EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

NanoSpace

Final COST NanoSpace Joint Scientific Meeting

Book of Abstracts

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Funded by the European Union

This publication is based upon the work from COST Action CA21126 – Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology).

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Tenerife, España

Sep 15–17, 2026

Final COST NanoSpace Joint Scientific Meeting

Book of Abstracts
Published by Instituto de Astrofísica de Canarias (IAC), La Laguna, Tenerife, Spain

Organized by
Instituto de Astrofísica de Canarias (IAC), La Laguna, Tenerife, Spain
COST action: CA21126 - NanoSpace

Edited by
Alexa Friederich Hidalgo
Domingo Anibal García Hernández

COST Action CA 21126

Carbon Molecular Nanostructures in Space

(NanoSpace)

Final COST NanoSpace Joint Scientific Meeting

Sep 15-17, 2026

Tenerife, España

Foreword

We are pleased to welcome you to the "**Final COST NanoSpace Joint Scientific Meeting"** taking place at IACTEC in La Laguna, Tenerife, Spain from 15th to 17th of Sep 2026. The meeting marks the culmination of this COST Action, bringing the NanoSpace community together to consolidate the scientific advances achieved throughout the Action, strengthen the interaction, learning, and collaboration among its members, and integrate young and ITC researchers into a shared understanding of the scientific challenges ahead.

With a programme of 42 talks (10 invited and 32 contributed) and 23 posters, we sincerely hope that this final meeting will be an excellent opportunity to share the latest research results as well as to discuss new developments and challenges in our research fields; all of them related to the NanoSpace scope. This is a unique opportunity for all of us to exchange ideas, learn from each other, and find new inspirations for our research. For the ITC researchers and young scientists, in particular, it will be a great opportunity for networking with other European and more senior researchers, respectively.

We warmly welcome all of you to this Final COST NanoSpace meeting in Tenerife. We hope that you will enjoy the programme, strengthening existing collaborations as well as establishing new ones.

Domingo Anibal García Hernández, Action chair

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Arturo Manchado - Instituto de Astrofísica de Canarias (IAC)
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Anselmo Sosa Méndez - Instituto de Astrofísica de Canarias (IAC) (NanoSpace Action Grant Holder Manager)

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JWST’s view on Cosmic Fullerenes

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The Universe is rich in carbonaceous compounds (molecules and dust grains) that appear in a bewildering variety of sizes, structures, shapes and chemical compositions. Fullerenes, a class of large carbonaceous cage molecules, are a fairly recent addition to the molecular inventory. The best-known member of the family is C_{60}("buckyballs"). First detected in 2010 with Spitzer in the otherwise inconspicuous planetary nebula Tc 1, fullerenes have since been discovered in a variety of objects -- from evolved stars to the diffuse ISM, reflection nebulae, young stellar objects, and meteorites. Fundamental questions remain about how these large, stable molecules form, whether they exist in the gas or solid phase, and what physical processes drive their excitation and IR emission.

In this presentation, I will discuss what we have learned from detailed and spatially resolved spectroscopic observations of Tc 1 (and some other sources) with JWST/MIRI and VLT/MUSE and what they may reveal about fullerene formation itself. The spectra are remarkably rich, and show the clear signatures of neutral $C_{60}$and C_{70}in addition to several weaker features. The fullerenes are clearly in the gas phase, with signatures of ^{13}C isotopic substitution. The fullerenes reside in the H II region -- where it was thought they would not survive but should photo-fragment. Electron attachment -- favoured by the high electron density and C_{60}'s strong electron affinity -- allows the molecules to survive; photodetachment then excites them, driving IR emission through a pathway not previously considered. The spectra also show unusual dust features that may be related to the formation of fullerenes. Finally, I will discuss the broader implications for large molecules -- including PAHs—in space.

Helium-tagging Spectroscopy of Molecular Ions and Ionic Clusters in the Visible and Infrared

Florian Foitzik,[1]Lisa Ganner,[1]Thomas T Lindkvist,[2]Franziska Hölzler,[1]Benjamin Felsner,[1]Vincent Richardson,[3]Gabriel Schöpfer,[1]Milan Ončák,[1]and Elisabeth Gruber [*1]

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Helium-tagging spectroscopy provides a highly sensitive approach for investigating the intrinsic optical properties of cold molecular ions and ionic clusters under well-controlled conditions, while only minimally perturbing the species under study. In our approach, ions are generated and efficiently cooled inside multiply charged helium nanodroplets (HNDs). Subsequent collisional heating of the droplets with helium buffer gas enables the formation of helium-solvated ions and ionic complexes at low temperatures. Following mass selection, resonant excitation of the target ions results in the evaporation of one or more weakly bound helium atoms. The corresponding helium loss is detected by time-of-flight mass spectrometry and serves as the action signal for recording electronic and vibrational spectra [1]. This technique allows the production and spectroscopic investigation of a broad range of species, including isolated molecular ions, weakly bound ionic complexes, and size-selected ionic clusters. In this contribution we focus on the spectroscopy of polycyclic aromatic hydrocarbons (PAHs) and fullerenes in both the visible and infrared spectral regions [2,3]. The implementation of a second ion source makes it possible to generate also multiply charged ions, extending the accessible systems to higher charge states [4]. This enhancement was successfully employed to record the vibrational and electronic spectra of doubly charged PAHs and fullerenes.

Furthermore, the setup has proven to be capable to spectroscopically probe products of ion molecule reactions, occurring inside HNDs. Here we want to present results on the formation of benzene from the stepwise addition of acetylene to the acetylene cation. The results suggest that this reaction might be a source for the benzene cation in space, which is considered to be an entry point for the formation of complex molecules in space [5].

