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Book of Abstracts

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Oral communications / 4**Photodeactivation mechanisms of graphene quantum dots****Author:** Sandra Gómez Rodríguez¹**Co-authors:** Alberto Martín Santa Daría ¹; Lola González-Sánchez ¹; Pablo G. Jambrina ¹¹ *Universidad de Salamanca***Corresponding Author:** sandra.gomez@usal.es

Graphene quantum dots (GQD) are nanoparticles consisting of a single or several layers of graphene sheets whose thickness does not exceed 100 nanometers. For their ease of preparation, biocompatibility and tunable absorption and emission properties, they have become extremely popular in optoelectronics, as nanocarriers for cancer therapy drugs and in bioimaging techniques.[1]

In this work, we focus on coronene, the smallest unit of a graphene nanoflake and a zero-dimensional quantum dot. Several studies have found that coronene shows fluorescence and phosphorescence in the visible range of the light spectrum.[2] As a starting point, we unravel the excited state deactivation pathways of a single unit of coronene using the ML-MCTDH method [3] and a vibronic coupling model for the nuclear Hamiltonian, including both singlet and triplet states.

Future work will look at expanding the system size, adding further layers and pondering the effect of functionalization to explain the strong emission found by our experimental collaborators in doped carbon nanoparticles. [4]

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Oral communications / 5**Charged nanosilicate Clusters and their Interaction with Oxygen: Astronomical Relevance****Author:** Joan Mariñoso Guiu¹**Co-authors:** Bianca-Andreea Ghejan ²; Joost Bakker ³; Sandra Lang ²; Stefan Bromley ⁴; Thorsten Bernhardt ²¹ *Universitat de Barcelona*² *Ulm University*³ *Radboud University*⁴ *Universitat de Barcelona and Institució Catalana de Recerca i Estudis Avançats (ICREA),***Corresponding Author:** joanmarinoso@ub.edu

Silicates are ubiquitously found as small dust grains in the interstellar medium, where they are processed due to high-energy processes, such as UV radiation absorption. These abundant nanosilicates are likely to play an important role in astrochemistry. In this work, we form small magnesium silicate clusters via laser vaporization of a binary Mg₂Si target in the presence of diluted molecular oxygen. The formed species are characterized via a combination of infrared multiple-photon dissociation spectroscopy (IR-MPD) and DFT calculations. Analysis of the spectra of MgSiO₉⁺ and Mg₂SiO₉⁺ reveal the preferred formation of a pyroxene monomer MgSiO₃⁺ decorated with two non-activated oxygen molecules. The remaining oxygen atoms bind to Mg₂SiO₉⁺ as a superoxide-like species,

but they form an ozone-like O₃ unit on MgSiO₉⁺. Due to the potentially high abundance of pyroxene monomers in the diffuse interstellar space, these findings could have important implications for the role of small silicates in explaining the missing oxygen in the diffuse ISM. Furthermore, in the Mg₂SiO₉⁺ cluster the second Mg atom is found to bind to the MgSiO₃ monomer core, which can be considered as the simplest initial step in silicate grain growth and thus indicates that small ionized pyroxenic clusters could assist in the initial stages of silicate dust re-birth in the ISM.

Poster Session / 6

Simulating interstellar temperatures in the laboratory to study the gas-phase OH+NH₂CHO reaction

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The kinetic study of neutral-neutral reactions in the gas phase at ultralow temperatures is undergoing a huge advancement over the last decades [1]. Such studies have exponentially increased due to the increasing number of new molecules detected in the interstellar medium (ISM), specially in the coldest regions (10-100 K). To model the chemistry occurring in these extreme environments, the formation and destruction routes for IS molecules have to be characterized by means of the rate coefficient, $k(T)$, a crucial parameter to be included in astrochemical networks. For most neutral-neutral reactions, $k(T)$ is usually extrapolated down to 10 K from kinetic data reported at high temperatures (>200-300 K). However, this procedure usually fails and $k(10\text{ K})$ is underestimated by several orders of magnitude, which obviously comes up with dramatic consequences in IS chemical modelling. For that reason, mimicking interstellar conditions in the laboratory and measuring accurate $k(T)$ are essential. First, a suitable technique, such as the so-called CRESU (French acronym for Reaction Kinetics in a Uniform Supersonic Flow) is used to achieve the very low temperatures of the ISM to determine $k(T)$ as a function of T [2]. In this work, a pulsed CRESU system has been employed to study the temperature dependence of $k(T)$ between 11.7 and 177.5 K for the reaction of formamide (NH₂CHO) with hydroxyl (OH) radicals, key intermediates in IS chemical processes. It is thought that NH₂CHO, which was first detected towards Sagittarius B molecular cloud [3], can play a crucial role in the formation of prebiotic molecules in space. The available experimental $k(T)$ for the titled reaction is scarce and only reported around 300 K [4,5]. However, theoretical calculations predict an increase of $k(T)$ when temperature decreases in the 200-350 K range [5]. Our kinetic study in the low-temperature range confirms that below 200 K, $k(T)$ increases when temperature is lower, with an increase of $k(T)$ in the whole temperature range with respect to $k(300\text{ K})$. The observed T-dependence of $k(T)$ will be discussed and an expression for its use in pure- and gas-grain astrochemical models will be provided.

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Poster Session / 7

Atmospheric impact of hydrofluoroethers (HFEs) at a global scale:

Can HFEs contribute to the global warming?

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Global concern about the high environmental impact of hydrofluorocarbons (HFCs) led the Kyoto Protocol to list these compounds as potent greenhouse gases. For that reason, hydrofluoroethers (HFEs) were proposed for substitution of HFCs in several applications, such as refrigerants, because of their relatively low global warming potential (GWP). Therefore, it is important to evaluate the impact of future HFE emissions on climate change prior to their widespread use. For that purpose, the most crucial physicochemical parameters to be determined are the rate coefficient for the gas-phase reaction with OH radicals ($k_{OH}(T)$), the main atmospheric diurnal oxidant, and the infrared (IR) absorption cross sections in the atmospheric window (1250-720 cm^{-1}), σ_ν .

In the present work, we present the first experimental determination of $k_{OH}(T)$ between 263 and 353 K for $CF_3CHFCF_2OCH_3$ (HFE-356mec3) and $CHF_2CHFOCF_3$ (HFE-236ea1). The pulsed laser photolysis/laser induced fluorescence technique was employed to generate OH radicals and to monitor their temporal profile.[1] A positive T-dependence of $k_{OH}(T)$ was observed in both reactions and it is well-described by following Arrhenius expressions:

$$\text{HFE-356mec3: } k_{OH}(T) = (1.18 \pm 1.07) \times 10^{-12} \exp[-(1046 \pm 27)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$\text{HFE-236ea1: } k_{OH}(T) = (7.76 \pm 4.26) \times 10^{-13} \exp[-(1417 \pm 28)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

According to the observed T-dependence of $k_{OH}(T)$, the OH-reactivity towards these HFEs decreases throughout the troposphere since T decreases with altitude. Based on the obtained kinetic results, the atmospheric lifetime of HFE-356mec3 and HFE-236ea1 due to OH-reaction (π_{OH}) was estimated to be 1.2 and 5.5 years, respectively, at sea level (T is considered 298 K). In addition, to evaluate the impact of the emission of 1 kg of the investigated HFEs, σ_ν were determined between 4000-500 cm^{-1} , allowing the calculation of the radiative efficiencies (REs) corrected with π_{OH} [2] and the GWP relative to CO_2 at a time horizon of 100 years. REs were 0.26 and 0.39 $W \text{ m}^{-2} \text{ ppbv}^{-1}$ and the resulting GWP at a time horizon of 100 years were 118 and 885 for HFE-356mec3 and HFE-236ea1, respectively. In conclusion, the contribution of HFE-356mec3 and HFE-236ea1 to global warming of Earth could still be significant if their emissions to the atmosphere increase. Despite this fact, HFCs with similar structures ($CH_3CF_2CH_2CF_3$, CHF_2CHFCF_3 , or $CH_2FCF_2CF_3$), contribute to the global warming of Earth in much larger extent than the investigated HFEs, presenting GWP between 804 and 8060 [2].

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Plenary Talks / 8

Recent developments of the Geant4-DNA extension of the Geant4 Monte Carlo simulation toolkit

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Modeling accurately biological damage induced by ionizing radiation at the scale of the DNA molecule remains a major challenge of today's radiobiology research (1). In order to provide the community

with an easily accessible mechanistic simulation platform, the general purpose and open source “Geant4” Monte Carlo simulation toolkit (2) is being extended in the framework of the “Geant4-DNA” project (3-7) with a set of functionalities allowing the detailed simulation of particle-matter interactions in biological medium. These functionalities include physical, physico-chemical and chemical processes that can be combined with nanometer size geometries of biological targets in order to predict early DNA damage. We will present an overview of the Geant4-DNA project and discuss on-going developments.

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Plenary Talks / 9

Ultrafast dynamics in microsolvated biomolecules

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Interactions between proteins and their solvent environment can be studied in a bottom-up approach using hydrogen-bonded biomolecule-solvent clusters. The ultrafast dynamics following UV-light-induced electronic excitation of the biomolecular chromophores, potential radiation-damage, and their dependence on solvation are important open questions. Specific and precise studies of the microsolvation effect are challenging due to the inherent mix of the produced gas-phase aggregates. We used the electric deflector to spatially separate different molecular species in combination with pump-probe velocity-map-imaging experiments, including applications of 3D “cameras” based on Timepix3. We demonstrated that this powerful experimental approach reveals intimate details, e.g., on the radiation damage of water-water and pyrrolewater dimers as well as on the UV-induced dynamics in the near-UV-absorbing prototypical biomolecular indole-water system.

We determined the time-dependent appearance of the different reaction products and disentangled the occurring ultrafast processes. This novel approach ensures that the reactants are well-known and that detailed characteristics of the specific reaction products are accessible –paving the way for the complete chemical-reactivity experiment.

1. <https://www.controlled-molecule-imaging.org/>

Poster Session / 10

Extreme-ultra-violet emission of W ions with open 4f-shell

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The plasma divertor for the International Termonuclear Experimental Reactor (ITER) will have target plates made out of tungsten (W) [1]. The inevitable W contamination will emit characteristic radiation that depends on the specific charge state balance, electron temperature and density conditions. Therefore, the respective emission spectra can be used as real-time diagnostics of the fusion reactor plasma physical conditions [1, 2]. Given the importance of the spectra of this elements, both its low and highly charged ions have already been extensively studied in the past in a wide range of the electromagnetic spectrum [2-5]. However, the emission of the open 4f-shell charges states, between 12+ and 28+, still remains largely understudied, as the emissions of this group of ions is usually observed mixed with each other. In our work, an Electron Beam Ion Trap (EBIT) was used to produce and individually observe the EUV spectrum (12-26 nm) of each of the charge states in the open 4f-shell complex. A slow electron beam energy scan between 300 and 1000 eV allowed us to observe the emissions for every individual charge state. The excellent resolution allows to retrieve each charge state contribution with the Non Negative Matrix Factorization (NNMF) method. The decomposed data was matched with the respective theoretical wavelengths of the Unresolved Transition Arrays (UTA) calculated with Flexible Atomic Code (FAC) [6]. In this regime, we observed the O-O transitions derived from N-O collisional excitations. This data is of great importance, as it can be incorporated in diagnostic models relevant for fusion plasma monitoring.

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Oral communications / 11

Proton diffusion in a benchmark entangled hydrogen bonding network

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Hydrogen-bonded networks sustain a broad range of structural and charge transfer processes in supramolecular materials. The modelling of the proton dynamics in these systems is challenging and demands insights into prototypical benchmark complexes. Intramolecular H-bonding in

3-hydroxyglutaric acid (M) provides an intriguing case study of entangled proton dynamics. We combine infrared action ion spectroscopy experiments with Born-Oppenheimer Molecular Dynamics computational modeling to expose and rationalize the vibrational signatures of intramolecular Grothuss-like proton diffusion triggered upon either the protonation or the deprotonation of M. Despite the formally similar symmetry of the $M\cdot H^+$ and $[M-H]^-$ frameworks, the relative proton affinities of the oxygen centers of the carboxylic and carboxylate groups with respect to that of the central carbohydroxy group lead to differentiated proton dynamics in the two systems. In $M\cdot H^+$, an arrangement of the type $HOCO\cdot HOH\cdot OCOH$ is preferred, with the two protons binding tighter to the central oxygen atom and forming two slightly asymmetric H-bonds. In $[M-H]^-$, the asymmetric $OCO\cdot HO\cdot HOCO$ configuration is most stable, with a stronger H-bonding on the bare carboxylate end. Both systems display nevertheless active backbone and concerted proton sharing dynamics, leading to distinct diffuse band structures in their vibrational spectrum.

Invited talks / 12

Laser excitation of the ground-hyperfine transition in muonic hydrogen

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The CREMA collaboration is pursuing a measurement of the ground-state hyperfine splitting (HFS) in muonic hydrogen (μp) with 1 ppm accuracy by means of pulsed laser spectroscopy to determine the two-photon-exchange contribution with 2×10^{-4} relative accuracy. In the proposed experiment, the μp atom undergoes a laser excitation from the singlet hyperfine state to the triplet hyperfine state, then is quenched back to the singlet state by an inelastic collision with a H_2 molecule. The resulting increase of kinetic energy after the collisional deexcitation is used as a signature of a successful laser transition between hyperfine states. We calculate the combined probability that a μp atom initially in the singlet hyperfine state undergoes a laser excitation to the triplet state followed by a collisional-induced deexcitation back to the singlet state. This combined probability has been computed using the optical Bloch equations including the inelastic and elastic collisions. Omitting the decoherence effects caused by the laser bandwidth and collisions would overestimate the transition probability by more than a factor of two in the experimental conditions. Moreover, we also account for Doppler effects and provide the matrix element, the saturation fluence, the elastic and inelastic collision rates for the singlet and triplet states, and the resonance linewidth. This calculation thus quantifies one of the key unknowns of the HFS experiment, leading to a precise definition of the requirements for the laser system and to an optimization of the hydrogen gas target where μp is formed and the laser spectroscopy will occur.

Poster Session / 13

Gas-phase reaction of 2-methyl-2-pentenal with Cl atoms: kinetic and product study

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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. In particular, the unsaturated aldehyde trans-2-methyl-2-pentenal (T2M2P) is emitted into the low atmosphere from several sources such as wildland fires, vegetation, and from some foods. Once in the troposphere, T2M2P can be degraded through gas-phase reactions initiated by diurnal oxidants such as hydroxyl radicals (OH) or chlorine atoms (Cl), important globally or

locally in marine atmospheres, respectively. Therefore, it is important to understand these reactions kinetically and to identify the products that are formed. The rate coefficient for the OH-reaction of T2M2P (k_{OH}) has been previously estimated [1], but neither kinetic measurements of the Cl-reaction nor detection of the reaction products have been reported in the literature up to date. Then, the aim of this work is, first, to evaluate the gas-phase reactivity of Cl atoms towards T2M2P at 298 K and 1 atm, by determining the rate coefficient (k_{Cl}) has been determined by the relative method in a smog chamber coupled to a Fourier Transform Infrared spectrometer to monitor the loss of T2M2P and a reference compound [2]. Secondly, the chemical characterization and quantification of the gas-phase reaction products have been performed in a smog chamber coupled to a Proton Transfer Reaction –Time of Flight –Mass Spectrometer [3] and a Fast Mobility Particle Sizer spectrometer has been used to monitor the formation of Secondary Organic Aerosols (SOAs) and to determine the SOA yield in the Cl+T2M2P reaction [4].

Finally, the atmospheric implications of the T2M2P reactivity will be discussed in terms of its lifetime due to the homogeneous reaction with Cl estimated from the determined k_{Cl} and the literature k_{OH} and in terms of the potential impact of the products generated on our health.

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Poster Session / 14

First-principles computations on guest-host (lattice) systems: He inclusion in hydrates

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He hydrates present an intriguing and relatively unexplored systems. As they may have significant implications in fields such as planetary science, exploration of novel ice phases, such as ultra-low density ices or superionic water ice, and the development of innovative materials with distinct properties and applications, such as solid electrolyte in batteries, understanding their fundamental properties is crucial for their future exploitation.

