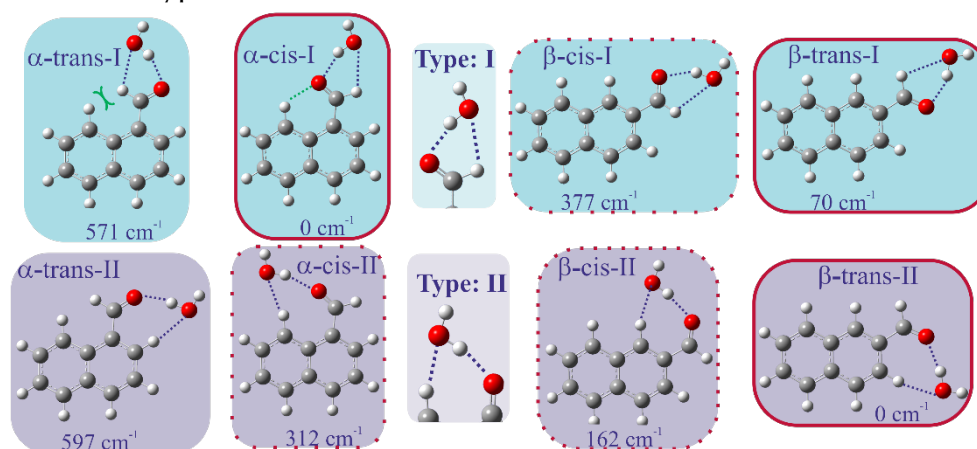
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Keywords: polycyclic aromatic hydrocarbons • structural determination • computational chemistry • atmospheric pollutants

Polycyclic aromatic hydrocarbons (PAHs) and their oxygenated products (oxi-PAH) are considered as important pollutants of the Earth's atmosphere since they are emitted by the combustion of fuels.<sup>1</sup> The study of their intermolecular interactions is essential to understand the formation of their aerosols. In this work, we have studied at molecular level the interactions present in the hydration of the oxi-PAH  $\alpha$ -naphthaldehyde. This study has been performed using a supersonic-jet Fourier transform microwave (FTMW) spectrometer in the 4-15 GHz range, with the support of theoretical calculations. The isolated  $\alpha$ - and  $\beta$ -naphthaldehyde species could present two possible structures: *cis*, the most stable one, and *trans*.<sup>2</sup> Our calculations show that there are three low energy monohydrates predicted for each conformer, *cis/trans*, in a range of 1500  $\text{cm}^{-1}$ . Experimentally, one conformer has been observed in gas phase for  $\alpha$  and two for  $\beta$ , corresponding to the calculated most stable structures. All species are stabilized by intermolecular hydrogen bonds between the water molecule and the aldehyde group of naphthaldehyde. For the  $\alpha$  isomer, the oxygen of the aldehyde acts as proton acceptor and the aldehyde hydrogen as proton donor (type I, see Figure 1); for the most stable  $\beta$  isomer, the oxygen of the aldehyde acts as proton acceptor and one of the ring hydrogens as a proton donor (type II).



**Figure 1.** Most stable structures of  $\alpha$ - and  $\beta$ -naphthaldehyde. The observed species are marked in red.

<sup>1</sup> G. Karavalakis *et al.*, *Sci. Tot. Environ.*, **2011**, 409, 738.

<sup>2</sup> M. Goubet *et al.*, *J. Phys. Chem. A*, **2020**, 124, 4484.

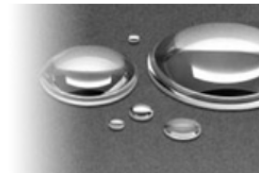


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