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The conformational dynamics of neutral naphthalene with H_2O, H_2S and CO_2molecules probed by infrared spectroscopy

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Carbon is ubiquitous in space, found in many environments and allotropic forms, including polycyclic aromatic hydrocarbon (PAH) species [1]. In the cold conditions of the interstellar medium (ISM), molecules are expected to be trapped in interstellar ices, with PAHs not an exception [2]. Such ices, while been composed to a large extent by water, have traces of other species, such as $CO_2$and H_2S. Crucial for the quest to understand the molecular composition of the ISM is to have precise laboratory information of relevant species, ideally covering the ranges where the James Webb Space Telescope (JWST) is most sensitive [3]. In this contribution, molecular beam experiments are presented with a focus on addressing the spectroscopic signatures of complexes of neutral naphthalene, a prototypical PAH, with H_2O [4], H_2S and CO_2molecules. The experiments reveal a complex dynamics of the adsorbed molecules on the PAH surface, even at the cold temperatures of molecular beams (≈20-40K), observed as broad absorption features in the far-IR. While static density functional theory (DFT) calculations cannot grasp the features seen experimentally, Born-Oppenheimer molecular dynamics (BOMD) simulations reproduce well the spectra, as shown in Figure 1.

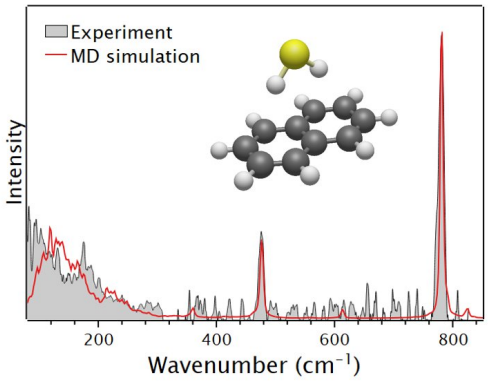


Figure 1: Measured far-IR spectrum of neutral napththalene-H_2S. The experiment is compared with dynamic BOMD simulations in red.

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Quantum Computational Spectroscopy of Endofullerenes

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Endofullerenes provide unique nanoscale laboratories in which molecular confinement gives rise to unconventional quantum phenomena that are directly accessible through high-resolution spectroscopy. We will present recent advances in the quantum computational description of light-molecule endofullerenes, with particular emphasis on $H_2O@C_{60}$ and $H_2O@C_{70}$. By combining multidimensional potential surfaces with rigorous full-dimensional quantum dynamics based on the multiconfiguration time-dependent Hartree (MCTDH) approach, it is possible to reproduce and interpret the intricate roto-translational-vibrational spectra of these confined systems. The calculations reveal how the interplay between molecular translation, rotation, vibration, and cage anisotropy determines the spectroscopic fingerprints of the encapsulated molecule. Special attention will be devoted to the origin of the experimentally observed symmetry breaking in $H_2O@C_{60}$, demonstrating that subtle distortions of the fullerene cage provide the most plausible explanation for the lifting of rotational degeneracies. We will also discuss the effects of the lower symmetry of the C_{70} cage, which produces a richer coupling between translational and rotational motions and leads to characteristic modifications of the energy-level structure. These studies illustrate how state-of-the-art quantum simulations establish a direct connection between microscopic intermolecular interactions and measurable spectroscopic observables, providing fundamental insights into molecular confinement and guiding future investigations of endofullerenes as model quantum nanosystems.

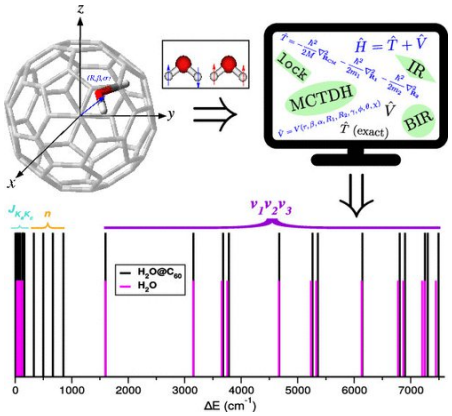


Figure 1: Coordinate systems used in this work to represent a water molecule inside the $C_{60/70}$ cage. Comparison of the rotational, translational and vibrational frequencies (see vertical sticks' positions) computed from the present 9D and 6D MCTDH calculations for the C_{60} encapsulated and isolated H_2O molecules.

Acknowledgements
The authors thank Centro de Calculo IFF/SGAI (CSIC), and CESGA, MICIN grant PID2024-155666-NB-I00, i-COOP Ref: COOPB25030,and COST Action CA21126 (NanoSpace)

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Gas-Phase Spectroscopy of $H_2O@C_{60}^+$ and $H_2O@C_{60}H^+$ in the Mid-Infrared: The Challenges of Searching for Endohedral Fullerenes in Space

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Given the prevalence of fullerenes in space,[1] it is plausible that there are also pathways for the formation of endohedral fullerenes, where a small species is enclosed within the hollow cavity of the fullerene cage.[2] In this work, mid-IR spectra are presented for the endohedral fullerenes $H_2O@C_{60}^+$ and $H_2O@C_{60}H^+$, obtained using action spectroscopy. These are the first gas-phase vibrational spectra of an endohedral fullerene containing an IR-active guest species. Both spectra look remarkably similar to those of the empty fullerenes,[3,4] with many of the same features present at slightly blue-shifted frequencies. Interestingly, the water bending mode is not observed in either of the spectra. This has been attributed to a polarisation of the pi-electrons of the fullerene cage, reducing the total dipole moment and the IR intensities. The similarity of the spectra with those of the empty fullerenes means that these species will be very hard to distinguish using only IR spectroscopy. This may have significant implications for the detection of $H_2O@C_{60}^+$, $H_2O@C_{60}H^+$, or indeed other endohedral fullerenes, in space.

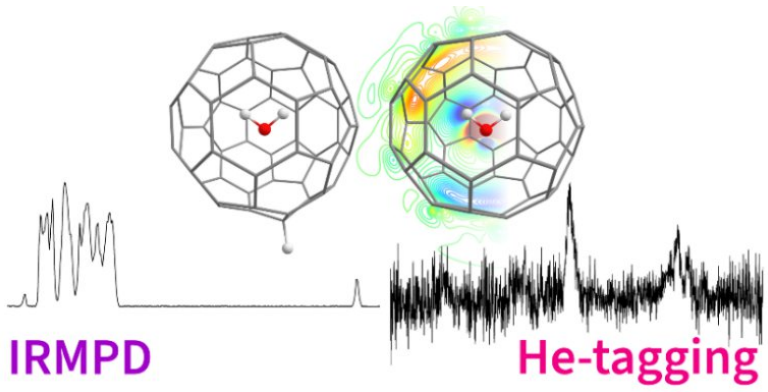


Figure 1: Experimental spectra of $H_2O@C_{60}H^+$ (left) and $H_2O@C_{60}^+$ (right).