Computational investigations on the He@hydrates were motivated by the recent experimental synthesis of He@sII [1], and in relation with the emerging research on new low-density ice polymorphs [2]. We performed quantum chemistry computations considering both aperiodic ice/clathrate-like finite-size structures <https://doi.org/10.1039/D1CP04935F> [3,4] and periodic 3D crystal frameworks [5]. In this way, we demonstrated the importance of conducting a systematic benchmark study of conventional and modern DFT-D approaches, including fundamental units (e.g. He-H₂O) and building block clathrate cages (e.g. 5¹² or 5¹²6⁴) or ice channels present in the most common sI, sII and sH clathrate hydrates or ice II and Ih. In turn, we analysed the stability of the cages forming the He@sII clathrate, considering single and multi-occupancy [6], through thermochemical calculations at a range of T-P conditions comparable to the experiment [1]. Finally, we explored the effects on the encapsulation of He atoms in the sI/sII crystal lattices by computing structural, mechanical and energetic properties in both empty and He-filled systems. For a more direct comparison with measurements on He@sII structural properties, multiple cage occupancy, similar to those established by diffraction experiments [1], is considered [7]. All these insights serve to better understand the role of the entire guest-guest, guest-host and host-host interactions in the stabilization of such clathrate hydrates, they address accuracy issues on weakly-bound systems, providing valuable reference data that can be utilized for developing future predictive data-driven models using either traditional fitting or emergent machine-learning techniques.

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Oral communications / 15

The cationic lithium dimer solvated in He clusters: Molecular Dynamics Simulations.

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The structures and energetics of Li+2-doped He clusters have been determined by means of evolutionary programming optimizations and classical molecular dynamics simulations 1. The underlying interactions in the HeN Li+2 complexes are described by sum-of-potentials ab initio-based models 2. The classical picture of the He atoms surrounding the cationic dimer shows a selective growth of the clusters. Figure below shows a contour plot of the probability distribution in the (z, ρ)-plane (right panel) and classical thermal conformer (left panel) for the N=30 cluster at T=2 K. The z axis is along the cationic dimer. Using the Feynman-Hibbs second order approach 3, quantum results are also presented and discussed.

Oral communications / 16

Ultralong-range Cs-RbCs Rydberg molecule: non-adiabaticity of dipole moments

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Triatomic ultra-long Rydberg molecules are formed by the interaction of a Rydberg atom, an excited atom with an electron with high principal quantum number, and a polar molecule. The study of Rydberg molecules is motivated by its interesting properties [1-3], and possible applications in ultracold chemical reactions 4 or quantum simulations 5. In this work, we investigate the electronic structure and properties of the Rydberg molecule Cs-RbCs.

A complete study of the adiabatic electronic potentials has been performed. The rovibrational structure is described beyond the Born-Oppenheimer approximation, and the coupled Schrödinger equation is solved by including the non-adiabatic coupling terms of the neighbouring electronic potential

curves. We explore the transition probabilities through the avoided crossing in the electronic structure, which characterize the ultracold chemical reaction of the Rydberg atom with the diatomic molecule. For the vibrational bound state, we provide the electric dipole moment and decay rates. For the experimental guidance, we identify the best states for photoassociation of this Rydberg molecules and provide the Franck-Condon factors.

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Poster Session / 17

High-wavenumber compressive Raman spectroscopy: a faster tool for melanoma diagnosis.

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Raman spectroscopy (RS) is a highly-sensitive optical technique based on specific vibrations of molecules, which enables non-invasive and non-destructive monitoring of biospecimens present in tissues, revealing disease-prompted variations and allowing to differentiate healthy from malignant samples with high accuracy, sensitivity and specificity. Nevertheless, pigmented tissues are inaccessible to conventional RS, because of laser-induced tissue fluorescence, unless infrared excitation is used. With these excitation wavelengths, Raman spectroscopy required very expensive pixelated detectors to achieve the necessary signal-to-noise ratio. These detectors are usually associated with liquid hydrogen cooling systems that make the equipment bulky, expensive and difficult to operate.

In order to solve these issues, this work details the design of a new Raman spectrometer, applying compressive sensing, based on spectral multiplexing by spatial light modulators (as a digital micromirror device) and on single-element detection. When applied to RS, these two components allow the acquisition of the same spectral information as in multichannel detectors but at a much higher acquisition speed, which is crucial for time constrained applications (as in clinical scenarios), lowering the cost of the equipment, and allowing for a small instrument since liquid cooling is no longer required. This offers new possibilities for the development of a much-simplified RS instrument that would promote a routine implementation of this technique in many different areas, including melanoma diagnosis.

Poster Session / 18

C5N– in collision with He: rotational transitions in the ISM

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In the last years, several C-bearing and (C,N)-bearing chains of molecular anions have been detected in the interstellar medium (ISM). Since experimental treatments are still challenging, computational methods have to be used to understand their chemistry. The C_5N^- anion is one of the largest (C,N)-bearing chains and, although there are several theoretical studies [1-3] that describe the dynamics of the smaller (CN^- , C_3N^-) + He/ H_2 systems, for the moment there has been no study reported for the collision between this molecular anion with He or H_2 .

We have performed quantum scattering calculations using a new ab initio potential energy surface (PES) where the interaction potential between C_5N^- and He was obtained using CCSD(T) approach and the complete basis set (CBS) limit (see Figure 1). Given the ISM conditions of this system, we calculate the state-to-state (de-)excitation cross sections and the respective rate coefficients as a function of temperature. These results have been also compared by those obtained for the $C_3N^-/C_5N^- + H_2$ system.

Oral communications / 19

Exploring space chemistry: quantum spectroscopic characterization of Ng-containing molecules through machine learning algorithms.

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For a long time, space was thought to be a hostile environment characterized by extreme conditions, in which the formation of any molecular system was highly unlikely, if not impossible. However, advances in three fundamental areas of molecular astrophysics (theoretical modeling, experimental laboratories, and observational missions), as well as, their joint effort are responsible for more than 290 molecules [1] have been already detected up to now. In that way, the intrigue grows with each new discovery, and the question “What comes next?” becomes more complex as the number of viable species increases. From this point of view, in the last decade, two of the most fascinating detections have been noble gas hydride cation complexes, HeH^+ and ArH^+ , due to their well-known high electronic stability [2, 33, 44, 5]. All this has generated a great deal of interest and a desire to learn more about the interstellar chemistry of noble gases.

In this vein, our main goal is to explore trends and models using quantum chemistry computations in order to collect data [46, 57, 6]. To accomplish this, we propose a machine learning-based approach to construct new accurate potential energy surfaces aiming to understand their chemical binding and electron exchange in clusters of noble gas hydride cations.

Poster Session / 20

On the Determination of Lipid Monolayer Langmuir Isotherms via Molecular Dynamics. Too big of a stretch?

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Lipid cellular membranes constitute a common factor to all known Life on Planet Earth. It is this commonness, and yet their distinctions based on cell type, organism, or age¹ what makes them attractive targets for a wide range of treatments. Therefore, it is of paramount importance to understand how these ubiquitous structures react to different stimuli. Specifically, their mechanical properties are of great interest in the pharmaceutical field, as the permeation of drugs is dependent on them.

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Traditionally, the in-plane expansion of lipid membranes has been studied with wet lab techniques, being the determination of Langmuir Isotherms for monolayers as membrane models a gold standard at that². On the other hand, Molecular Dynamics has proven to be an invaluable tool at giving insight on the molecular mechanisms that govern the mechanics of lipid membranes³. In this work we attempt to design new simulation protocols to mimic Langmuir trough experiments using Umbrella Sampling MD. Our results point to agreements, but also to differences, to typical results obtained in a lab; and help to shed light on the nanoscopic-scale processes that are involved in membrane mechanics, while paving the way towards new approaches for their study with in-silico techniques.

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Invited talks / 21

Single photon autoionization of aromatic molecules in solution

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The ionization of molecules in the condensed phase is driven by the interactions established with the environment. In fact, for some aromatic molecules dissolved in water, the formation of the fully separated charges (cation+electron) has been found after exciting at the onset of their electronic absorption, well below the gas-phase ionization potentials.[1,2] By using transient absorption methods based in femtosecond pulses, we have induced and tracked the relaxation dynamics of aromatic molecules solvated by H-bonded protic solvents. The research aims to address the nature of the initially formed electronic-excited state and the intermediate steps toward the fully separated charges, and to establish the influence of the specific solute-solvent interactions on them.³ Understanding this relaxation channel opens the possibility of controlling the generation of charges in solution.

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Oral communications / 22

Simulation of Pm-Like Bismuth Spectra in an EBIT

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We use a multiconfiguration Dirac-Fock code [1,2] to calculate electronic excitation cross sections and radiative decay transition probabilities for a large number of atomic levels in Pm-like bismuth. By numerically solving a set of equilibrium equations we were able to obtain the level populations of the $4f^{14}5s$, $4f^{13}5s5f$, $4f^{13}5s5d$, $4f^{13}5s5p$, and $4f^{13}5s^2$ configurations and synthesized spectra for a number of electronic density values in an EBIT for 640 keV incident electron energy.

The synthesized spectrum we obtained for 10^{10} cm^{-3} electronic density agrees qualitatively with the experimental data of Kobayashi et al. 3. We found significant differences between our simulations and Kobayashi's for several electronic density values.

The emission lines position and relative intensity can also be compared with laser produced plasma spectra, to improve the identification of the Pm-like ions and provide experimental values of electron density at those plasma conditions.

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Oral communications / 23

Using a 125 μm thick COBRA to increase the light yield of He-CF₄ gas mixtures

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Many state-of-the-art optical readout micro-patterned gaseous detectors (MPGDs) are equipped with standard Gas Electron Multipliers (GEMs), which are 50 μm thick. The COBRA_125, a 125 μm thick, triple-electrode MPGD has the potential to further increase the optical gain of these detectors: whereas in a GEM, the Electroluminescence light is only produced in the holes, the two independent stripped electrodes imprinted on the bottom face of the COBRA_125 define a second high-field region that produces additional light. Furthermore, the increased thickness of the COBRA_125 adds electrical robustness, meaning that higher voltages can be applied across the holes before the onset of microdischarges.

In this work, we compare the absolute light yield of He-CF₄ mixtures produced by a 125 μm COBRA to the one obtained with a standard GEM (50 μm thick). The detector, operated in flow-mode, was irradiated with X-rays from a ⁵⁵Fe source. A Large Area Avalanche Photodiode (LAAPD) was used to readout the light produced by the COBRA_125 and by a standard GEM. Our results show that the COBRA_125 is able to increase the light yield of a standard GEM by an order of magnitude, proving to be a strong solution for future optical MPGDs.

Oral communications / 24

Exploring the secondary structure of Host Defense Peptides in their biological environment. A Molecular Dynamics approach.

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Host defense peptides (HDPs) are short cationic peptides that have a critical role in the innate immune response across all living organisms ¹. Their primary mode of action does not depend on protein receptors, but instead on their ability to target and disrupt the membranes of various pathogenic and pathological cells, such as those found in cancer, bacteria, or even our own senescent cells. These structures are characterized by their specific compositions, typically containing a relatively high concentration of anionic lipids. Upon encountering a pathogenic/pathological lipid membrane, the peptide's secondary structure undergoes a transformation, promoting its adsorption through electrostatic and hydrophobic interactions ². The membrane's functionality is compromised depending on the concentration of HDPs, which may also lead to the disruption of its structure. The general interaction mechanism between HDPs and lipid membranes is still not fully understood; however, understanding the peptide's structure in the presence of the membrane is a critical initial step towards synthesizing new artificial peptides with enhanced activity.

Predicting the secondary structure of HDPs from their sequences is particularly challenging, primarily due to the significant influence of the environment, specifically the presence of the membrane. Furthermore, there is a significant lack of structural information available for HDPs: solving the structure of a peptide in the presence of a membrane is a difficult task, resulting in sparse data compared to that for proteins. The use of Molecular Dynamics (MD) simulations may compensate the shortage of experimental results, as it is able to describe the complex interactions between the peptide and the environment and reach the typical microsecond scale of the folding processes.

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Poster Session / 25

DIRAC-FOCK CALCULATIONS OF AUGER SPECTRUM IN Au: IMPACT ON SENSITIZED RADIOTHERAPY WITH NANOPARTICLES

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Several studies show that the combination of high-Z nanoparticles (NPs) and external radiotherapy (RT) leads to an increased radiation effect in tumoral cells without an increase of the patient dose [1,2]. Among the various elements with sensitizing potential, Au NPs have been the most studied due to the greater biocompatibility of gold. In this technique, Au NPs are incorporated inside tumor cells with the aid of biomolecules with specific affinity for each cell type. Thus in an RT treatment it is possible to produce additional secondary radiation enhancement in the tumor tissues internalized with Au NPs. This additional radiation results mostly from electronic collisions of the external beam used in RT with the NPs. Particularly relevant is the ionization of internal atomic shells that lead to a cascade of transitions. The low-energy component of the Auger spectrum produces electrons with a very short range (smaller than the cell dimensions) and, therefore, contribute significantly to the local radiosensitizing effect of NPs.

Dosimetric calculations of RT with NPs are based on Monte Carlo (MC) simulations using well-known codes 3. These typically use libraries of atomic parameters calculated several decades ago with outdated models. Since the low-energy component of the Auger spectrum is particularly sensitive to correlation effects, we present in this paper new calculations based on the Multiconfiguration Dirac-Fock method. For this, the code developed by Desclaux and Indelicato [4,5] was used to compute radiative and radiationless transition rates as well as photoionization cross-sections for different energies relevant in RT. The Auger spectrum is simulated using an MC-based method to produce the atomic de-excitation cascades. The impact of the new calculations will be discussed based on simulations of the radial dose profile in a water sphere using the TOPAS code [6,7].

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Oral communications / 26

A new analytical potential energy surface for (H₂⁺)He cluster**Authors:** José Bretón¹; Javier Hernández Rojas²; Antonio Sarsa³¹ *Departamento de Física e IUdEA. Universidad de La Laguna*² *Departamento de Física e IUdEA. Universidad de La Laguna, 38200, La Laguna, Tenerife. Spain*³ *Departamento de Física, Universidad de Córdoba.***Corresponding Author:** jhrojas@ull.edu.es

We present a new potential energy surface (PES) for the interaction between the Hydrogen molecule ion and the Helium atom in its electronic ground state. The PES of (H₂⁺)He cluster is represented by 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 dispersion-repulsion forces characterized by an “atom-bond” potential between the bond of H₂⁺ and the He atom. All parameters of this new PES have been chosen and fitted from post Hartree-Fock calculations at CCSD(T) level and performed with the NWChem Quantum Chemistry Software. By assuming pair-wise interactions and considering the Aziz-Slaman potential for the interaction between Helium atoms, we define a PES for H₂⁺(He)_N clusters and study their energetic and structural properties employing classical and quantum simulations.

Invited talks / 27

Quantum Stereodynamics of cold collisions between two aligned molecules**Author:** PABLO GARCÍA JAMBRINA¹¹ *Universidad de Salamanca***Corresponding Author:** pjambrina@usal.es

One of the most fundamental questions in molecular dynamics is the dependence of a collision outcome on the relative orientation/alignment of the reactants, i. e. the stereodynamics of a collision process. For bimolecular gas phase reactions, it is possible to address this question by polarizing the reactants bond-axis and/or rotational angular momentum.[1-4]

Here, we will illustrate how the outcome of a collision can be controlled by selecting the relative geometry of the colliding partners before they start to interact. In particular, we will focus on the collisions at low energies, which proceed with contributions from just a few partial waves, such as those between two aligned D₂ molecules, whose angular distributions have been measured recently by Zhou et al. 2. Our results based on full-dimensional coupled-channel scattering calculations reveal that the experimental angular distribution is caused by a L=4 resonance, and that key features of the experimental angular distributions are only captured when four-vector correlations in aligned-aligned molecular collisions are accounted for.

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Oral communications / 28**Understanding the formation of aromatic compounds in the interstellar space****Author:** CASTIÑEIRA REIS MARTA Not Supplied^{None}**Co-authors:** Emilio Martínez Núñez ¹; Antonio Fernández Ramos ¹¹ *University of Santiago de Compostela***Corresponding Author:** marta.castineira.reis@usc.es

Understanding the formation of PolyAromatic Hydrocarbons (PAHs) can shed light on the origin of the prebiotic Earth and even on the origin of life.¹ Unfortunately, to date, the formation of organic compounds in space is a scarcely understood area.