Acknowledgements
The authors acknowledge financial assistance from the Royal Society and EPSRC. This research work has been funded in memory of Dr Brian R. Phillips.

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Unravelling the Structure of Monocyclic Carbon Ring Cations through Vibrational Spectroscopy

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Laser vaporisation of graphite generates a diverse range of carbonaceous clusters including linear chains, monocyclic and bicyclic rings, and fullerenes.[1]Whilst several linear chains and fullerenes have been studied spectroscopically, and detected in the interstellar medium,[2]the structure and spectra of many monocyclic carbon ring structures are still unknown.

Recent infrared (IR) spectroscopic studies of C_{4n}^{+}(n = 5-11) monocyclic rings have revealed intense infrared resonances which have been attributed to localised Kekulé-type bond distortions across the ring.[3]In this study, we report the IR spectra of a series of monocyclic carbon ring cations (C_{4n}^{+}, n = 2-7) including previously-uncharacterised C_{16}^{+}, $C_{12}^{+}$and C_{8}^{+}. Two clear trends are observed - the frequency of the GIRR redshifts linearly, and increases in intensity as the ring size increases. However, for smaller ring systems, such as $C_{12}^{+}$and C_{8}^{+}, clear deviations from these trends are observed. The experimental data is compared to a series of quantum chemical calculations, which suggests the observed trends can be explained by changes to the bond length alternation of these structures. Finally, the likelihood of detecting these structures in the interstellar medium is evaluated.

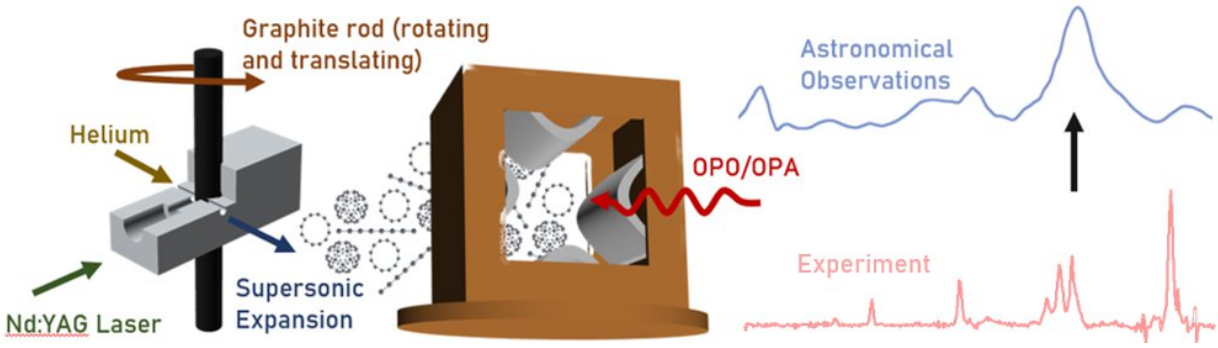


Figure 1: Simple schematic of the home-built apparatus in our laboratory which is used to generate and spectroscopically characterise astrochemically-relevant molecular ions.

Acknowledgements
The authors acknowledge the financial assistance from the Royal Society and Engineering and Physical Sciences Research Council. This research work has been funded in memory of Dr Brian R Phillips. This article is based upon work from COST Action CA21126 (NanoSpace).

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Gas-Phase Infrared Spectroscopy of Ethynyl-Bearing PAHs from Electrical Discharge using FELIX

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Reactions of the interstellar C_2H radical with aromatic hydrocarbons represent an efficient growth pathway toward molecular complexity in cold clouds [1]. Several ethynyl- and cyano-substituted aromatics have been detected in TMC-1, including ethynylbenzene [2], cyanonaphthalene [3], and a recent detection of a $C_{11}H_8$ species [4]. Gas-phase infrared fingerprint spectra of these molecules are essential complements to radio detections, enabling structural identification in infrared observations with JWST.

We apply IR-UV ion-dip spectroscopy using the free-electron laser FELIX, coupled with mass-selective two-colour 1+1' resonance-enhanced multiphoton ionization (REMPI), to characterize ethynyl aromatic products formed by the electrical discharge of bromobenzene and 1,2-dibromopropane precursors in a supersonic expansion.

Ethynylnaphthalene (m/z 152), as seen in Figure 1, serves as both a confirmed spectral assignment and a DFT calibration anchor. Our experiments additionally yield a range of higher-mass products arising from distinct radical pathways, with distributions that partly overlap and partly diverge from those observed in naphthalene-based discharge experiments [5,6] and structural assignments are ongoing.

The validated approach is now being applied to $C_{11}H_8$ (m/z 140), motivated by the recent TMC-1 detection of the cyclopenta-fused isomer 1H-cyclopent[cd]indene [4]: our discharge is expected to populate ethynyl-substituted indene isomers of the same mass, and a spectral unmixing pipeline is used to disentangle the isomeric contributions.

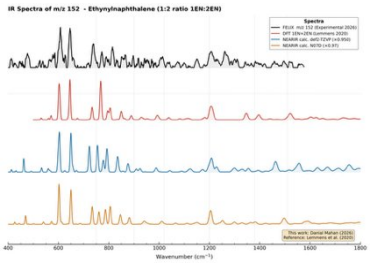


Figure 1: IR-UV ion dip spectrum of m/z 152 (ethynylnaphthalene, 1EN:2EN 1:2) compared with calculated spectra and with the reference spectrum of Lemmens et al. [5].

Acknowledgements

We thank the HFML-FELIX staff for their technical assistance and beam time, and NWO for supporting the FELIX Laboratory. D.M. acknowledges a Short-Term Scientific Mission grant from COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology), in support of this work.

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Characterization of Methyl Acetate Through the Interplay of Vibrational Spectroscopy and Quantum Chemical Calculations

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Methyl acetate (CH_3COOCH_3), the simplest saturated ester, was first detected in the molecular cloud Orion KL in 2013 [1], and very recently confirmed toward the Galactic Center molecular cloud G+0.693 [2]. Being the second most stable species within the $C_3H_6O_2$isomeric family [2], methyl acetate is a complex organic molecule (COM) of particular interest in astrochemistry due to its potential involvement in the reaction mechanisms that lead to the formation of ester-bearing molecules and prebiotic species, both in icy mantles and warm gas of the interstellar medium (ISM). Given this importance, its spectroscopic characterization is therefore crucial to contribute to the spectroscopic databases that might help observation in the interstellar gas and ices.

In the present work, the vibrational and ro-vibrational properties of methyl acetate are studied by state-of-the-art quantum chemical calculations. Equilibrium geometries and harmonic frequencies are computed by CCSD(T) based composite schemes [3], which are then augmented through anharmonic contributions evaluated in the frame of density functional theory [3]. From this hybrid force field, excited state rotational constants and vibrational transition frequencies and absorption intensities are worked out by resorting to vibrational perturbation theory to second order. Simulated spectra were used to assist the analysis of the gas-phase infrared (IR) spectrum, recorded in the 150–6500 cm^{-1}region at a resolution of 0.5 $cm^{-1}$by using a Bruker Vertex 80v equipped with a 199 mm cell with polyethene and KBr windows for the far- and medium-IR region, respectively. Finally, the full characterization of the IR features was completed with the experimental determination of absorption cross sections over the same region, by using spectra acquired at sample pressures in the 9 – 100 hPa range.

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Small hydrocarbons and radicals in C-rich evolved sources: JWST and Spitzer views of proto-PAH chemistry

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Carbon-rich evolved stars are important stellar factories of carbonaceous material in the interstellar medium. As these stars evolve beyond the asymptotic giant branch (AGB), ultraviolet radiation and shocks can further process their circumstellar gas and dust. Small hydrocarbons and radicals provide observational clues to the chemistry accompanying this processing and its possible connections to the formation of polycyclic aromatic hydrocarbons (PAHs).

I will present the first secure detection and quantitative characterization of the neutral methyl radical (CH_3) in the highly evolved carbon-rich source SMP LMC 011, using JWST/MIRI-MRS observations from the Proto-PAH project [1]. Multiple absorption features between 16.3 and 20 μm establish the presence of CH_3, while spectral modelling constrains its physical conditions such as rotational excitation and column density.

I will then discuss the origin and possible chemical fate of this abundant CH_3reservoir. Comparison with existing gas-phase photochemical models motivates an additional source, potentially supplied by UV- or shock-driven erosion of hydrogenated amorphous carbon (HAC) grains. The large benzene reservoir in SMP LMC 011 also makes this source particularly interesting for exploring subsequent aromatic chemistry: photochemical processing of benzene could supply aromatic radicals that react with $CH_3$to form more complex species. These pathways remain to be tested quantitatively.

Finally, I will present preliminary results from Spitzer/IRS spectra of 11 Galactic carbon-rich evolved sources, comparing their small-hydrocarbon inventories and examining candidate CH_3signatures to place SMP LMC 011 in a broader observational context.

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From atoms to aromatics: unraveling PAH growth from C and H

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With the increasing detection of polycyclic aromatic hydrocarbons (PAHs) in space, the question of their formation in such a chemically hostile environment remains a central issue in astrochemistry. Together with coworkers, we recently proposed a pathway for forming the first aromatic building blocks, $C_5H_6$and C_6H_6, in dense molecular clouds [1,2], and for their subsequent growth via carbon addition [3]. However, these mechanisms are likely feasible only in cold, dense molecular clouds, and cannot account for PAH formation in other regions of space. Furthermore, neither the neutral nor the cationic forms of the PAHs known to be present in dense clouds appear to be responsible for the long-standing diffuse interstellar bands (DIBs) -- a set of absorption features spanning from the near-IR to the visible, observed along lines of sight toward more diffuse, UV-exposed regions of space.

We propose to investigate the structure of PAHs, formed in the most unbiased manner possible, using electronic spectroscopy with our newly built instrument [4]. These PAHs are produced by laser ablation of carbon graphite in a H-atom-rich environment. We also compare this PAH production to that obtained from laser ablation of an analogue of hydrogenated amorphous carbon (polystyrene). Finally, we aim to investigate the possibility of forming hydrogenated carbon cages in space, as these are also considered promising DIB carrier candidates.

Acknowledgements

The work was funded by the French "Agence Nationale de la Recherche" (ANR) under Grant No. ANR-22-CE29-0013 (Project iSELECTION). Additional financial support was provided by the Paris Ile-de-France Region (DIM ORIGINES, project DIBsFINDER). This work was also supported by the Programme National "Physique et Chimie du Milieu Interstellaire" (PCMI), a research grant (VIL71404) from VILLUM FONDEN, and support of the Académie Spatiale d'Île-de-France through a PhD fellowship.

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The Evolution of Aromatic Chemistry in the Interstellar Medium

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Polycyclic Aromatic Hydrocarbons (PAHs) are thought to sequester a large fraction (10-25%) of all carbon in the Universe. While strong circumstantial evidence for their presence in space has existed since the 1980s, it is only in the last few years that the first individual PAH species have been definitively detected. In this talk, I'll describe the synthetic and spectroscopic laboratory work, computational approaches, and observational efforts which have led to these discoveries, discuss our current understanding of the formation and molecular evolution of PAHs in space, and describe the growing body of evidence that these species, in no small part, influence the inventory of raw organic material delivered to early planets. I'll conclude by taking a critical look at open questions related to PAH chemistry in space and the prospects for the field going forward.

Laboratory simulations of dust formation at astrophysical conditions

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Evolved stars are the molecular factories of space. In their atmospheres, cosmic dust grains are produced, and they play a crucial role in the cosmic cycle of matter (see Figure 1). However, dust formation is still poorly understood and laboratory simulations contribute to gain insight into the dust formation process.