In this arena, automated protocols for the identification of reaction mechanisms show great potential to aid in the learning of how PAHs are formed in space. Taking advantage of the AutoMeKin [2,3] program, we have found thousands of potential paths that account for the formation of the simplest PAH: benzene. We have not only uncovered several direct paths, for which reactants have been detected in space, but also some more indirect paths in which well-known intermediates such as benzyne or the very acetyl radical play a crucial role.

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Oral communications / 29**Variational principle to regularize machine-learned density functionals****Author:** Pablo del Mazo Sevillano^{None}**Corresponding Author:** pablo.delmazo@uam.es

Practical density functional theory (DFT) owes its success to the groundbreaking work of Kohn and Sham that introduced the exact calculation of the non-interacting kinetic energy of the electrons using an auxiliary mean-field system. However, the full power of DFT will not be unleashed until the exact relationship between the electron density and the non-interacting kinetic energy is found. Various attempts have been made to approximate this functional, similar to the exchange-correlation functional, with much less success due to the larger contribution of kinetic energy and its more non-local nature. In this work we propose a new and efficient regularization method to train density functionals based on deep neural networks, with particular interest in the kinetic-energy functional. The method is tested on (effectively) one-dimensional systems, including the hydrogen chain, non-interacting electrons, and atoms of the first two periods, with excellent results. For the atomic systems, the generalizability of the regularization method is demonstrated by training also an exchange-correlation functional, and the contrasting nature of the two functionals is discussed from a machine-learning perspective.

Poster Session / 30

Molecular Dynamics Simulations Shed Light on Antimicrobial Peptide Interactions with COVID-19 Altered Membranes

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In recent years, the COVID pandemic has garnered a great deal of attention, focusing mainly on the acute phase of the disease. However, this is only the beginning, as some patients continue to experience persistent symptoms, known as Post-COVID Condition (PCC), and an estimated 20% of those affected do not recover. The presence of this condition shows a number of obstacles, including the lack of suitable therapeutic options and the long-term consequences for survivors of the disease.

While the study of genome sequencing and the protein composition of the virus membrane is of undeniable value for vaccine development, there are other aspects that have been overlooked. One of these is the lipid profile of patients with COVID-19. The lipid profile plays a crucial role not only during the acute phase, but also throughout disease progression and during medium- and long-term effects^{3,4}. There appears to be a potential connection between the lipid profile and COVID-19, suggesting that the innate immune system, specifically antimicrobial peptides (AMPs), may be responsible for this association⁵. Therefore, understanding the importance of the lipid profile and how AMPs function at the interface of lipid membranes affected by COVID-19 could improve our understanding of the disease and potentially contribute to the development of better treatments.

To investigate the interaction between antimicrobial peptides and infection-affected membranes, we performed Molecular Dynamics (MD) simulations with various AMPs and models of altered and unaltered membranes. The findings of this study may provide deeper insight into the role of AMPs in the lipid profile of patients with COVID-19 and PCC, which could lead to the development of more effective treatments.

Acknowledgments

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Invited talks / 31

Theoretical-computational comparative study of the persistent organic pollutants: adsorption, detection and permeability

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In today's world, the great pollution puzzle is undoubtedly the greatest challenge facing the world's population. Dioxins and dibenzofurans are persistent organic pollutants (POPs); the more toxic forms correspond to their tetrachlorinated derivatives, 2,3,7,8-tetrachloro-p-dibenzodioxin (TCDD) and 2,3,7,8-tetrachlorodibenzofuran (TCDF). The reduction of their emissions, the elimination of pollution already generated and the study of the interaction of these contaminants with living beings are the three fundamental pillars in research related to this particular problem of pollution. In this sense, the computational modelling of these systems ranges from the study of their biological activity to the search for an effective detection method and sustainable treatment.

In this contribution, a complete computational research encompasses: the adsorption of these two "dioxin-like" compounds on new 2D materials, such as white graphene, structurally analogous to graphene but consisting of borazine rings acting more actively as filters or adsorbents, or hybrid boron-nitrogen-carbon (h-BNC) structures; and their subsequent molecular detection using optical spectroscopy, namely, Surface Enhanced Raman Spectroscopy (SERS).

The theoretical work is completed with the study of their behavior in biological media, since the most toxic pollutants accumulate mainly in fatty tissues due to their hydrophobic character. In this way, cell membranes behave as storage reservoirs for pollutants, becoming an internal source of chronic exposure to contamination. Therefore, for a description of the uptake process as well as the changes induced in the membranes at molecular level, the intermolecular interactions between the contaminants and the membranes must be known in detail.

This theoretical research allows for a complete vision of the problem; covering the action, detection and treatment of these substances.

Acknowledgements

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Poster Session / 32

Lipid monolayers as membrane models for cancer and infection: a synergic in-vitro/in-silico study

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Lipid membranes are highly complex and dynamic systems formed by hundreds of different types of lipids combined in specific ratios. Many pathological cells exhibit significant alterations in the lipid composition of their membranes when compared to healthy cells. For example, lipid profile singularities have been found in cancer, bacterial and viral infections and even in senescent cells 1. All the properties of a cell membrane (the internal structure, the dynamic correlation between different lipids, and the thermodynamic stability of the whole system) are endowed by its molecular composition. Mechanical perturbations could irreversibly destroy the cell or could be transitory if the membrane spontaneously repairs itself. Thus, the vulnerability of pathological membranes to certain perturbations could be exploited as a therapeutic strategy. However, the connection between

membrane composition and the associated properties is poorly understood.

Lipid monolayers have been extensively used as minimalistic models for cell membranes, being lipidic composition essential for the determination of their structure and mechanical properties. Particularly, the determination of adsorption isotherms for Langmuir monolayers can be easily performed by both computational and experimental methods [2, 3]. Molecular Dynamics (MD) simulations at atomic scale can provide high resolution results not available through wet-lab experiments [4], realizing the synergistic potential of a combined in-silico/in-vitro approach in the characterization of the mechanical membrane destabilization process.

In this work, the results obtained from MD simulations and Langmuir trough experiments will be presented, aiming to understand the response of different models of bacteria and cancer cells to mechanical efforts.

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RAMAN THERMOMETRY OF CONFINED GAS MICRO-FLOWS

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Microfluidics devices with internal gas flows are nowadays subject of a rapid development. These devices often operate in rarefied gas flow regimes, since the ratio of the molecular mean free path over the channel dimensions becomes non-negligible. In those rarefied flows, effects like temperature-jumps near the wall are expected to occur. However, there is a lack of experimental techniques capable of measuring the internal properties, such as temperature, in gas flows confined in small channels [1].

Raman spectroscopy is a powerful non-intrusive technique to probe gas jets at the molecular level with high spatial resolution, as we have demonstrated in the Laboratory of Molecular Fluid Dynamics of the IEM [2].

Here we present a first proof-of-concept application of Raman thermometry to the gas flows within the millimetre channels. For this work, we have designed several channels with forced thermal gradients, and demonstrated that the gas temperature in the flow can be retrieved, with high spatial resolution, from the rotational and vibrational Raman spectra of molecules like N₂, CO₂ and acetone.

Acknowledgements

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Exploring the Interaction of Endogenous Therapeutic Peptides with Lipid Membranes: Insights from Biased calculations.

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Understanding the behaviour of endogenous therapeutic peptides (ETPs), short cationic peptides that have the ability to target and disrupt the pathological membranes, which typically contain a high concentration of anionic lipids, is crucial for the development of effective therapeutic strategies [1,2]. This study investigates multiple ETPs and their interaction with model lipid membranes. The main objective of this research is to characterise the free energy profiles associated with the interactions between various ETPs and lipid bilayers. Here, we employ advanced computational techniques, including Metadynamics 3, which allows a comprehensive exploration of the configurational space, overcoming the limitations of conventional molecular dynamics methods, where the system can be trapped in local or global minima, which leads to poor sampling of the configurational space. Using Metadynamics, we can effectively capture the peptide-membrane approach, the tilt or rolling motion of ETPs and obtain a more accurate sampling of their membrane interaction states. Energy calculations play a key role in this study, as they allow us to assess the relative stability of different conformations and interaction states. The resulting free energy profiles provide valuable information on the favourable interactions between ETPs and lipid membranes. These findings are crucial for identifying ETPs, thus facilitating the rational design and development of therapeutic peptides. As a result, an optimized, reproducible and easy to automate protocol to get the free energy profile corresponding to the interaction between ETPs and lipid bilayers is obtained. The protocol here presented is sensitive both to the ETP sequence and the lipid composition of the membrane model.

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Oral communications / 35

Status and recent results of the XENONnT experiment

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The detection of particle dark matter (DM) remains an unresolved challenge in contemporary physics. The XENONnT experiment, located at the Laboratori Nazionali del Gran Sasso, in Italy, utilizes a multi-tonne liquid xenon time projection chamber to probe DM interactions. With an active target of 5.9 tonnes, low background, and keV-level threshold, XENONnT completes its science program with other rare-event searches such as solar neutrinos, solar axions, bosonic DM, and rare nuclear decays. In this talk, I will present an overview of the XENONnT detector, its subsystems, and the key results from its first science run.

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Investigating the Catalytic Mechanism of β -Cyclodextrin Dimer in Previtamin D3 Isomerization

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The sigmatropic isomerization reaction of previtamin D3 to vitamin D3, when encapsulated within a dimer of β -cyclodextrin, exhibits a 40-fold enhanced rate compared to its counterpart in an isotropic organic solution¹. Despite several hypotheses, the exact mechanism by which β -cyclodextrin dimer catalyzes the reaction remained elusive.

We have conducted a rigorous investigation of the isomerization dynamics of previtamin D3 within a β -cyclodextrin dimer through a combination of molecular dynamic simulations and statistical multi-structural transition state theory to address this knowledge gap. Two key programs in the field of Chemical Kinetics, namely *TorsiFlex* [2,3] and *Pilgrim* 4, play a crucial role in facilitating our investigations. *TorsiFlex* allows for an extensive conformational search encompassing both previtamin D and the reaction transition state, while *Pilgrim* enables precise calculations of thermal rate constants within systems comprising multiple conformations.

Our results verify the experimental observations and provide unprecedented insights into the β -cyclodextrin dimer catalytic mechanism.

Acknowledgements

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TRIGGERING EXCITED STATE DYNAMICS IN GRAPHENE QUANTUM DOTS: THE ABSORPTION SPECTRUM OF CORONENE AND CIRCUMCORONENE

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Graphene quantum dots (GQD) are nanoparticles consisting of a single or several layers of graphene sheets whose thickness does not exceed 100 nanometers. GQD have become extremely popular in optoelectronics as nanocarriers for cancer therapy drugs and in bioimaging techniques, mostly due to their ease of preparation, biocompatibility and tunable absorption and emission properties¹.

This work is focused on coronene (Fig. 1), the smallest unit of a graphene nanoflake and zero-dimensional quantum dot. Several studies have found that coronene shows fluorescence and phosphorescence in the visible range of the light spectrum 2. As a starting point, the excited state deactivation pathways of a single unit of coronene are unraveled using the ML-MCTDH method 3 and a vibronic coupling model for the nuclear Hamiltonian, including both singlet and triplet states. This study has been extended to circumcoronene in the direction towards graphene where promising results have been found.

Future work will look at expanding the system size, adding further layers, and pondering the effect of functionalization to explain the strong emission found by our experimental collaborators in doped carbon nanoparticles 4.

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Measuring physical quantities of CO₂ by Raman spectroscopy

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In the present work, static and dynamic quantities of carbon dioxide (CO₂) are studied by means of Raman spectroscopy in gas flows.

CO₂ is a molecule of great importance in several current challenges, like characterization of exoplanets atmospheres, development of accurate climate models or synthesis of fuels through plasmas. Most of these problems involve non-local thermodynamic equilibrium (nLTE) conditions. Therefore, deep understanding of relaxation (and excitation) processes is needed in order to work on the aforementioned questions.

Supersonic jets in the laboratory provide an ideal medium to investigate these mechanisms. Combined with Raman spectroscopy, information on the evolution of the populations of the molecules can be retrieved and a detailed study of its relaxation along the jet can be made [1,2]. Nevertheless, this experimental method raises another problem: Raman spectroscopy strong dependency on the polarizability transition moments of the molecule under study. Although this quantity is well-known for CO₂ rotational Raman transitions, reliable data for vibrational transitions is missing 3.

We present a set of results for both problems. On the one hand, by generating high-temperature flows of CO₂ in thermodynamic equilibrium, a set of measurements of the polarizability transition moments have been obtained for more than 30 vibrational Raman transitions. On the other hand, we probed several supersonic jets of CO₂ from hot nozzles by Raman spectroscopy, obtaining a set of state-to-state rate coefficients for rotational relaxation for a wide range of temperatures.

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Improvement and benchmarking of atomic data for kilonova modeling

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Given the recent detection of multiple neutron-star merger events, in particular the AT2017gfo observation, in which the ejection of hot and radioactive matter, termed kilonovae, was detected as an electromagnetic signal. It is critical to combine a more comprehensive description of nuclear and atomic properties with advanced astrophysical simulations in order to produce accurate predictions of r-process nucleosynthesis yields and electromagnetic signals when compared with observational data.

Since the luminosity and spectra of the radiative emission depend significantly on the atomic opacities of the heavy elements ejected [1,2], in this work we provide results for large-scale calculations of data needed to compute those opacities for lanthanides and actinides. The atomic data was calculated utilizing the Flexible Atomic Code (FAC) 3, as it allows for structure, radiative and collisional data, needed for kilonova modeling. Structure calculations are carried out by FAC employing a configuration interaction approach and a central potential improved with existing experimental data utilizing machine learning methods. In this work we also performed benchmarking tests on our atomic data to investigate the implications of using this central potential model in our calculations.

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The Plasma Window as a Vacuum-Atmosphere Interface for Measurements of Stellar Neutron-Induced Reaction Cross Sections

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Neutrons play a dominant role in the stellar nucleosynthesis of heavy elements. We review a scheme for the experimental determinations of neutron-induced reaction cross sections using a high-intensity neutron source based on the $^{18}\text{O}(p,n)^{18}\text{F}$ reaction with an ^{18}O -water target at SARAF's upcoming Phase II. The quasi-Maxwellian neutron spectrum with effective thermal energy $kT \approx 5$ keV, characteristic of the target (p,n) yield at proton energy $E_p \approx 2.6$ MeV close to its neutron threshold, is well suited for laboratory measurements of MACS of neutron-capture reactions, based on activation of targets of astrophysical interest along the s-process path. ^{18}O -water's vapour pressure requires a separation in between the accelerator vacuum and the target chamber. The high-intensity proton beam (in the mA range) of SARAF is incompatible with a solid window in the beam's path. Our suggested solution is the use of a Plasma Window, which is a device that utilizes ionized gas as an interface between vacuum and atmosphere, and is useful for a plethora of applications in science, engineering and medicine. The high-power dissipation (few kW) at the target is expected to result in one of the most intense sources of neutrons available at stellar-like energies. Preliminary results

concerning proton beam energy loss and heat deposition profiles for target characteristics and design, a new full-scale 3-dimensional computer-aided design model of the Plasma Window (as well as its operation principles) and the planned experimental scheme, will be reviewed.