In this talk, I will introduce the Stardust machine, a unique facility composed of six independent ultra-high vacuum modules which mimic the physico-chemical conditions of the circumstellar envelope (CSE) of Asymptotic Giant Branch stars (AGBs) (see Figu). It enables both the synthesis of nanoparticles of cosmic dust analogues and their in-situ characterization[1].

To show the outstanding capabilities of Stardust I will present some exemplary results on the dust formation process that have been obtained with this facility. In particular, I will present the formation of carbonaceous cosmic dust analogues through the interaction of atomic carbon and molecular hydrogen[2], the most abundant gaseous species in the CSEs, as well as the formation of silicon carbide grains, for which $H_2$is crucial[3]. Carbonaceous grains and silicon carbide dust are the main constituents of cosmic dust in carbon rich AGBs.

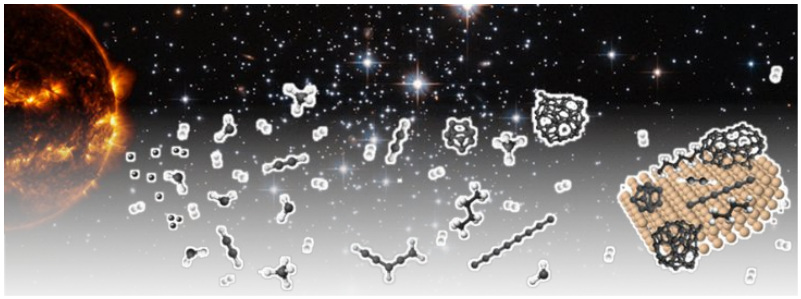


Figure 1: Pictoric representation of the CSE of a AGB star.

Acknowledgments
Support from the Severo Ochoa Centres of Excellence Programme (Grant No. CEX2024-001445-S) and MICIU/AEI/10.13039/501100011033 (Grant No. PID2023-149077OB-C31) are acknowledged.

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Laboratory studies of ice morphology, structure and chemistry under interstellar conditions

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Interstellar dust and molecular clouds, the regions where new stars and planetary systems form, are home to surprisingly complex chemistry. In spite of the very low temperatures and pressures characterizing these clouds more than 350 molecules have so far been detected. Ice-covered nanoscale dust grains are expected to play a dominant role as catalysts for this molecular complexity. The last 20 years have seen major advancements in our understanding of interstellar reactions, specifically with regards to simple molecules, however, the degree of chemical complexity attainable via such reactions is still under exploration. Recently it was shown that the simplest amino acid, glycine, can form under interstellar conditions. In this case a non-diffusive reaction mechanism in interstellar ices was proposed. Erosion reactions directly involving carbonaceous dust grain surfaces provide an alternative pathway to complex molecule formation under interstellar conditions. Here I discuss recent advances in experimental surface and solid-state astrochemistry with focus on direct imaging of abundant interstellar ice species and on non-diffusive and erosion reaction pathways to formation of interstellar complex organic molecules.

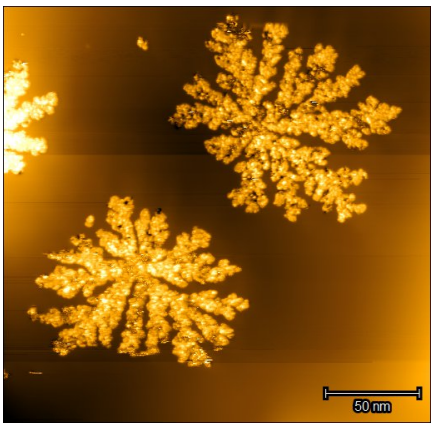


Figure 1: Scanning Tunneling Microscopy image of amorphous solid water clusters on a graphitic surface. The water clusters were grown at 45 K and imaged at 8 K.

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Swift heavy ion irradiation of astrochemical model systems with in situ analysis for cosmic radiation simulation

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Complex organic molecules have been detected in the interstellar medium (ISM) and in protoplanetary discs, both in the gas phase and increasingly also in the solid phase through observations with the James Webb space telescope (e.g.[1–3]. These molecules are thought to form in the solid phase, where particles and molecules are exposed to various types of electromagnetic and particle radiation.

Among these, heavy ions are of particular interest because they deposit large energy densities in highly localized regions. This leads to very specific effects on sputtering and radiolysis of molecules, as well as on the morphology and structure of cosmic dust analogs. Although heavy ions represent only a minor fraction of cosmic radiation, their specific interaction mechanisms must be considered separately to obtain a complete picture of chemical processes in the ISM.

Here, we provide an overview on the in situ experimental techniques available at the M-Branch of the GSI heavy ion accelerator facility, including ice deposition, FTIR and Raman spectroscopy, X-ray diffraction and time-of-flight mass spectrometry for the detection of secondary ions and neutrals. We highlight selected results from various experimental user campaigns on the radiolysis and desorption of complex organic molecules. Additionally, we discuss the role of dust grain surfaces in promoting the formation of new molecular species in irradiated ices, an aspect that is often neglected in studies on the effects of cosmic radiation (cf. section 37 in [4]), and present new results on evolution of ices on cosmic dust analogs and the analogs' surface properties, obtained both at M-Branch and IRRSUD at the GANIL facility in Caen, France.

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DESIREE: A tool to study the formation and survival of carbonaceous molecules in space

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Cryogenic electrostatic ion-beam storage rings provide unique opportunities to investigate the properties of gas-phase ions and their reactions under conditions that closely resemble those found in space. The DESIREE facility at Stockholm University [1] enables studies of collisions between oppositely charged internally cooled ions with precise control of the collision energy down to the sub-electronvolt regime [2-4]. Such low-energy ion–ion reactions are expected to play a significant role in the chemistry of dilute environments where anions, rather than electrons, serve as the dominant negative charge carriers. In addition, the exceptional vacuum conditions achieved in DESIREE enable investigations of the intrinsic properties and dynamics of atomic, molecular, and cluster ions on timescales exceeding minutes and in unprecedented detail [5-9].

In this talk, I will present recent results obtained at DESIREE and discuss how these contribute to our understanding of the formation, evolution, and survival of carbonaceous molecules in astrophysical environments.

Acknowledgements
This work was performed at the Swedish National Infrastructure, DESIREE (Swedish Research Council Contracts No. 2021-00155 and No. 2023-00170), supported by the Knut and Alice Wallenberg Foundation (contract No 2018.0028) and the Swedish Research Council (individual project grant with contract No 2024.0134), and is based upon work from COST Action CA18212—Molecular Dynamics in the GAS phase (MD-GAS) and COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology).

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IRPD Spectroscopy of the Phenanthrenequinone Cation ($C_{14}H_8O_2^+$) and its Dissociation Products

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Oxygen-substituted polycyclic aromatic hydrocarbons (OPAHs) are thought to play a role in the interstellar medium, with OPAHs proposed as potential carriers of the 6.0 μm feature observed in the infrared spectra of many astronomical objects [1]. We present results from a combined theoretical and experimental study of the phenanthrenequinone cation (PHQ^+, $C_{14}H_8O_2^+$) and its dissociative ionization fragments. Sequential CO loss was reported for protonated PHQ [2], motivating molecular dynamics simulations of the dissociation of PHQ^+. These predict sequential CO loss as the dominant fragmentation pathway for PHQ^+, yielding the fluorenone cation ($C_{13}H_8O^+$) and a $C_{12}H_8^+$ species as the primary daughter products, before further breakdown into smaller hydrocarbons. We compare these predictions against gas-phase infrared predissociation (IRPD) spectra recorded with the FELion cryogenic 22-pole ion trap [3] at the FELIX free-electron laser facility, and report experimental infrared spectra for fragments at m/z = 208, 180, 152, and 76. The m/z 152 fragment is of particular interest, as the same mass is produced in the dissociative ionization of the unsubstituted PAHs anthracene and phenanthrene, both of which yield a common acenaphthylene cation [4]. Whether OPAH isomers converge to a common m/z 152 daughter product upon dissociation has direct implications for PAH lifecycle models in photodissociation regions and top-down formation routes to small aromatic molecules observed in TMC-1. We discuss our spectroscopic assignments in this light.

Acknowledgements
This work was supported by the Max Planck Society, the Arnold and Mabel Beckman Foundation, and Schmidt Family Futures. The authors gratefully acknowledge the support of Radboud University and of NWO for providing beam time at the FELIX Laboratory as well as the skillful assistance of the FELIX staff. The authors thank the Cologne Laboratory Astrophysics group for providing the FELion ion trap instrument for the current experiments and the Cologne Center for Terahertz Spectroscopy, funded by the Deutsche Forschungsgemeinschaft (DFG, Grant SCHL 341/15-1), for supporting its operation.

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Unexpected reactive dynamics of carbon-based molecules under intense interstellar-like ionizing radiation

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Exposure to ionizing radiation produces highly excited and ionized molecular systems that commonly undergo rapid fragmentation. However, dissociation is not the only possible outcome. Competing ultrafast processes, occurring on femtosecond timescales, can lead to molecular isomerization and chemical reactivity, opening pathways to the formation of new molecular species and the growth of molecular aggregates (see, e.g., [1-6]).

While these ultrafast processes have been extensively investigated, studies of ionization-induced dynamics occurring on much longer timescales remain relatively scarce. In this contribution, we focus on delayed fragmentation, a process in which highly excited molecular ions dissociate long after the initial ionization event. Recent results on photoionized ethanol [7] will be presented as a model system to investigate how deposited energy is redistributed before dissociation takes place. We will also discuss recent observations of delayed fragmentation and competing isomerization pathways in nitrogen-substituted polycyclic aromatic hydrocarbons (PAHs) following ion-impact ionization [8]. Finally, ongoing work on ionization-induced reactions in molecular clusters will be discussed [9]. Particular attention will be given to the radiation-driven formation of nitrogen-containing polycyclic aromatic hydrocarbons.

Together, all these results suggest that ionization opens alternative pathways toward increased molecular complexity and chemical evolution in radiation-rich astrophysical environments. These studies combine state-of-the-art experiments with high-level quantum chemical simulations to provide a molecular-level understanding of the underlying mechanisms.

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Lessons from 25 years of multidisciplinary computer modelling

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Computer modelling has become one of the most powerful tools in the physical sciences to predict, rationalize and guide the discovery of molecular and materials properties. Modelling provides a valuable bridge between molecular-scale mechanisms, laboratory characterization and space-relevant phenomena.

Drawing on more than 25 years of multidisciplinary work, I will discuss, in an accessible and non-technical way, key choices in computational modelling, together with their strengths and limitations when addressing real-world problems. The presentation will follow a trajectory from early studies of functionalized carbon nanotubes, highlighting how the field has changed over the last two decades in terms of accuracy, system size, chemical complexity and predictive power [1]. I will also discuss examples of polymeric systems, with particular emphasis on covalent organic frameworks, where simulations can rationalize the complex growth of twisted structures on graphite [2] and reveal the emergence of moiré two-dimensional materials [3].

Special attention will be given to carbon-based nanostructures of potential relevance to NanoSpace, including nanographenes and their structural, electronic and magnetic properties [4], as well as formation routes involving sequential cyclodehydrogenation [5]. Finally, I will discuss the computational characterization of very large novel π-conjugated systems, such as ultralong graphene nanoribbons [6].

These examples provide useful conceptual and computational models for understanding the formation, transformation and stability of extended carbon nanostructures under different conditions. Overall, the contribution aims to illustrate how computer modelling can support the identification, characterization and rational design of carbon nanostructures.

Acknowledgements

The author acknowledges the support of CICECO – Aveiro Institute of Materials and the University of Aveiro. This contribution is framed within the scientific scope of the COST Action NanoSpace, CA21126, Carbon molecular nanostructures in space.

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Simulation of complex organics in astrophysical environments using machine learning

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Organic compounds containing carbon, hydrogen, and oxygen (CHO) are among the most abundant molecular building blocks in the universe and play a central role in astrochemical evolution, from interstellar clouds to protoplanetary disks. Hydrocarbons and hydrogenated amorphous carbon (HAC) materials play a key role in shaping interstellar medium chemistry. Species including fullerenes, polycyclic aromatic hydrocarbons (PAHs), carbon chains, and HAC have been detected and proposed as important constituents of the interstellar medium [1]. Understanding their microscopic structure is essential for linking formation pathways to observable spectroscopic signatures. Because direct observations provide only indirect structural information, there is a pressing need for accessing detailed interatomic interactions and understanding structural transformation processes through computational modeling.