Poster Session / 42

Magnetic resonance spectroscopy and imaging in the CASPEr dark matter experiment

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An overview of our experimental program to detect QCD axions and axion-like-particles (ALPs) as possible candidates for dark matter (DM) using NMR techniques within the cosmic axion spin precession experiment (CASPEr) is presented. ALPs are hypothetical particles that could also solve the strong CP violation problem, and it is predicted that the axion field would behave as a classical field: it would oscillate at a mass-dependent frequency. ALPs also have derivative interactions with the SM fields. Nuclei that are interacting with the background axion DM acquire time-varying CP-odd nuclear moments such as an electric dipole moment (EDM). In analogy with NMR, these moments cause spin precession in a material sample induced by coupling between the ALP field and the axial nuclear current, in the presence of an electric field. Precision magnetometry can be used to look for such a precession. The signals from these particles will be very weak so all possibilities for signal enhancement need to be considered and for that, the chosen nuclei are ¹²⁹Xe that are hyperpolarized using the spin-exchange optical pumping (SEOP) technique inside a large optical cell. In this method, polarization is transferred to the Xenon via Fermi contact interactions with an optically pumped alkali metal, Rubidium. Especially for investigations of the nuclear spin resonance of liquid Xe as a fundamental physics experiment, a non-metallic variable temperature insert (VTI) is needed. This VTI should be suited for immersion in liquid helium. The sapphire sample holder is to hold on a level of $165 \text{ K} \pm 1 \text{ K}$ by a gaseous flow of temperature-stabilized nitrogen. Xenon has a much higher spin density when it is liquid, thus it has to be kept in that narrow temperature range. The hyperpolarized Xenon is then to be placed in an external magnetic field that will be swept from ultra-low field up to 14.1 T looking for the resonance with the axion field, while the Xenon nuclei undergo precession due to the gradient interaction. The first-generation experiments explore many decades of ALP parameter space beyond the current astrophysical and laboratory bounds. It is anticipated that future versions of the experiment could ultimately cover the entire range of masses up to $\sim \mu\text{eV}$, complementary to cavity searches.

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Time evolution of natural orbitals in ab initio molecular dynamics

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One-particle reduced density matrix (1RDM) functional theory is an alternative formalism to both density functional and wavefunction based methods. A pragmatic approach results in approximate

functionals of the 1RDM in its diagonal form, that is, the use of natural orbitals and its occupation numbers as the fundamental variables, which define a natural orbital functional (NOF).

In this talk, I will first introduce the recently proposed 1 global NOF (GNOF). The latter has shown a balanced treatment of electron correlation effects in molecular systems with different spins, including complete dissociation curves; as well as an adequate treatment of the strong electronic correlation regime in challenge systems [2,3]. The NOF theory is currently an active research field, which can already be applied to large molecular systems of general chemical interest [4,5] using open-source software like DoNOF 6.

Secondly, I will present a GNOF-based ab initio molecular dynamics (AIMD) within the Born-Oppenheimer approximation. The most prominent feature of GNOF-AIMD is the ability to display the real-time evolution of natural orbitals, providing detailed information on the time-dependent electronic structure of complex systems and processes, including reactive collisions. The quartet ground-state reaction $\text{N}(4\text{S}) + \text{H}_2(1\Sigma) \rightarrow \text{NH}(3\Sigma) + \text{H}(2\text{S})$ is taken as validation test. Collision energy influences on integral cross sections for different initial ro-vibrational states of H_2 and rotational-state distributions of NH product are discussed, showing a good agreement with previous high-quality theoretical results.

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Computational Ingredients to Model Biological Processes

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The computational 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 conformational sampling. In the case where the process under investigation takes place in a long-time scale, the application of enhanced sampling approaches may also be needed. In this contribution, the modeling of several physical processes occurring in different biological media will be discussed, including the permeation of drugs across lipid membranes ¹, electron-transfer events on DNA strands in terms of reduction potentials ², and the binding of photoswitches to ion channels ³.

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Benzimidazole: One molecule - two photoreactions

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Benzimidazole: One molecule - two photoreactions

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Monomers of benzimidazole trapped in an argon matrix at 15 K were characterized by vibrational spectroscopy and identified as 1H-tautomers exclusively. The photochemistry of matrix-isolated 1H-benzimidazole was induced by excitations with a frequency-tunable narrowband UV light and followed spectroscopically. Hitherto unobserved photoproducts were identified as 4H- and 6H-tautomers.¹ Simultaneously, a family of photoproducts bearing the isocyano moiety was identified.¹ Thereby, the photochemistry of benzimidazole was hypothesized to follow two reaction pathways: the fixed-ring and the ring-opening isomerizations.

The former reaction channel is initiated by cleavage of the NH bond and formation of a benzimidazolyl radical and an H atom. The latter reaction channel involves cleavage of the five-membered ring and concomitant shift of the H-atom from the CH bond of the imidazole moiety to the neighboring NH group, leading to 2-isocyanoaniline (ICA) and subsequently to isocyanoanilinyl radical (and an H-atom). Recombination of the radical pairs yields a variety of photoproducts. The mechanistic analysis of the observed photochemistry will be presented, demonstrating that the photochemistry of benzimidazole occupies an intermediate position between the earlier studied prototype cases of indole² and benzoxazole,³ which exhibit exclusively the fixed-ring and the ring-opening photochemistries, respectively.

Acknowledgements:

All researchers involved in the studies cited in this work are kindly acknowledged. The Chemical Process Engineering and Forest Products Research Centre (CIEPQPF) is supported by the Portuguese Science Foundation (Fundação para a Ciência e a Tecnologia, FCT) through projects UIDB/EQU/00102/2020 and UIDP/EQU/00102/2020.

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Poster Session / 46

A computational study of the mode of action of the DAD photo-switch in the NaV1.5 channel

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Azobenzene derivatives are becoming increasingly popular in pharmacology due to their improved selectivity based on trans-cis isomerization upon light irradiation. In the context of ion channels, one of the conformations may block ion conduction, while the other allows it. We studied an azobenzene derivative, DAD, designed with the aim of avoiding excitation wavelengths in the UV region of the electromagnetic spectrum. Two binding pockets of DAD in the cardiac sodium channel were

obtained by means of Gaussian Accelerated Molecular Dynamics combined with free-energy calculations, showing that the most relevant ligand-protein interactions were of electrostatic nature. Comparison of the absorption spectra reveals similar results in water and in the binding pockets. The photoisomerization mechanism is analogous to azobenzene: it begins with the population of the second excited state (S₂), fast crossing to S₁ and relaxation along the rotation of the azo dihedral to a S₁/S₀ conical intersection that connects the trans and cis geometries on the ground state. However, it seems more favourable in the case of DAD.

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Unveiling the photosensitivity mechanisms of UVB filter PABA

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Para-aminobenzoic acid is a formerly used UVB filter that was found to react with the DNA when exposed to sunlight.¹ Molecular Dynamics (MD) and Umbrella Sampling simulations show that the neutral species of PABA binds favourably DNA by intercalation between two nucleobase pairs, while the binding of the anionic species is not feasible from the thermodynamic and kinetic points of view. Simulation of the joint PABA-DNA absorption spectrum by Quantum Mechanics/Molecular Mechanics (QM/MM) calculations on top of a MD ensemble of geometries, followed by transition density analysis, suggests that charge transfer states could play a role in the deactivation of the system and lead to the formation of radical species that might trigger DNA lesions.² Moreover, the identification of relevant deactivation routes of excited PABA in vacuum revealed the favourable population of a long-lived triplet state, which can participate in photosensitising mechanisms, such as energy transfer processes to thymine or to molecular oxygen.³

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Oral communications / 48

Effect of the intersystem crossings in the S⁺+H₂ reaction

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SH⁺ is a widespread molecular ion in diffuse interstellar clouds, and has also been detected in emission toward the Orion Bar photodissociation region (PDR). In warm and dense PDRs, SH⁺ is thought to form by exothermic reactions of S⁺ with vibrationally excited H₂ ($v>1$). The viability of this hypothesis have been confirmed by theoretical simulations reaction which demonstrate that for vibrational level $v=2$ or higher of H₂, the reaction exhibit high rate constants¹.

From an experimental point of view, scarce data are available². As the reaction of the ground state ion is endothermic by almost 1 eV, the SH⁺ product is observed only at high collision energies where translational energy brings the needed energy to reach products, as predicted by the theoretical simulations. Interestingly, it appears from this experimental study that spin-orbit couplings between

the quartet and first doublet state of the H₂S⁺ system may play a significant role on the reaction, motivating a new theoretical study of the reaction, now including the spin-orbit interactions.

Exact quantum dynamics calculations show that spin-orbit interaction does indeed play an important role in this reaction, and that three electronic states are involved in the reaction mechanism.

Acknowledgments: This work was supported by the Grants No. PID2019-107115GB-C21 and PID2021-122549NB-C21 from MICINN (Spain).

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Poster Session / 49

The Raman spectrum of diacetyl revisited

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We have revisited and enlarged the vibrational analysis of diacetyl or 2,3-butanedione by means of state-of-the-art Raman spectroscopy 1 and quantum chemical computations. The Raman spectra were obtained previously only in condensed phases 2 and hence hindered low-energy vibrational modes were undetected. Here we measured the Raman spectra of diacetyl in all the gas and liquid phases and cooled in supersonic expansions. Some new bands have been observed for the first time. Differences in the band progression and widening are discussed. The measured bands were assigned by means of density functional theory incorporating the anharmonic Generalized Vibrational Perturbative Theory of Second Order (GVPT2) correction and Born-Oppenheimer Molecular Dynamics. Discussion on the accuracy of the computational methods to describe Raman intensities and vibrational mode centers in such centrosymmetric molecule are examined.

Acknowledgement

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Oral communications / 50

Interstellar detection of carbonic acid (HOCOOH) at last

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The joint journey of rotational spectroscopy and radioastronomy is firmly pushing the frontiers of interstellar chemistry based on the detection of new molecules with ever-higher degrees of molecular complexity. However, for several families of compounds (e.g., carboxylic acids) the census of

identified interstellar species has remained untouched for almost a quarter century. Herein, we present the discovery of *cis-trans* carbonic acid (HOCOOH) toward the molecular cloud G+0.693-0.027, which ranks as the first interstellar molecule containing three oxygen atoms and the third carboxylic acid detected in the interstellar medium to date. Although the available laboratory measurements ended at 65 GHz, we have used our spectral line survey as a “conventional” laboratory spectrum and managed to detect several clear and unblended spectroscopic features directly in the 3mm radio astronomical data. Hence, we were able to improve its set of rotational spectroscopic constants. We derive a column density for this conformer of $N = (6.4 \pm 0.4) \times 10^{12} \text{ cm}^{-2}$, which translates into an abundance with respect to H_2 of 4.7×10^{-11} . We also report the nondetection of the more stable *cis-cis* HOCOOH, showing an upper limit to the molecular abundance with respect to H_2 of $\leq 1.2 \times 10^{-9}$, because of the huge impact that its low dipole moment (about fifteen times lower than that of the *cis-trans* form) has on the overall detectability of the conformer. Nevertheless, we suggest that it may be efficiently generated under interstellar conditions, most likely via -OH radical addition of HOCO on the surface of dust grains, although it is nearly imperceptible to radio astronomical observations. We derive a *cis-cis* / *cis-trans* ratio of ≤ 25 , consistent with the smaller energy difference between both conformers compared with the relative stability of *trans*- and *cis*-formic acid (HCOOH). Finally, we analyze the abundance of carboxylic acids in different astronomical environments, including star-forming regions, asteroids and comets, which enabled us to prove an overall good correlation between their relative molecular abundance; these acids seem to survive the star-formation process.

In summary, the interstellar detection of carbonic acid, HOCOOH, deepens our understanding of the levels of interstellar chemical complexity, and will be of great relevance to unveil the role of HOCOOH within both carbon and oxygen interstellar chemistry. This research work will also open a window to perform further coordinated observational, theoretical and laboratory efforts aiming to discover molecules with an extremely low dipole moment, based on the detection of other moderately higher-in-energy conformers with sizable dipole moments. This fact will be of great relevance for high-Tkin sources such as Galactic Center molecular clouds (i.e. G+0.693), hot cores and corinos, which are able to populate these high-energy species efficiently.

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Non-Covalent Interactions in Carbon Dioxide Clusters: Comparison Between the Thiophenol-CO₂ and Benzylmercaptan-CO₂ Dimers Using Microwave Spectroscopy

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Non-Covalent Interactions in Carbon Dioxide Clusters: Comparison Between the Thiophenol-CO₂ and Benzylmercaptan-CO₂ Dimers Using Microwave Spectroscopy

Carbon dioxide (CO₂), as a greenhouse gas causing global warming, has received great attention concerning its pollution effects and reactivity.¹ Hence, various strategies have been implemented to reduce the atmospheric concentration of CO₂ for instance, separation, storage, and utilization.² The investigation of the noncovalent interactions involving CO₂ could help understanding CO₂ aggregation and reactivity in the atmosphere. Presently, only a few clusters of CO₂ and sulfur molecules have been studied using rotational resolution.³ In this work, we have measured the microwave spectra of the clusters of thiophenol-CO₂ and benzylmercaptan-CO₂ using broadband chirped-pulsed microwave spectroscopy. Only one isomer was observed for both clusters, with dominant C⋯π and C⋯S non-bonding interactions. The experiments are supplemented density functional theory and

Natural Bond Orbital (NBO) calculation. Details of the experimental and computational results on this problem will be offered during the conference.

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On the use of in-situ non-invasive spectroscopic techniques to unveil ancient artistic materials

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Heritage science has one of its most interesting fields of research on the analysis of colour materials of what ancient Artworks are made of. In the last few years, special attention has been given to in-situ non-invasive approaches, such as the use of mapping elemental analysis (MA-XRF) and molecular analytical techniques (UV-Vis-NIR-FORS and hyperspectral imaging analysis). In this work, the use of these approaches at HERCULES Lab will be presented, highlighted with some case studies involving the analysis of ancient artworks, such as the analysis of ancient Ivory or the characterization of pigments and dyes in medieval and renaissance illuminated manuscripts.

Invited talks / 53

Application of X-ray spectroscopy instrumentation in Forensic Sciences

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Most forensic studies deal with the identification and characterization of a sample, which is the evidence of some crime activity, comparison of samples coming from different sources, and interpretation of the results obtained in the context of the events. X-ray instrumentation has been commonly used in forensic science and also in some related fields such as Cultural Heritage objects authentication. Main strengths are its non-destructive nature, thus preserving crime evidences and materials integrity, its ability to identify chemical compounds, to determine elemental chemistry and, in some cases, elemental speciation. Moreover, the versatility of the X-ray techniques permits the analysis of very diverse materials, -inorganic, organic, metals-, in powder, solid or liquid forms.

Different X-ray spectroscopy based tools, just as many other analytical techniques, have been applied for the analysis of crime evidences. Classical X-ray based techniques used in forensic work are X-ray powder diffraction (XRD), X-ray fluorescence (XRF), X-ray imaging and energy dispersion X-ray emission linked to an electron microscope (SEM-EDX). These complementary techniques are mainly used for micro- and macro- trace analysis. Conventional macro-XRF, whilst attractive for the forensic analyst, sometimes cannot be applied because in the majority of cases crime scene specimens are microscopic in nature. The common bench-top XRF systems have analysis spot of perhaps 2–4 cm, and are unsuited to perform, for instance, analysis of a 100 µm pieces or even less size.

During the last decades, noticeable development was made in the instrumental aspects of X-ray spectrometry, especially in the improvement of X-ray optics and detection systems. All this resulted in a wide variety of instrumentation becoming available nowadays. Significant advances in focusing optics (development of collimators and polycapillary lenses) have promoted the design of micro beam sources for the analysis of small regions by conventional X-ray instrumentation. The use of

automatized XYZ stages allows the possibility to choosing point, line profile or mapping analyses. A microscopic particle from a crime scene can be directly analysed without any sample preparation, simply located using optical cameras, and subsequently characterized for elemental content.

Poster Session / 54

Chemical characterization of microplastics by small-spot Energy Dispersive X-ray Fluorescence

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The presence of (micro)-plastics in different aquatic environments is a matter of world concern that has been gaining importance in recent years due to its potential impact on the environment and human health. (Micro)-plastics have been found in practically all types of water bodies and the presence of metals in these materials, either due to their manufacture or through adsorption processes, can be very harmful. Some toxic metals such as Pb, Hg, Cd and Cr present in (micro)-plastics can be released into the water and this fact can negatively affect ecosystems due to their persistence.

The most commonly used methods for the determination of metals in (micro)-plastics require carrying out acid digestions with microwave ovens and subsequent analysis with spectroscopic techniques and therefore require a previous treatment of the sample in which dangerous and harmful reagents such as strong acids and oxidizing agents are used.

The main objective of the work is the development of a non-destructive analytical methodology focused on the use of X-ray fluorescence spectroscopy (XRF) for the multi-elemental analysis of (micro)-plastics. In order to develop this method, it was necessary to determine the elemental composition of a set of plastic samples through their digestion and subsequent analysis by means of ICP-OES, in order to use them as standards to calibrate the micro- XRF instrumentation.

Once the quality of the results obtained with the methodology developed through the analysis of certified reference materials was verified, the method was applied to the analysis of (micro)-plastic samples collected in the Mediterranean Sea and the Atlantic Ocean. The results obtained have been promising and the determination of metals in the samples has been achieved without the need to treat previously the sample. It has been observed that the elements most present in these samples are Ca, Ti, Fe, Cu and Zn. However, in some samples it was also possible to determine appreciable contents of more toxic metals such as Cr and Pb.

Poster Session / 55

Exploring Chemical Pathways in Molecular Clouds: Unraveling CS Chemistry through CH + S, CS + H, and C2 + S Reactions

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Carbon monosulphide (CS) is among a few sulfur-bearing species that have been widely observed in all environments, including the most extreme ones such as diffuse clouds. Moreover, it has been widely used as a tracer of gas density in the interstellar medium in our Galaxy and external galaxies. Therefore, a full understanding of its chemistry in all environments is of paramount importance for the study of interstellar matter. We performed ab initio calculations to characterize the main features of all the electronic states correlating to the open shell reactants. For CH + S, we calculated the full potential energy surfaces (PES) for the lowest doublet states and the reaction rate constant using a quasi-classical method. For C2 + S, the reaction can only occur through the three lower triplet states, all of which exhibit deep insertion wells. A detailed study of the long-range interactions for these triplet states allowed us to apply a statistical adiabatic method to determine the rate constants 1.

Our comprehensive theoretical study of the CH + S → CS + H reaction provides valuable insights into its temperature dependence. We have observed that the reaction rate remains nearly constant within a wide temperature range of 10–500 K, with a consistent value of $5.5 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ at temperatures above 100 K. Notably, this rate is consistently lower by a factor of approximately 2-3 compared to the rate predicted by the capture model. In contrast, the rate of the C2 + S → CS + C reaction exhibits pronounced temperature dependence. At lower temperatures, the rate is approximately $2.0 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$, gradually increasing to around $5.0 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ for temperatures exceeding 200 K. Importantly, our detailed modeling, which takes into account electronic and spin states, yields a rate that is approximately twice as high as the currently employed rate.

1 Carlos M. R. Rocha, Octavio Roncero et al. <https://arxiv.org/pdf/2307.00311.pdf>

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Poster Session / 56

Water-Induced Energy Reordering of the Equilibrium States in an Imine-Based Molecular Switch

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Imine-based molecular switches were recently developed, and so their properties remain largely unexplored¹. Their potential to perform multi-step unidirectional rotations make them an important addition to the existing nanomotor toolbox². 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. The different energies of the various conformations means that, when in equilibrium, they exist with a given distribution. In solution, the interactions between the solvent molecules and the solute can alter the energetic balance of the conformers³. In this contribution we present a rotational study of a chiral camphorquinone imine. From our investigations we uncovered the structure of the open (E) and closed (Z) configurations of the switch and their first and second order microsolvated species, which were validated using experimental isotopic information. The predicted favoured stability of Z over E in the gas phase is experimentally shown to reverse in the presence of water, with increasing abundance of E over Z with increasing cluster size. In an attempt to understand the origin of this reversal, we used quantum chemistry calculations to interpret the observed change in stability for isolated versus

solvated scenarios. We will discuss our findings and the suitability of rotational spectroscopy to engage in structural studies of highly functional micro-solvated molecular systems.

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Invited talks / 57

Laser-induced breakdown spectroscopy: challenges and perspectives for scientific, technological and industrial applications

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Laser-induced breakdown spectroscopy (LIBS) has emerged as a versatile technique for elemental analysis, offering high-resolution and real-time measurements, while being minimally destructive. This powerful analytical technique holds significant promise in various fields, including academia, technology, and industry. However, several challenges hinder its widespread adoption and limit its potential impact in these sectors.

In INESC TEC we work closely with all these domains trying to identify and address these challenges while exploring the prospects for LIBS in different applications. Some examples of LIBS implementation in prospection and geology 1, in cork 2 and wood industries and in electrodes assessment for Li batteries will be shown. The main challenges such as quantification, lack of data analysis algorithms, integration with complementary techniques and adaptation to diverse sample matrices, among others, will be addressed.

Despite the challenges, several promising opportunities are emerging in the LIBS landscape. The conviction that gold standard techniques are always the best option is getting more and more contradicted. Novel methods, such as LIBS, are often fit for purpose offering enough data quality, but also unsurpassed savings in time, labor and price.

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Poster Session / 58

Laser-induced breakdown spectroscopy as a sorting tool for high quality recycled wood chips in industrial environment

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Particleboard (PB) is produced using 50% to 75% recycled wood, with the possibility of reaching 100% recycled content, while Medium Density Fiberboard (MDF) is mostly made with virgin wood ¹. The presence of physical and chemical contaminants in wood waste may compromise its incorporation in recycling facilities. While physical contaminants as nails, joints, glass, textiles, etc., are easier to detect, chemical contaminants are more challenging and need good quality analytical techniques for detection and identification.

This work aims to develop an innovative industrial-scale sorting tool to produce high quality recycled wood chips from used MDF and other non-hazardous wood waste, minimizing the risk of incorporation of contaminated chips/fibers into PB or MDF production. Taking advantage of its undeniable speed, portability, low capital and maintenance costs associated, Laser-induced breakdown spectroscopy (LIBS) was chosen as the best technique to perform this task.

A LIBS system with a Q-Switch Nd:YAG laser (1064 nm), operating at 20 Hz with pulses of 8 ns duration and ~51 mJ was used. Acquisition range was between 180 and 926 nm. Wood samples from different processing states were placed in a sample holder and analysed by LIBS, obtaining an elemental distribution map with a step size of 1 cm. To help reduce the number of spots analysed, and consequently the time of analysis, a SLIC algorithm was applied to create super-pixels based on the color and spatial distances, creating delimitations similar with the sample shapes better defining the areas to be analysed. Preliminary results shown that Titanium (Ti) and Lead (Pb) were present in the samples under study, particularly in the wood painted areas. Results were displayed using a combination of photogrammetry with spectral imaging techniques ². LIBS showed to be a powerful technique to detect heavy elements in the wood waste, identifying contaminated wood pieces that must be discarded instead of being used for particleboard fabrication.

Figure 1.

! [A. LIBS generated map for the distribution of Pb (405.85 nm) in an agglomerate of wood waste. B. Superpixels obtained applying the SLIC algorithm to a photograph of the sample. C. Superpixels filled with the average intensity of LIBS for each cluster. D. Interactive 3D model of the wood sample overlaid with the spatial distribution of Lead.]

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Figure 1. <https://drive.inesctec.pt/s/sf93YmHny4JW8bw>

Poster Session / 59

Unveiling the molecular conformation of 2-(2-pyridyl)benzo[b]thiophene using jet-cooled rotational spectroscopy

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Sulfur-containing heterocycles hoard a major scientific interest for its key role in natural and pharmaceutical products [1,2]. One of these compounds is 2-(2-pyridyl)benzo[b]thiophene, a heterobiarylic molecule whose structural insights are addressed here using computational methods and rotational spectroscopy.

Theoretical calculations have included density functional predictions (B3LYP-D3 and B2PLYP-D3) for the title molecule and its monohydrate, using Ahlrichs (def2-TZVP) and Pople basis sets (6-311G(d)). The investigation of the rotational spectrum used chirped-pulse broadband Fourier transform microwave spectroscopy in a supersonic jet expansion, operating in the 2-8 GHz region.

Two conformers were detected in the rotational spectrum. The cis-locked geometry has emerged as preferential by ca. 2.25 kJ mol⁻¹, although transitions associated with the trans species have been also detected. The rotational constants and the nuclear quadrupole coupling constants determined experimentally present a satisfactory agreement with the computational predictions. Both conformers are effectively planar, with a small inertial defect caused by low-frequency vibrations. Finally, the non-covalent interactions have been rationalized using the non-covalent interactions index and natural bond orbitals calculations. Both methods confirm the role of the N...S interaction to drive the molecular orientation.

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Poster Session / 60

NEXT - An international network for Nonlinear Extreme ultraviolet to hard X-ray Techniques

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Extreme Ultraviolet (EUV) table-top sources and soft to hard X-ray Free Electron lasers (XFELs) have opened a new era in science, providing ultrashort, coherent, and tunable pulses that are used to perform cutting-edge experiments in Atomic and Molecular physics, Condensed Matter Physics, Biology and Chemistry. However, most of the reported studies rely on linear light-matter interactions, which are fundamentally limited in the dynamical information they can provide. On contrary, nonlinear radiation-matter interactions have proven to be a powerful tool to unravel hitherto inaccessible properties.

The NEXT collaboration will capitalize on pioneering promising results, reported over the last decade, to create the first concerted experimental and theoretical effort aimed at implementing EUV/X-ray nonlinear spectroscopies at lab-based and large-scale facility short-wavelength sources, especially XFELs.

In this short presentation we would like to advertise this new initiative and the recently funded COST Action (CA22148), which will be located in Spain (IMDEA Nanoscience) and should become active in autumn 2023. We would like to particularly encourage the research groups in Spain and Portugal to consider joining the Action and contribute to this new endeavour.

Oral communications / 61

Ultrafast X-ray and optical studies of charge carriers dynamics in colloidal quantum dots

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The interest in CuInS₂ (CIS) quantum dots (QDs) has increased significantly in the past few years due to broad range of their potential applications, such as photodynamic therapy or solar cells¹. This owes to extraordinary optoelectronic properties of this material, such as broad photoluminescence with a large Stokes shift and long charge carrier lifetimes. To elucidate the origin of these unique features, several mechanisms for the radiative recombination in CIS QDs have been proposed theoretically and experimentally.

In this work we aim to understand and confirm the possibility of observing the radiative recombination resulting from an electron in the conduction band and a hole in the so-called confined hole state [2-3], next to the effects of stoichiometry and Zn doping on the passivation of the QDs and the formation process of the CHS⁴. The range of such possible hole trapping states would explain the broad photoluminescence and the large Stokes shift.

We approached these questions through a combination of ultrafast laser and XFEL pump-probe techniques complemented with steady-state synchrotron measurements. The element and oxidation state specificity of X-ray techniques will serve as a direct probe to track recombination and localization dynamics of photogenerated holes, while optical probes will follow the electron dynamics. We focused our X-ray studies on following the oxidation state of Cu via femtosecond-resolved Cu K-edge XANES and comparing the electronic and geometric structures of different samples obtained from static XANES and EXAFS at Cu, Zn and S K-edges. This allowed us to gain insights and correlate the observed charge carriers dynamics with the underlying CIS QD structures, the degree of their surface passivation and the different Zn doping levels.

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Invited talks / 62

NEXT: a neutrinoless double beta experiment

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NEXT (Neutrino Experiment with a Xenon TPC) is an experiment that searches for neutrinoless double beta decay in ¹³⁶Xe using a high pressure xenon (HPXe) gas time projection chamber with

electroluminescent (EL) amplification. The aim is to determine whether neutrinos are Majorana particles (i.e. they are their own antiparticle) or not, having huge implications in cosmology and particle physics.

The NEXT collaboration has established a path towards the accomplishment of this task through different phases. The NEXT-White (NEW) detector was a prototype that operated at Laboratorio Subterráneo de Canfranc (LSC) between 2016 and 2021 to validate the HPXe-EL technology in a large-scale detector. Its main goals were fulfilled: validation of the background model¹, demonstration of a great energy resolution² and topological discrimination³, and measurement of the two-neutrino double beta decay half-life⁴. NEXT-100 is a double sized version of NEW, currently under construction at LSC. It is expected that NEXT-100 will achieve, in the search of neutrinoless double beta decay, similar limits to those of its main competitors in the hundred-kilogram scale. Nevertheless, sensitivity to longer half-lives requires detectors with larger exposures. NEXT-HD is a future tonne-scale HPXe that will pursue the goal of the experiment after NEXT-100.

In this talk I will review the latest NEXT-White results, the construction status of NEXT-100, and R&D efforts toward future tonne-scale detectors.

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Unveiling the Aggregation Patterns of Curcumin and Piperine Mixtures in different Polar Media: A Molecular Dynamics Investigation

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Curcumin, a natural yellow pigment derived from the rhizome of turmeric (*Curcuma longa* L.), possesses significant biological properties. Nonetheless, its therapeutic potential is hindered by its limited bioavailability.¹ To address this challenge, and thus enhance the bioavailability and pharmacological efficacy of curcumin, one proposed strategy is the co-administration of curcumin with piperine, a bioactive compound of black pepper (*Piper nigrum* L.).² Regardless of the extensive scientific research that has been conducted on the curcumin and piperine systems, it is still clear the lack of knowledge at the molecular level of these compounds behavior in solution.³ In this study, by employing molecular dynamics (MD) simulations, we intend to contribute to a better understanding of the aggregation patterns of curcumin (both enol and keto tautomers) and piperine in water, ethanol, and water-ethanol mixture. In particular, we investigated the influence of piperine on the self-aggregation of curcumin, while analyzing the structural characteristics of the resulting aggregates. For the characterization of the formed aggregates, a range of properties were calculated, such as: radial distribution functions; distances between molecules or atoms; interaction energies and the number of hydrogen bonds; clustering analysis. In the MD simulations involving two solute molecules a rapid formation of curcumin dimers in water was observed, as a result of its low solubility, while piperine formed less stable dimers. In contrast, both curcumin and piperine showed limited ability to form dimers in the presence of ethanol. Larger and more complex aggregates were obtained when additional solute molecules were introduced in water solutions, characterized by stacked or cage-like structures.

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Atomic Calculations and Data Using the MultiConfiguration Dirac-Fock General Matrix Elements (MCDFGME) code

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The current accuracy of atomic calculations is impressive, allowing us to explain and probe novel and extremely rich physical phenomena. In turn, novel experiments constantly allow us to validate and adjust our theories and calculations. The atomic data we can calculate encompasses many physical interactions, providing a wide range of fields with the necessary data for their own studies.

The theory is there for us to use, however we must apply it in a practical manner for a variety of bound systems, which oftentimes require hundreds of thousands of separate calculations. This brings the question of how are we going to, in a more practical and autonomous manner, implement our theories to produce usable atomic data?

In this talk I will show you how we currently utilize the MCDFGME code 1 to perform atomic calculations on a variety of atomic systems and obtain useful, reliable and accurate atomic data. I will also bring attention to a few details of the calculation method which, if not considered, could result in erroneous calculations and atomic data. Finally, I will show you recent atomic data that we have calculated using this code, which can also be obtained experimentally.

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Poster Session / 65

The Innovative PISA Concept in Medical Imaging

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Medical imaging plays a crucial role in the diagnosis and treatment of various diseases and conditions. It allows healthcare professionals to visualize internal structures and processes of the body

without the need for invasive procedures. Medical imaging techniques include x-ray, computed tomography (CT), magnetic resonance imaging (MRI), and ultrasound, among others. Position sensitive gas detectors are a type of detector used in medical imaging applications to detect and measure ionizing radiation. They are particularly useful in detecting high-energy particles such as gamma rays and x-rays, which are commonly used in medical imaging. They work by ionization of the gas medium inside the detector, and then measuring the resulting signal to determine the location and intensity of the event. These detectors have a number of advantages over other detectors and techniques, including good spatial resolution, fast response times, easy scaling-up to large detection areas at a lower cost, making them ideal for medical imaging applications. In this presentation, we will explore the application of the Photon Induced Scintillation Amplifier (PISA) concept as a position sensitive gas detector in medical imaging. We will show some preliminary results of the studies performed so far.