Machine learning interatomic potentials (MLPs) provide a unified framework capable of capturing these interactions comprehensively, bridging applied materials science and astrophysical chemistry within a single model. I will present our general-purpose CH MLP [2], covering the formation of simple and complex alkanes, aromatic hydrocarbons, hydrogenated amorphous carbon, and CH systems under extreme conditions. I will show how these models enable near first-principles atomistic simulations over system sizes and timescales relevant to the evolution of complex carbonaceous materials. I will then demonstrate how this potential is extended to a broader range of CHO materials, including amorphous carbon networks as analogues for interstellar dust grains. Finally, I will describe how experimental observables from the actual experiments can be incorporated to simulate the structures of carbonaceous dust analogues [3].

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Spectroscopic Modelling of Small Heteroatomic Carbon-Chain Molecules using Gaussian Process Regression

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Gaussian process regression (GPR) [1,2] provides a flexible machine-learning framework for modelling molecular properties from sparse *ab initio*data. Unlike purely interpolative fits, GPR provides prediction uncertainties, which allow the reliability of the model to be assessed and can guide the selection of additional geometries. We use a Matérn 5/2 kernel with hyperparameters optimized by maximizing the marginal likelihood. One important advantage is the possibility of active learning, in which the predictive variance identifies regions where additional calculations are most useful.

As a pilot application, one-dimensional potential energy curves are constructed along the terminal C–X stretching coordinate for short heteroatomic carbon chains (C_nX), which are relevant to astrochemistry and carbon-rich interstellar environments. The curves are generated from separated fragments and a limited number of *ab initio*points at the MRCI(Q)/aug-cc-pVQZ level [3]. The GPR analysis is used to extract dissociation energies and C–X stretching frequencies and to investigate their dependence on chain length, heteroatom identity, and charge state. The relationship between accuracy and the number and distribution of training points is examined in order to establish a compromise between computational cost and predictive reliability.

This workflow represents a transferable tool for generating molecular input data for spectroscopic and astrochemical studies. Although it is limited here to a single coordinate, it provides a basis for future extensions to multidimensional surfaces, for example by incorporating bending or C–C stretching coordinates. Such extensions would enable a more comprehensive spectroscopic characterization while preserving the efficiency gains achieved through uncertainty-aware interpolation.

Acknowledgements
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Data-driven potential energy surfaces for astrophysical molecules: the case of [Ar-H-He]+

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Not long ago, space was thought to be too hostile and empty for molecules to form. However, the field of molecular astrophysics has completely transformed this perspective: we now know of more than 300 different molecules in the interstellar medium [1], and each new discovery seems to raise more questions than it answers. One of the most unexpected findings has been the discovery of noble gas hydrides such as HeH and ArH [2,3]. These demonstrate that even++ elements we consider completely inert can form bonds under the right astrophysical conditions, prompting us to rethink the limits of chemistry in space. The problem is that studying these systems in the laboratory is extremely difficult, and performing high-level quantum calculations in all possible configurations is prohibitively expensive. This is where machine learning (ML) comes in. ML-based potential energy surfaces offer a practical solution: they provide near-ab initio accuracy at a reasonable cost, enabling dynamic simulations and the prediction of spectra that would otherwise be unattainable [4]. Specifically, we developed a three-dimensional ML potential for the [Ar–H–He] cation using a breeding core Hilbert space (RKHS) approach,+ trained with high-level CCSD(T)/CBS reference energies [5]. We paid particular attention to the generation and validation of the training data to ensure that the surface is uniform and reliable across the configurational space required for quantum dynamics. With this potential, we performed MCTDH calculations to obtain accurate vibrational energy levels for the main [Ar–H–He] isotopes. The results provide concrete spectroscopic predictions that could guide future+ astronomical searches and, moreover, demonstrate how machine learning methods can help connect quantum chemistry with real-world observations of space.

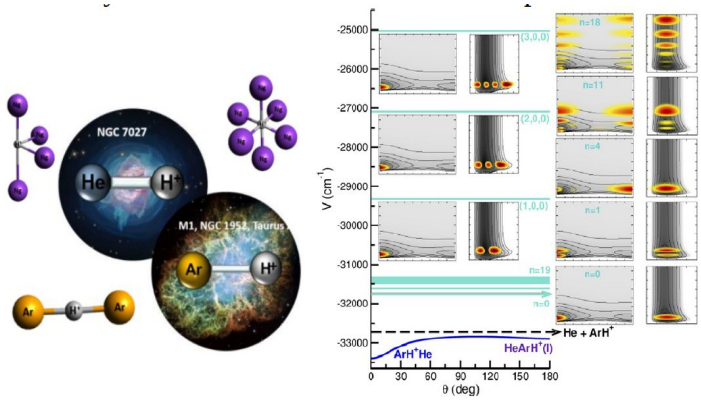


Figure 1: (Left)Visual description of HeH+ and ArH+ discoveries [2,3], as well as higher-order noble gas containing molecules. (Right) Bound vibrational energies for [ArHHe]+ calculated with the corresponding CCSD(T)/CBS[56] RKHS ML-PES from the MCTDH computation [5].