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Absolute primary scintillation yield in Xe for electrons and alpha particles

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Primary scintillation in Xe for electrons and alpha-particles Content Gaseous xenon (GXe) is playing an increasingly significant role in important areas of neutrino physics such as double beta decay and double electron capture experiments and is a potential alternative to MeV-region γ -ray imaging. The precise knowledge of the xenon response to radiation interactions in both scintillation and ionization channels is of utmost importance for the exact understanding and modulation of xenon radiation detectors. The primary scintillation yield, i.e. the mean energy required to produce a scintillation photon, w_{sc} , of GXe is far less understood than the ionization yield due to the limited number of studies in the literature. While for 5.5-MeV α -particle interactions the w_{sc} -value was measured to be in the 34-60 eV range, for electrons, measuring the primary scintillation produced by x- and γ -ray interactions, the w_{sc} -value was measured to be in the 61 - 111 eV range. The average energy expended per excited atom in GXe is expected to be similar for x-, γ -rays or electrons and almost equal to that obtained for α -particles. However, the results presented in the literature are inconsistent with that expectation and not fully understood, as can be only partially ascribed to the different gas density and/or drift field conditions. One may also pose the question of a dependence of w_{sc} with photon energy. We carried out a systematic study on the absolute primary scintillation yield in Xe under reduced electric fields in the 70–300 V/cm/bar range and near atmospheric pressure, 1.2 bar, using a Gas Proportional Scintillation Counter. Our results are supported by a robust geometrical efficiency simulation model. Our experimental w_{sc} -values agree with both state-of-art simulations and literature data obtained for α -particles.

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Strong Field QED Analysis With Bayesian Model Selection for He-Like Ions

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Quantum Electrodynamics (QED) effects have been tested and measured in multiple systems, including free electrons, atomic and highly charged ions systems. Frequentist statistical analyses either point to a possible deviation from the theory prediction 1 of $n = 2 \rightarrow 1$ transitions energy in two-electron systems with a dependency of Z^3 , Z indicating the nuclear charge, or find no disagreement [2-5]. We present a Bayesian statistical approach method using the nested sampling algorithm, implemented in the nested fit code package 6, to quantitatively evaluate different deviations via probability inference from Bayesian evidence. The deviations are modeled as aZ^n and aZ^{n+b} functions, a and b being free parameters, for the measurements of multiple transitions on helium-like ions for $Z = 12 - 92$. We evaluated these modeled deviations from the current theory predictions [7, 8] for the $1s2p\ 1P1 \rightarrow 1s2\ 1S0$ (w), $1s2p\ 3P2 \rightarrow 1s2\ 1S0$ (x), $1s2p\ 3P1 \rightarrow 1s2\ 1S0$ (y), and $1s2p\ 3S1 \rightarrow 1s2\ 1S0$ (z) radiative transitions. We found that the function with highest probability corresponds to a deviation with $n \approx 4.5$, but has a marginal statistical significance of 2.7σ with respect to the zero model with no deviation from the theory. The additional analysis of the $n = 2 \rightarrow 2$ ($Z = 5 - 92$) transitions provided an even lesser evidence for either a constant or power model deviations. Finally, we investigated on the impact of possible future high-accuracy experiments on high- Z ions. In particular, we determine the minimum required accuracy for a meaningful test of possible deviations. We construct hypothetical measurement data in the Z region of interest, vary its uncertainty and value, and survey the behaviour of the probability distribution over the selected models for each combination. Such an analysis will allow for a better design of future experiments for the search of new QED contributions or even new physics, like milli-charged particle interactions.

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Real-time observation of conical intersection in biomolecules

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Conical intersections (CIs) are regions of the potential energy landscape of a molecule where the electronic and nuclear degrees of freedom become strongly mixed and the Born–Oppenheimer approximation breaks down. CIs are ubiquitous features in the photophysics and photochemistry of molecules and can be considered as “doorways” through which the photoexcited wavepacket is efficiently funneled to a lower-energy electronic state. CIs play a dual role in the interaction of biomolecules with light: either to promote efficient conversion from a reactant to a product state in a photochemical reaction or to enable efficient dissipation of excess electronic energy, preventing a potentially harmful photochemical reaction 1. An example of the first case are visual opsin proteins, in which the photoexcited retinal chromophore exploits a CI to promote ultrafast photoisomerization to a ground-state photoproduct which triggers visual transduction. An example of the second case are nucleobases, the building blocks of DNA, for which CIs are used to promote rapid dissipation of excited state energy, preventing photoreactions which could damage the genetic code. Given the extreme speed of the processes leading to CIs, ultrafast optical spectroscopy is the elective tool for their observation. However, the direct visualization of a wavepacket passing through a CI is

challenging, because the energy gap between the interacting levels changes very rapidly over a short time, calling for the combination of high temporal resolution and broad spectral coverage. In this talk I will present examples of real-time visualization of CIs in biomolecules (opsin proteins 2 and nucleobases [3, 4]) using a specially developed ultrafast transient absorption spectroscopy system combining sub-20-fs time resolution with broad frequency tunability, from the UV to the infrared 5. I will also discuss the potential of X-ray free-electron lasers to open new spectroscopic windows for the detailed study of the CI dynamics, via element-specific probing of ultrafast electronic and structural dynamics.

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Strategies for improved light detection in noble element radiation detectors

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The development of radiation detectors has seen significant advancements over the past decades, particularly in those relying on electroluminescence. Optical time projection chambers (OTPCs) have become the preferred choice in the field of direct dark matter searches (more specifically in WIMP searches), having also been considered for neutrino experiments. Dark matter experiments examples include XENON, LZ, DarkSide, and CYGNO where directional information is expected to be explored. Moreover, these detectors have found applications in nuclear physics, such as in the study of $\beta\beta_{0\nu}$ decay (NEXT) and 2p-decay and related processes (Warsaw-TPC).

Even though significant progress has been observed in the development of these detectors since the first works in the 1960s, the optimization of the light collection efficiency remains an important concern. Historically, these structures were mostly made up of meshes or conventional micro-pattern gas detectors (MPGDs) designed for avalanche mode and working mainly in quenched gases.

Given the expected scalability of most of the aforementioned detectors, light production and collection pose unique challenges. Dealing with alignment, and the use of meshes or wires spanning large areas presents practical limitations. In most cases, relying on scintillation originated in charge avalanches will affect not only the energy resolution but also impact the attainable spatial resolution. In addition, the use of lenses, while enabling the reduction of the number of optical sensors required to read large areas and improvement of the optical gain, may limit the spatial resolution attainable, introducing undesirable optical effects (e.g. aberrations). Nevertheless, it is important to consider techniques that can mitigate potential adverse effects associated with the current amplification structures and readout.

In this work, a brief overview of the evolution of electroluminescence studies is given, along with strategies to address some of the main challenges faced in the development of such detectors. Alternative structures, GEM-based, capable of providing higher optical gains without relying on avalanche multiplication, thus enhancing energy resolution and detector stability (while eliminating ion back-flow), will be presented.

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Real-time imaging and control of electron motion in molecules: towards attochemistry

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Photoinduced electron transfer and charge transfer processes occurring in organic and inorganic materials are the cornerstone of technologies aiming at the conversion of solar energy into electrical energy and at its efficient transport. The early stages of these processes occur in the attosecond time scale, the natural time scale for electronic motion in atoms and molecules. Accessing this time scale requires the use of light pulses with a duration below the femtosecond, which were first produced in the lab at the dawn of this millennium. The first attosecond experiments aiming at the observation of electronic motion in organic molecules date from 2014 ¹. The usual approach in these experiments is to employ an attosecond pulse to generate an electronic wave packet that subsequently evolves under the influence of the nuclear motion and to interrogate the system with a second pulse at a given time delay in order to obtain a picture of the system at that particular time. By varying the delay between the two pulses, one can thus obtain a sequence of frames or the “movie” of the electronic motion.

The experiments usually record photoelectron and/or fragmentation yields as a function of the temporal delay between the two pulses with attosecond resolution. However, in spite of the successful observation of sub- and few-fs dynamics in the recorded yields [1-4], it is not yet clear how the early electron dynamics leaves its signature in molecular fragments that may be created long after those initial steps (usually after going through a series of non adiabatic processes) or why one should expect a reminiscence of such electron dynamics at all. To answer these questions, one must understand i) the electronic excitation or ionization induced by the first pulse, ii) the coupled electron and nuclear dynamics that follows, iii) the interaction of the second pulse with a molecular system in a coherent superposition of states, and iv) the coupled electron and nuclear dynamics that follows the last step and eventually leads to fragmentation of the molecule. Every step is in itself a theoretical and experimental challenge for molecules containing more than two nuclei. In this talk I will review recent experimental and theoretical efforts to account for these four steps and discuss the optimum conditions to visualize electron dynamics in molecules ⁵.

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Poster Session / 71

X-ray Imaging with GEM-based detectors using Single-Pixel Imaging techniques

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X-ray imaging is an invaluable tool for noninvasive analysis in many fields ranging from basic science to medicine and security. The development of low-dose large area imaging solutions still represents an important challenge for various applications.

One solution to the imaging of large areas lies in the development of novel computational imaging systems that can overcome the limitations imposed by hardware, relying instead on numerical processing power. The single-pixel detector, depending on the application, may offer a competitive edge over conventional cameras (being a cheaper alternative to the multi-pixelated solutions). In addition, the single-pixel detector can be used to achieve improved detection efficiency, faster timing response, and good spatial resolution with low radiation dose. Moreover, this technique enables detectors to image through diffuse mediums, increasing the image quality at significant depths, solving the depth penetration issues of other imaging methods.

Another advantage of single pixel imaging is that it can be combined with compressive sensing, which significantly reduces the data storage and data transfer requirements, an important consideration for remote sensing applications or when the problem is high dimensional such as hyperspectral imaging.

In this work, we explore the application of single-pixel imaging techniques to produce two-dimensional images with high temporal resolution, using only a single detector (bulk detector). The setup, based on the application of Hadamard patterns, showed promising results, proving the ability of the system to acquire 4x4 pixel images using thin PLA masking (up to 5 mm thickness). Both simulation, using GEANT 4, and experimental setup, based on a time projection chamber (TPC), used in this work to demonstrate this technique will be reported here along with the first results.

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Exploring Quantum Tunneling in Organic Reactions

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For nearly a century, the role of quantum mechanical tunneling (QMT) in organic chemistry remained barely unrecognized. The interpretation of chemical selectivity has been done solely based on the classical paradigms of thermodynamic and kinetic control. However, it has recently been shown that these paradigms do not cover all aspects of chemical reactivity and QMT can also direct chemical selectivity.¹ QMT is very sensitive to the potential energy barrier width of a reaction, which is measured by the mass-weighted displacement of the atoms involved on it. Reactions that occur exclusively through higher, yet narrower, potential energy barriers than other alternative paths operate through tunneling control. There is the perspective that tunneling control will be essential to fully understand chemical reactivity.²

Direct observation of QMT organic reactions has been accomplished in experiments performed at cryogenic temperatures, under which thermal activation is impossible.³ In the present communication, two representative examples of such experiments, related to reactions of aryl nitrenes, will be showcased through a multidisciplinary approach involving organic synthesis, spectroscopy, photochemistry, kinetics and computational chemistry. i) A novel approach where H-tunneling is activated by narrowband IR light irradiation.⁴ Those results provide the proof-of-concept of an exciting novel strategy to attain control over QMT, opening new avenues to direct chemical transformations. ii) An unprecedented occurrence of two simultaneous conformer-specific reactions that occur through QMT, which selectivity can only be interpreted based on tunneling control.⁵ Those results highlight the current limitations of the classical paradigms of chemical reactivity and the need to develop a thoroughly understanding of QMT implications in organic reactions.

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Present and Future of the ALBA Synchrotron

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Synchrotron light is a key instrument for the scientific approach towards a sustainable world, and the ever-growing communication among the different synchrotron facilities boosts their scientific and socio-economic impact at regional and global levels.

Over the past decade, the ALBA Synchrotron, the Spanish 3rd generation light source, has become an important pillar of the Spanish and European Research Area, providing research capabilities and a wide range of state-of-the-art instrumentation to a community of more than 7000 academic and industrial users. With its ten operational experimental beamlines, while four more are being put into operation and with the creation, in collaboration with other institutions, of an electron microscopy center, it is an essential tool to address society's most urgent challenges.

ALBA is prepared to leap to the 4th generation, aiming at increasing its performance, reinforcing its role on the user community and on the industrial use of the instrumentation, as well as its educational vocation and training capacity. ALBA II, whose project has just started and is planned to be fully operative in the '30s, will combine the upgrade to low-emittance storage ring with the construction of new fully-optimized beamlines, the refurbishment of part of its instrumentation, and the evolution of the data infrastructure.

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Optical negative ion drift operation at nearly atmospheric pressure

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We are going to present for the first time Negative Ion Drift (NID) operation in He:CF₄:SF₆ at nearly atmospheric pressure within a Time Projection Chamber (TPC) with optical readout via PMTs and scientific CMOS camera (sCMOS). These results have been obtained in the context of the CYGNO/INITIUM project, for the development of high precision 3D TPC for directional direct Dark

Matter searches. NID operation is a peculiar modification of the TPC principle by which, thanks to the addition of an highly electronegative dopant to the gas mixture, anions act as image carriers rather than electron, strongly reducing down to the thermal limit (or below) the diffusion during drift. This characteristics allows for the use of longer drift distances, combined with improved tracking. We are going to illustrate the analysis of both PMTs and sCMOS data, that are not only able to reproduce He:CF₄:SF₆ mobility as from previously published papers with charge readout, but also display an impressive reduction of the diffusion during drift, as much as half of classical electron drift with He:CF₄ along 12.5 cm. The observed features can significantly boost the performances of any experimental approach that requires high precision imaging TPCs, such as, among the others, X-ray polarimetry, neutron spectroscopy, Migdal effect measurements and tracking in high energy physics.

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Modelling Enzyme Activity Behind Antimicrobial Resistance

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please see attached

Oral communications / 76

Photophysics of protonated vanillin in the gas phase: a laser action spectroscopy and theoretical approach

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Protonation and deprotonation processes in derivatives of aromatic systems play an important role in various areas of chemistry. The 'competition' between different centers to accept or donate a proton depends on a number of parameters, including electron density effects. This competition can result in the formation of different tautomers, each one having a different photophysical behavior. Vanillin serves a model system with three functional groups exhibiting distinct characteristics (see Figure 1). In this work, we first set out to determine the protonated tautomers formed in vanillin from an electrospray source, using different laser action techniques (such as IRMPD room temperature and UVPD in cryogenic ion trap). The results indicate that protonation predominantly occurs at the oxygen atom of the carbonyl group (C=O). Moreover, through the analysis of the results, we were able to unambiguously determine the configuration of the observed protonated tautomer. These results are partially in agreement with the order of stability predicted by theoretical calculations with DFT and MP2 methods. We will discuss apparent deviations from theoretical predictions concerning the observed isomer. Furthermore, both theoretical calculations and experiments reveal a spectroscopic pattern similar to that of protonated benzaldehyde (benzene with HC=O group) in terms of electronic absorption, highlighting the significant influence of the HC=O group on the photophysics of the system. Finally, we will briefly address the challenges encountered in the analysis of the deprotonated species, such as the interpretation of the IRMPD spectrum.

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Investigating Heavy Metal Elemental Distribution in Zebrafish (Danio Rerio)

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In this study, we investigated the elemental distribution of heavy metals in Zebrafish (*Danio rerio*) using an X-ray fluorescence system that relies on a gaseous detector. The primary objective was to analyze the presence and spatial distribution of heavy metals within the tissues of Zebrafish specimens. The employed X-ray fluorescence system, which incorporated a THCOBRA detector, allowed for precise and non-destructive analysis of the elemental composition in the Zebrafish samples. This advanced technique provides valuable insights into the bioaccumulation and localization of heavy metals in this important animal model, aiding in the assessment of potential environmental contamination and its implications for aquatic ecosystems.

Poster Session / 78

Photodissociation dynamics and alignment of CH₂BrI in the third absorption band at 193 nm

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The photodissociation of dihalomethanes have received significant attention due to its role in producing pollutant species and ozone depletion.¹ Moreover, CH₂BrI presents an intricate structure of excited electronic states and a high bond selectivity. For instance, the A absorption band was attributed to C-I dissociation, while the A' band corresponds to C-Br bond fission.² However, the third band (B band) has not been investigated deeply.³

The detection of atomic iodine I(²P_{3/2,1/2}) and bromine Br(²P_{3/2,1/2}), using a combination of laser pump-and-probe and slicing imaging techniques coupled to (2+1) REMPI, show the presence of two main contributions. Combining the experimental results with high ab initio calculations, we assigned the faster contribution to a predissociation through the 9A' state. Meanwhile, the slower contribution was attributed to a secondary dissociation after absorbing a second 193 nm photon. Due to geometrical restrictions, this process was favored through the C-Br dissociation rather than the C-I bond cleavage. The calculated anisotropy parameter supports the proposed mechanism.

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Poster Session / 79

Comparison of the photodissociation dynamics of alkyl nitrites in the A and B absorption bands

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Alkyl nitrites (R–ONO, R=CH₃, *n*-C₃H₇, *t*-C₄H₉) have been widely studied due to the efficient photodissociation and formation of NO fragment.[1,2] The absorption spectra of all these molecules present two bands. A first band characterized by a clear vibronic structure, and a second more intense band which extends to the VUV energy region.[2,3] In this work, three different alkyl nitrites were studied, CH₃ONO, *n*-C₃H₇ONO, and *t*-C₄H₉ONO, so a comparison of the hydrocarbon chain on the photodissociation dynamics could be made.⁴ The study was performed in the two absorption bands (A and B) independently. Pump-probe experiments using nanosecond laser pulses in combination with velocity map imaging detection of NO by (1 + 1) REMPI were carried out.

The results in the A band show a shift in the kinetic energy distributions as higher vibrational states for a fixed rotational quantum number $J = 19.5$ of the NO fragments were detected. By comparing the three molecules, a larger shift in energy is also present, a displacement previously observed in the studies of alkyl halogen molecules.⁴ Several differences in the shape of the kinetic energy distributions, and in the angular distributions, were also detected. Meanwhile, the B band shows a parallel transition in contrast to the perpendicular transitions observed in the A band. In this case, several contributions could be observed for each of the measurements performed.

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Dynamics of the photodissociation of methylamine: H and CH₃ displacement channels

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Due to its similarity with ammonia (NH₃) and because it has been observed in the interstellar medium,¹ methylamine (CH₃NH₂) has received considerable attention in the last decades. The molecular photodissociation of methylamine was studied using the pump-probe method with nanosecond laser pulses. The molecule was excited in the 198 – 203 nm range, and the generated photofragments were detected with the velocity map imaging (VMI) technique, studying the H-atom elimination and the N–C bond fission channels separately, combining experiment and theory.

On the one hand, the H-atom displacement channel presents two main dissociation pathways. One is attributed to the formation of CH₃NH(X) via a conical intersection (CI),^[2,3] while the other to CH₃NH(A), observed for the first time. On the other hand, the recorded images for the NH₂ + CH₃ channel show unstructured Boltzmann-type distributions; however, the speed-dependent anisotropy parameters reveal the presence of two dissociation mechanisms. With a similar landscape of the computed potential energy curves to the N–H bond fission, prompt dissociation of the C–N bond through the CI is proposed as a minor channel. In contrast, the kinetic energy distribution reflects a major slow dissociation in the ground state, which can arise from frustrated N-H bond cleavage trajectories or vibrationally-hot ground state NH₂ fragments.

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THCOBRA detector performance in mixtures of Kr/Xe mixtures

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The application of THCOBRA based detectors for X-ray imaging has been studied. The optimization of detector performance is intrinsically related with the study of the gas mixture capable of providing the better image quality. When operating in gas flow mode with a gas mixture of Ne/CH₄ (95/5), a charge gain of 10⁴ was achieved, together with an energy resolution of about 22% (@ 8 keV), and a spatial resolution close to 1.2 mm (for about 4 keV) were achieved. For pure Kr, in a sealed detector, the achieved energy resolution was 23% (@ 5.9 keV) and the spatial resolution was 650 μm (for 16.5 keV) ², allowing to improve detector performance when compared with its operation in Ne/CH₄ [3, 4]. In this work, detector performance in terms of charge gain, energy and spatial resolutions were studied, for different gas mixtures of Kr and Xe, namely 98/2, 95/5, 90/10 and 85/15. Results will be presented and compared with the previously achieved.

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Plenary Talks / 82

Surprising reaction dynamics of radical cations following electron ionization

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Femtosecond time-resolved measurements have provided the timescales of bond breaking and bond forming processes for a wide range of chemical reactions. Some chemical reactions such as those that

involve a collision with an atom or an electron, however, are very difficult to study by time resolved methods. This talk will focus on the reaction dynamics of radical cations far from equilibrium following electron scattering, a situation that occurs in electron-ionization mass spectrometry. These types of measurements are important because they can help refine methods for predicting molecular fragmentation patterns, which are essential for molecular identification. Lack of experimental dynamic information has prevented scientists from determining how fast the energy distributes and how it affects bond breaking and bond forming processes. Therefore, currently predicting the fragmentation pattern of a given molecule remains a challenge. We have developed a method for tracking multiple fragmentation pathways simultaneously following strong-field ionization. This talk will include examples of unexpected pathways that include roaming moieties, concerted dynamics, and intramolecular rearrangements, many occurring prior to intramolecular energy redistribution.

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Poster Session / 83

Molybdenum disulfide coated gold nanostructures for biosensing using SERS

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Molybdenum disulfide (MoS₂) is a two-dimensional (2D) semiconductor that has attracted significant attention due to its properties, such as a band gap energy dependent on the layers' number and a large specific surface area prone to chemical functionalization. These properties make 2D MoS₂ an excellent platform for optical sensing applications [1,2]. For example, the combination of MoS₂ layers with plasmonic metals (e.g. Au) allows the fabrication of materials with potential to detect a variety of biomolecules by exploring the surface-enhanced Raman scattering (SERS) effect [3,4].

Herein, we report our research on MoS₂ nanosheets prepared by a hydrothermal method that subsequently have been deposited on different types of substrates. These nanocomposites were firstly assessed for their SERS performance by using the dye rhodamine B (RhB) as the analyte, under a range of operational conditions, which included the deposition method and the type of underlying substrate used in such deposition process. The most intense Raman signal due to chemisorbed RhB was observed for the Au substrates coated with the MoS₂ layers. Hence, these platforms have been investigated to detect lactate in buffer medium, as an important biomarker used for sports performance monitoring. Hence, the immobilization of lactate dehydrogenase (LDH) on neat gold substrates was firstly performed envisaging the indirect detection of lactate using SERS. The vibrational data obtained in these experiments have been interpreted considering the specific recognition of lactate by the biofunctionalized substrates. Finally, we discuss preliminary research on the MoS₂ coated Au nanostructures in the SERS detection of lactate via the enzyme immobilization method mentioned above (see scheme in appendix).

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Exploring materials chemistry in flatland by applying surface spectroscopic methods

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Two-dimensional materials are comprised of single- or few-layers of atoms arranged in a crystalline lattice structure. These materials exhibit unique properties due to their ultrathinness and the ability to adjust the number of layers. The research field surrounding these materials has gained significant interest since the discovery of graphene and its derivatives 1. Recently, other 2D materials, such as few-layered transition metal chalcogenides, have also been explored 2. Moreover, researchers have been exploring surface chemical modifications on these layered materials, taking advantage of their large surface-to-volume ratios. In our research, we have investigated surface chemical modifications for graphene oxide and molybdenum disulfide colloidal suspensions. This talk emphasizes the application of spectroscopic methods in monitoring such surface modification processes aiming at developing functional 2D nanostructures. Specifically, we used Raman and fluorescence spectroscopies to study selected functionalized layered nanosystems, that were designed to respond to the presence of target analytes in solution. Overall, this research aims to contribute to the development of spectroscopic methods applied to 2D materials for optical sensors.

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Breakthroughs in Solar-Powered Lasers

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Solar-powered laser systems directly convert free broadband and incoherent solar radiation into narrowband and coherent laser radiation through an active medium, being considered as one of the most promising technologies in renewable energy research.

Our research group, led by Prof. Dr. Dawei Liang, was established more than a decade ago with the aim of substantially improving the performance of solar-powered lasers. Currently, we have been seeking high solar laser performance through the development of alternative prototypes for pumping laser crystals with broader absorption spectrum in the visible region (Ce:Nd:YAG), whose outcomes will be addressed in this invited talk, and which resulted in the following breakthroughs:

- The side-pumping of a Ce:Nd:YAG laser rod at NOVA solar facility led to 1.6 times increase in solar laser collection and conversion efficiencies compared to that with Nd:YAG laser rod under the same pumping conditions. This work demonstrated the great potential of the Ce:Nd:YAG laser material as a gain medium for solar-pumped lasers, being featured in *Journal of Photonics for Energy*.
- Maximum continuous wave solar laser power of 40 W was registered by adopting a side-pumping configuration with a rectangular light guide, being the highest laser power level reported from a solar powered Ce:Nd:YAG laser medium.
- Records in collection, slope, and solar-to-laser conversion efficiencies of 41.3 W/m², 7.64%, and 4.64%, respectively, were recently attained by end-side-pumping three thin Ce:Nd:YAG laser media simultaneously within a common pump cavity. This system allowed the concentrated solar radiation to be shared by the three laser rods, ensuring not only a substantial alleviation of the thermal lensing effects but also a significant rise in solar laser efficiency. This breakthrough was spotlighted in *Laser Focus World*.
- The lowest threshold pump power of 29.2 W was obtained with the first Ce:Nd:YAG solar laser pumped under a cloudy sky. The cloud-filtered sunlight enabled notable improvements in the solar laser efficiency by lessening the thermal lensing effects.

In addition to the abovementioned breakthroughs, innovative solar laser schemes were also both numerically and experimentally performed for high stable solar laser emission with enhanced efficiency, thermal performance, and tracking error compensation capacity. Through experimental work, large enhancement in solar laser tracking error compensation capacity was confirmed for the first time with a dual-rod side-pumping scheme.

Since this technology can be operated using only renewable energy, it may bring an important economic advantage for countries with high solar availability and for the future development of sustainable industrialization, either on Earth or in Space.

Invited talks / 86

Unveiling the interstellar grain surface chemistry by means of quantum mechanical simulations

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The Universe is molecularly rich 1. Its chemical diversity and complexity are reflected by the more than 290 molecular species detected in the gaseous phase by means of radioastronomy 2 and the

different solid-state phases in the form of dust grains³. The presence of the gas-phase molecules cannot be explained uniquely by reactions taking place in the gas phase but chemical reactions occurring on the surfaces of grains are essential to rationalize the interstellar chemistry. However, combining astronomical observations with astrochemical modelling and laboratory experiments is not enough to fully unveil the grain surface chemistry and its role to the chemistry of space because they hold some intrinsic limitations [4,5,6]. Quantum chemical simulations can partly alleviate these limitations as they provide reliable, quantitative atomic-scale information (structure, energetics, and dynamics) of chemical processes taking place on the surface of grains, this way allowing us to determine the actual role of the grains on them, i.e., chemical catalysts, reactant concentrator and/or third bodies. This contribution aims to present some of the potentialities of current state-of-the-art computations developed in our group to obtain unique and fundamental information that help improving our know-how on the interstellar grain surface chemistry. To this end, examples on simulations of i) modelling realistic grain surfaces for silicates and ices⁷, ii) the adsorption of astrochemically-relevant species [8,9], iii) chemical reactions forming interstellar complex organic molecules [10,11], and iv) the fate of the extra energy released in interstellar exothermic reactions [12,13], will be presented.

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Complex forming reactions at the low temperatures of interstellar medium: from statistical to statistical methods

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The molecular complexity in the interstellar medium increases in cold molecular clouds, at approximately 10 K. It is then important to establish the reactivation rate constants in chemical networks taking place in gas phase, as alternative to those taking place on cosmic ices. At 10 K, quantum effects, such as tunneling and zero point energies are very important. Complex forming reactions are particularly challenging, because they involve the formation of long lived complexes which are difficult to treat with dynamical methods. In this talk I will briefly present some recent results obtained using statistical methods, quantum/adiabatic statistical approach¹ or capture/RRKM method², and dynamical methods, such as Ring Polymer Molecular Dynamics for reactions presenting relatively shallow wells and barriers³. In this last case, the role of dimers between reactants formed at low temperatures will be also described⁴, as an alternative explanation for the fast increase of the reaction rates with decreasing temperature measured in CRESU experiments for a large variety of organic molecules with OH radical.

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Ultrafast inter-system crossing in triply fused porphyrin - nanographenes

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We present recent results on the photophysics and optical properties of nanographenes. The first part of the talk focuses on the photophysics of cove-edge hexa-peri-hexabenzobis-peri-octacenes. The remarkable light emission properties and lack of excited state absorption upon solvation give rise to net stimulated emission and amplified spontaneous emission, largely enabled by the cove-edge pattern. Therefore, this nanographene system stands as a promising optical gain medium in laser cavities.

In the second part of the talk, we will focus on a family of edge-fused nickel porphyrin-nanographenes. Porphyrins are appealing building blocks for solar energy applications, although their photosensitization capability is limited by their large optical energy gap, resulting in a mismatch in absorption for efficient harvesting of the solar spectrum. Porphyrin π -extension by edge-fusing with nanographenes can be employed to narrow their optical energy gap, enabling the development of porphyrin-based panchromatic dyes with an optimized energy onset for solar energy conversion in dye-sensitized solar fuel and solar cell configurations. Combined pump-probe measurements with time-dependent density functional theory demonstrate that photoexcitation in these nickel porphyrin-nanographenes leads to a lowest ligand-centered singlet state, which undergoes ultrafast intersystem crossing (1.2 ps) towards an intermediate (d,d) triplet level, unaffected by the symmetric conjugation expansion. Remarkably, this triplet level delocalizes into a ligand centered triplet state in 18 ps, an asset for sunlight-to-energy conversion. This observation implies that the decoration of the porphyrin moiety with nanographenes, while significantly impacting the absorption onset of the novel dye, promotes the formation of a ligand-centered lowest triplet state with a large spatial extension, potentially interesting for boosting interactions with electron scavengers.

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Azobenzene Molecules Towards the Creation of Molecular Photonics

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² Azobenzene molecules present TRANS-CIS isomerization capabilities about the N=N bound, which can be induced with light. The TRANS conformation, naturally the most energetically stable at room temperature, can be converted into CIS conformation under the action of light, with the rate of TRANS-CIS-TRANS conversion for a given molecular system dependent on temperature and light, namely light intensity, wavelength, and light electric field direction with respect to molecular dipole moment. This process is accompanied by molecular reorientation can be used to optically induce birefringence and to create relief grating in the medium containing azobenzene molecules. The main use of materials is in photonics, namely in optical storage, sensors, energy conversion devices and information processing, reason for which these materials have been widely investigated over the past years. A general overview of these materials features will be drawn, its applications and trends.

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Poster Session / 90

New insights on the non-adiabatic dynamics of the ultrafast photodissociation of the methyl iodide cation

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The development of light sources in the extreme ultraviolet (XUV) based on high harmonic generation has opened new avenues for the investigation of time-resolved photodynamics in cationic excited electronic states of polyatomic molecules. Here, an XUV pump-infrared (IR) probe scheme with femtosecond time resolution is employed to study the dynamics of dissociative ionization in methyl iodide 1.

A time-delay-compensated XUV monochromator is employed to isolate the 9th harmonic of the fundamental 800 nm (13.95 eV, 88.89 nm), which is used as a pump pulse to prepare the cation in several electronic states. A time-delayed IR probe pulse is used to probe the dissociative ionization dynamics on the first excited \tilde{A}^2A_1 state. Photoelectrons and photofragment ions are detected by velocity map imaging. The experimental results are complemented with high-level ab initio calculations of

potential energy curves (PECs) of the electronic states of CH_3I^+ as well as full-dimension on-the-fly trajectory calculations on the $\tilde{\text{A}}^2\text{A}_1$ state, considering the presence of the IR pulse. CH_3^+ and I^+ transients reflect the role of the IR pulse in probing the photodynamics of CH_3I^+ in the $\tilde{\text{A}}^2\text{A}_1$ state, mainly through the coupling to the ground state $\text{X}^2\text{E}_{3/2,1/2}$ and to the excited B^2E state manifold. Oscillatory features are observed and attributed to a vibrational wave packet prepared in the $\tilde{\text{A}}^2\text{A}_1$ state. The IR probe pulse induces a coupling between electronic states leading to a slow depletion of CH_3^+ fragments after the cation is transferred to the ground $\text{X}^2\text{E}_{3/2,1/2}$ states and an enhancement of I^+ fragments by absorption of IR photons yielding dissociative photoionization.

Complementary experiments have been carried out at the synchrotron SOLEIL using double imaging photoelectron photoion coincidence (i^2 PEPICO) spectroscopy to study the valence-shell dissociative photoionization of methyl iodide. The measured threshold photoelectron spectrum for CH_3^+ reveals that the ν_5 scissors vibrational mode promotes a transfer of population from the initially populated first excited state ($\tilde{\text{A}}^2\text{A}_1$) into the ground cationic state, leading to the formation of CH_3^+ . Additional high-level ab initio calculations of PECs reveal the presence of an elusive conical intersection mediating this internal conversion.

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Poster Session / 91

Probing molecular dynamics using ultrafast XUV transient spectroscopy

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Attosecond probing of core-to-valence electronic transitions is a powerful tool for real-time observation of chemical dynamics.¹ Here, ultrafast extreme ultraviolet (XUV) transient absorption spectroscopy is employed to investigate the electronic and nuclear dynamics on small polyatomic iodinated molecules. The dynamics induced by one- or two-photon absorption using either few-femtosecond visible pulses, ranging between 500 nm and 900 nm, or 20-fs UV pulses around 260-280 nm is probed by XUV attosecond isolated pulses through iodine-4d core-to-valence transitions.

This method allows us to directly map in real time the motion of the wavepacket on the excited states, due to the strong shift of the XUV core-to-valence transitions with internuclear separation and the high sensitivity of the wave packet to the electronic configuration. The result presented will involve the direct visualization of time-resolved photodynamics from a diatomic system (I_2) to polyatomic molecules.

First, coherent nuclear motion in the B excited state of molecular iodine is visualized with great detail² including the wave packet spreading and later recompression, at the outer and inner turning points, respectively. Second, the photodissociation dynamics of alkyl iodides such as CH_3I , $\text{C}_2\text{H}_5\text{I}$ and $\text{C}_3\text{H}_5\text{I}$, following one-photon absorption into the A band, is imaged in real-time [3, 4]. In particular, the wave packet bifurcation at the conical intersection is mapped. Structural effects, with special attention to the presence of a double bond, on the dissociation dynamics will be considered.

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Poster Session / 92

Ultra-Thin Converter Layers for Gas Based Neutron Position Detectors

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Gaseous neutron detectors are crucial tools to many scientific fields, as neutrons are used to probe matter, revealing structures and functions not accessible by other imaging means. ³He filled multi-wire chambers are being replaced by novel instruments coated with thick layers of boron, as ³He is now almost exclusively used for security applications. I will present a novel approach which relies on sub-micrometer boron layers for neutron conversion. It is a counter intuitive choice which profits from momentum conservation of the neutron capture reaction and provides superior information. Recent results and developments will be presented, showing the potential to achieve unmatched position resolutions, intrinsic full gamma-ray suppression and a strong reduction of the exposure time.

Invited talks / 93

AMBER: an experiment for Hadron structure

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AMBER (Apparatus for Meson and Baryon Experimental Research) is an experiment located on the M2 beam line of CERN SPS. The understanding of the origin of the visible mass in the universe is one of its physics goals. It is known that the Higgs boson mechanism alone is not sufficient to explain the mass of a nucleon. Another phenomenon must interplay with it to explain the emergence of the hadron mass. The AMBER collaboration proposes a broad physics program to address that question under different aspects and learn more about QCD. This talk will focus on the Drell-Yan lepton pair, Charmonium and prompt photon production measurements dedicated to the determination of the partonic structure of the pion and the kaon to complement and to compare to the one of the proton in the aim of shedding light onto the emergence of hadron mass mechanism.

Poster Session / 94

Neutral bremsstrahlung emission spectrum in argon

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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 referred to as Neutral Bremsstrahlung and is possible even in noble atoms due to their induced dipole moment. Neutral bremsstrahlung in noble gases has been neglected in favor of excimer-based Vacuum-Ultraviolet emission, being only recently studied in argon and xenon. In this study, we present preliminary results of the neutral bremsstrahlung emission spectrum obtained experimentally in pure argon at 1.2 bar, covering the 150–550 nm wavelength range, and under reduced electric fields within the 0–2 kV/cm/bar range.

Plenary Talks / 95

Nuclear Fusion Challenges and the Portuguese contribution

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The production of electricity from nuclear fusion has been a long-term challenge addressed by many research teams around the world. Recent records from inertial fusion and in magnetic confinement fusion experiments open great perspectives for a successful outcome in this quest. ITER construction is being accompanied by a vibrant fusion research program in many countries but, in particular in Europe, carried out by the consortium Eurofusion. The private investment in fusion is also growing considerably promising an ecosystem where innovation will accelerate the path towards fusion energy. In the EUROfusion roadmap, DEMO is foreseen as an intermediate step between ITER (under construction) and commercial power plants. Large tokamaks like ITER and the many different DEMO devices being designed will require to solve enormous engineering problems. This lecture will provide insights into the advancements and challenges surrounding nuclear fusion as the energy source of tomorrow. The lecture promises to delve into the world of nuclear fusion and the Portuguese contributions to this endeavor. This contribution will present some of the multiple engineering and physics challenges addressed while designing components for nuclear fusion devices. Using as example some of the Portuguese contribution, particular focus will be given to diagnostic development, control and data acquisition but also on experimental physics and understanding of the plasma.

Poster Session / 96

Evaluation of matrix effects on Formalin Fixed Paraffin Embedded tissue samples using μ -EDXRF

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Every time an intervention is performed, the total (biopsy) or a portion (surgery) of normal and tumor tissue is retrieved and processed as Formalin Fixed Paraffin Embedded (FFPE) blocks for the diagnosis and after they are stored for safekeeping. These FFPE blocks contain precious information regarding the elemental composition of normal/tumor tissue that is not harvested because there is no suitable analytical tool for elemental analysis of these samples. In what regards EDXRF, paraffin embedding process alters the sample's matrix permanently, hindering the application of common quantitative approaches based of Certified Reference Materials (CRMs).

In this work we have analyzed 12 sets of mirrored tissue samples, processed as pellets or after FFPE, in order to develop calibration curves and parametrize the influence of paraffin in the intensity of elemental peaks in the EDXRF spectrum.

Measurements were performed using Bruker M4 Tornado EDXRF system with Rh anode X-Ray tube. Calibration curves for S, Ca, Fe, Cu and Zn were obtained with and without correcting the intensities for the Rh Ka Compton to Rayleigh ratio. A 13th set of samples was used for validation, comparison of the intensity obtained in the FFPE tissue block and as pellet (true value).

Results show that using both uncorrected and corrected approaches the obtained intensities present a bias towards the true value lower than 13%. On the other hand, precision of the method is still too low, so there is a need to increase sample size and reduce the uncertainty of the method.

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Study of gaseous argon scintillation in the 160-650 nm range

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Argon gaseous detectors have been widely used in dark matter search and neutrino experiments over the last decade, owing to their unique ionization and scintillation characteristics. The primary and secondary scintillation in argon mainly result from the radiative de-excitation of singlet and triplet excimer states produced at gas pressures above 100 mbar. This well-known light production mechanism dominates the argon scintillation spectrum, consisting of Gaussian-like emission, centered at 128 nm, with a 10-nm width, commonly referred to as the 2nd continuum. On the other hand, alternative scintillation mechanisms, such as neutral bremsstrahlung and 3rd continuum emission, have been less studied due to their lower scintillation yield compared to the 2nd continuum. Despite this fact, their longer wavelength region, covering from the near vacuum ultraviolet to the near-infrared range, is typically more accessible to current photosensors, thus eliminating the need for wavelength shifters. In this work, we conducted a systematic study on the yield and time properties of the primary and secondary scintillation emissions in gaseous argon within the 160-650 nm wavelength region. In addition to the fast emission, we observed a slow component with time constants of the order of tens of microseconds. The yield and time properties of the slow contribution was studied for a wide range of electric fields values.

Poster Session / 98

A Gas Proportional Scintillation Counter with annular geometry

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Electroluminescence (EL) is the phenomenon of light emission, by a material, following electron impact in the presence of an external electric field. Gas Proportional Scintillation Counters (GPSC) use this effect in noble gases as an amplification process of the ionization signal induced by radiation interaction in the gas. Several geometries have been proposed and developed for this type of radiation detectors, the most common being the double grid assembly defining two different regions, the absorption and the electroluminescence region. One limitation in this type of detector is the ratio between the size of the detector radiation-window to the size of the photosensor reading out the EL. This restricts the large-window operation as the solid angle subtended by the photosensor relative to the electroluminescence region is dependent on the location of the radiation interaction in the gas medium. In this work, we propose the use of an annular electroluminescence region from which the solid angle of the EL production in respect to the photosensor is constant. This enables the use of a large radiation window area as the photon emission position is independent from the position of the primary interaction. Other advantages are inferred such as the simpleness of the detector design along with the low power electronics possibility, contributing both to a portable GPSC solution. We report on the latest results for the energy resolution capabilities for 5.9, 22.1 and 56 keV following the latest improvements in the electric system and in the light collection, reporting a GPSC with a radiation window area of 50 cm² and a photosensor sensitive area of 18 cm² for Xenon gas at 1.09 bar. Also reported are the results for large area capabilities for several ratios between the window size and photosensor active area, presenting an exceptional performance for six times the radiation window area, in respect to the photosensor sensitive, 2 cm² area, using an LAAPD. Several results are also presented from a comprehensive simulation study of the detector obtaining a good agreement between the simulated and experimental performance, the latter obtained using the x-rays interacting directly with the LAAPD to calculate the electroluminescence yield. This type of portable room-temperature detector, with large-detection-area and large-detection-volume, can compete with solid-state detectors in x-ray astronomy applications.

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Determination of the absolute primary scintillation yield of pure krypton

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Gas Proportional Scintillation Counters (GPSC) are gas-filled detectors in which the charge signal produced by radiation interaction is amplified by secondary scintillation promoted by electron impact (electroluminescence) taking place in the gas. Primary electrons produced by the interacting radiation are driven towards a scintillation region, where the applied electric field is high enough to excite but not ionize the noble gas atoms, producing a scintillation pulse through atom de-excitation proportional to the number of primary electrons and, thus, proportional to the incident x-ray energy. Additionally, the primary scintillation light produced is used as the event trigger in several present experiments. In order to decide what gas to use in a given experiment, it is of utmost importance to determine parameters such as the electroluminescence yield and the primary scintillation yield for each candidate. Pure noble gases are an obvious choice for this kind of experiments. Krypton is

denser than argon, much less expensive than xenon, presenting even the highest absorption cross section for x-rays in the 14–34 keV energy range. These are advantages in applications where large detection volumes and high pressure are required. Using a GPSC coupled to a photomultiplier tube we have performed experimental studies on the primary scintillation yield for krypton. Preliminary results were obtained for 5.9- and 14.3-keV x-rays.

Poster Session / 100

Application of WLS fibers for xenon scintillation readout

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Wave-Length Shifting (WLS) fibers are optical fibers specially designed to shift the wavelength of incident ultraviolet or blue light to longer wavelengths, namely green light. The usage of WLS fibers for xenon scintillation readout offers several advantages, including enhanced light yield due to efficient conversion of UV/blue scintillation photons to visible light, reduced sensitivity to electromagnetic interference and improved spatial resolution, rendering them valuable for precise detection in xenon-based particle physics experiments. Xenon is extremely important in experiments regarding rare event detection, specifically in experiments for neutrinoless double beta decay and direct dark matter searches. To conduct research on the readout of WLS fibers, simulation studies will be performed to assess some characteristics of the fibers, namely their overall losses. For that purpose, an optical, light-tight box has been assembled to house a system consisting of WLS fibers and optical detection instrumentation for experimental validation of the simulated results.

Invited talks / 101

MOLECULAR STRUCTURE ELUCIDATION AND BEYOND WITH MICROWAVE ROTATIONAL SPECTROSCOPY

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Since the dawn of the chirped-pulse era ¹, rotational spectroscopy emerged as an outstanding tool for structure-solving, enabling novel exploratory approaches with unprecedented tracing capabilities ². The enhanced sensitivity and broadband capabilities of chirped-pulse microwave spectroscopy unlocked investigations into increasingly intricate molecular species ³, including notable examples such as artificial molecular motors ⁴. Leveraging the inherently narrow line widths of rotational transitions, microwave spectra are unique molecular fingerprints, facilitating unambiguous determination of precise three-dimensional structures and even enabling identification and quantification of enantiomers through recently developed strategies [5,6]. In this contribution, we will discuss recent findings showcasing the wide-ranging applications of broadband rotational spectroscopy, in the realm of molecular structure elucidation and beyond.

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Poster Session / 102

Development of organic scintillators for neutron detection

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The detection of ionizing radiation is of vital importance in various branches of science, medicine, border security and environmental monitoring, among others. The development of new detection systems that have versatility of applications, of easy production and manipulation with viable costs has been one of the fields of application of many recent studies, namely in the field of neutron detection, since the main system to detect these particles is still based on helium 3, which is scarcely available, and its availability has progressively been decreased over time. Liquid and plastic scintillators are a viable alternative, as they are relatively easy to produce and can be produced in large sizes and formats. This work presents the study and development of different systems of organic scintillators with application in the detection of fast and thermal neutrons. Exploring different compositions for scintillators (plastic and liquid), making use of different compounds containing Boron or Lithium, incorporated into the scintillator matrix in a homogeneous and heterogeneous way is the aim of this work. Some preliminary results of this development are presented.

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Optimization of a drone-mounted gamma scintillation detector for radiation mapping, surveillance and search operations

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In this Poster, we will present a proposal for a robust gamma radiation detector system for aerial mapping and radiation surveillance. It entails assembling and calibrating the detector using four high-resolution crystals and studying the effects of a VETO system. The detector will be equipped

with real-time communication capabilities and AI algorithms for data analysis and source identification. Additionally, the suitability of crystals with high intrinsic background radiation will be explored, aiming real time energy calibration. Ultimately, the project aims to generate radiation maps for specific areas in the United Arab Emirates.

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Opening Session

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The PISA Photosensor for Multi-Ton Rare Event Detectors

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The search for dark matter is one of the highest priorities in contemporary modern particle physics roadmaps. Direct detection experiments employing noble liquid detectors are currently limited by the radioactivity from the detector materials, mostly from the specially radio-clean photomultiplier tubes (PMTs), contributing to the background at ~ 80% level. Large area avalanche photodiodes and SiPMs have limited gain or too small active areas to be alternatives to PMTs. We propose a simple concept, the Photon Induced Scintillation Amplifier (PISA), as an innovative high-gain photon-multiplier with imaging capability. Instead of a multi-element stack of micropattern electron multipliers, in the PISA a true photon-multiplier is conceived. The secondary scintillation produced in the charge avalanches that take place inside the holes of the micropattern electron multiplier will be read out by suitable photosensors, like SiPMs. The PISA will be cost effective and allow for area coverage above 80%, maximizing the photon detection efficiency. The SiPMs can be distributed in a 2D array with a pitch suitable for the imaging capability. The PISA concept offers an attractive alternative to PMTs and other photon-detector concepts for dark matter direct detection and other high-energy physics experiments.

Poster Session / 108

MICROSOLVATION OF α -PINENE OXIDE AS OBSERVED BY BROAD-BAND ROTATIONAL SPECTROSCOPY

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α -pinene is the most abundant monoterpene in the atmosphere and its oxidation yields to several oxygenated species that play a major role in the formation of secondary organic aerosols. α -pinene oxide ($C_{10}H_{16}O$) is generated from the reaction of ozone with α -pinene and has been shown to contribute to the formation of organosulfates under atmospheric conditions. Thus, understanding its interactions with atmospheric molecules is crucial to explain the first steps of molecular aggregation in the aerosol formation. Here, we present the investigation of the hydrates of α -pinene oxide, $C_{10}H_{16}O \cdots (H_2O)_n$ ($n=1,2$), using two different chirped-pulse Fourier transform microwave spectrometers operating in the 2-18 GHz frequency range,^{1,2} supported by quantum chemical calculations. The hydrates consist of water chains anchored to the oxygen atom of α -pinene oxide by a primary $O-H \cdots O$ hydrogen bond and further stabilized by secondary $C-H \cdots O$ interactions. The structures of these hydrates have been further confirmed by the analysis of the rotational spectra of their ^{18}O water isotopologues and compared with those of related species.

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