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Effect of the charge state on the reactivity and relaxation pathways of ionized C_4H_6 and its clusters

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Charge state and molecular environment determine how ionized 1,3-butadiene dissipates excess energy. We combine coincidence measurements, *ab initio* molecular dynamics (AIMD), and potential energy surface (PES) calculations to compare isolated $C_4H_6^+$ and $C_4H_6^{2+}$ with ionized butadiene clusters. For the isolated ions, both charge states display rapid H migration and hydrogen scrambling, but their neutral emission pathways differ significantly. The radical cation relaxes predominantly through atomic H loss, whereas the dication shows a pronounced propensity for H_2 formation and emission. The dication can additionally undergo sequential neutral loss before Coulomb explosion [1]. Thus, double ionization does not merely enhance fragmentation; it redirects the dynamics toward rearranged structures that enable H_2 release. In clusters, neighbouring molecules redistribute charge and internal energy, partly suppressing direct fragmentation and opening intermolecular hydrogen transfer and molecular growth pathways [2-4]. AIMD and PES calculations indicate that ionized 1,3-butadiene clusters can undergo Diels-Alder cyclization to long-lived cyclic products, including the 4-vinylcyclohexene radical cation and precursors associated with $m/z = 68^+$ and 79^+, species relevant to PAH-growth chemistry [5]. Our results establish a charge- and environment-dependent hierarchy of relaxation: H-atom emission dominates the isolated cation, H_2 emission is strongly enhanced in the isolated dication, and clustering redirects part of the deposited energy toward stabilization, hydrogen transfer, and new C-C bond formation.

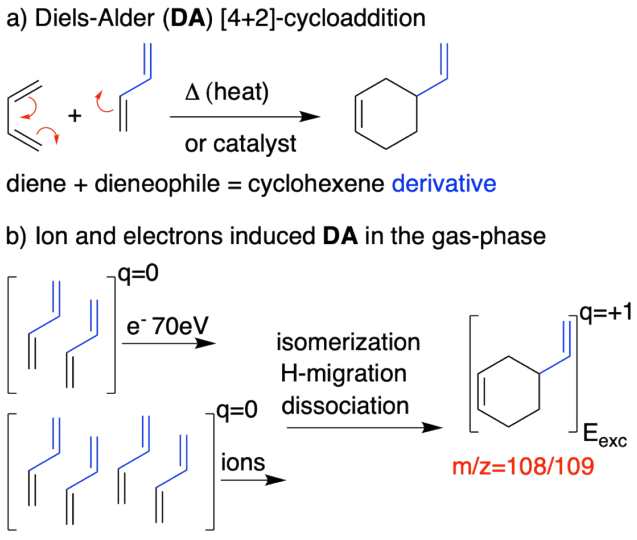


Figure 1. (a) general scheme of the Diels-Alder mechanism and b) our approach.

Acknowledgements

This work was supported by the National Science Centre, Poland, grant no. 2022/47/D/ST4/03286 and COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace).

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JWST insights into the complexity of molecules, ices and dust grains in buried galactic nuclei

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Nowadays, it is widely accepted that most galaxies undergo an active phase during their evolution. The energy released by active galactic nuclei (AGN) can strongly impact the interstellar medium of their host galaxies. At nuclear scales, obscuring structures connect the AGN feeding reservoir with the host galaxy gas cycle. Recent observations have shown that these regions are not simple dusty structures, but complex multiphase environments composed of dust, molecular gas, and icy mantles.

In this context, I will present new JWST results revealing an unprecedentedly rich molecular chemistry in the nuclear dusty structures of obscured AGN. The advent of JWST has revolutionized the study of deeply obscured nuclei, providing access to their molecular and solid-state composition through NIRSpec and MIRI spectroscopy. These observations have revealed a diverse inventory of molecular tracers, including H_2O, CO, CO_2, HCN, small hydrocarbons, and H_3^+, together with ice features, enabling detailed constraints on extinction, excitation conditions, ionization, and the geometry of deeply embedded sources.

Molecular absorption is found to arise from compact, warm, and dense environments associated with buried AGN and compact obscured nuclei (CONs), where extreme dust and gas columns hide the central power source from optical and X-ray observations. These studies also suggest that the erosion and fragmentation of hydrogenated amorphous carbonaceous (HACs) grains and polycyclic aromatic hydrocarbons (PAHs) play a key role in producing small hydrocarbons in these nuclear environments.

These JWST results demonstrate the power of infrared molecular spectroscopy to probe the innermost regions of AGN and reveal the complex multiphase nature of nuclear obscuring structures. They also highlight the need for new generations of dusty AGN models that incorporate molecular and ice components to accurately describe these extreme environments.

Acknowledgements
IGB is supported by the Programa Atracción de Talento Investigador ``César Nombela" via grant 2023-T1/TEC-29030 funded by the Community of Madrid, and acknowledges support from the COST Action CA 21126 Carbon molecular structures in space (NanoSpace), supported by the European Cooperation in Science and Technology, and the research project PID2024-159902NA-I00 funded by the Spanish Ministry of Science and Innovation/State Agency of Research (MCIN/AEI/10.13039/501100011033) and FSE+. IGB also acknowledges support from.

Dust production and survival from stellar remnants to high-redshift galaxies

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Dust plays a central role in the evolution of galaxies, regulating gas cooling, molecule formation, star formation, and the interpretation of observations across cosmic time. However, the origin and survival of dust in galaxies remain highly debated, particularly at high redshift, where large dust reservoirs are observed in some cases only a few hundred million years after the Big Bang. At the same time, there are also high-redshift galaxies that appear to be nearly dust-free. In this contribution, I present a connected view of dust evolution across different astrophysical environments, linking dust formation and processing in stellar remnants with the emergence of dusty galaxies in the early Universe.

I will discuss our recent work on dust formation and destruction in circumstellar and interstellar environments, including nova eruptions, and supernova remnants [1]. These systems are laboratories for understanding how fresh dust is injected into the surrounding medium, how it is processed by shocks, and radiation, and under which conditions it can survive long enough to enrich the interstellar medium. I will then connect these small and intermediate scale processes with the broader problem of dust enrichment in young, compact, star-forming galaxies at high redshift. In particular, I will address how intense stellar feedback can both promote and suppress the build-up of observable dust reservoirs by shaping the multiphase structure of the interstellar medium, driving outflows, and exposing grains to destructive shocks [2].

By combining hydrodynamical modeling, dust-evolution calculations, and multi-wavelength observational constraints, this work aims to bridge the gap between the microphysics of dust processing in stellar ejecta and the macroscopic evolution of dusty galaxies. This approach highlights the importance of treating dust not as a passive tracer, but as a dynamically and chemically evolving component whose survival depends on the interplay between stellar feedback, gas density structure, metallicity, and galaxy evolution.

Finally, I will also briefly present our work on Diffuse Interstellar Bands as tracers of the dusty and molecular interstellar medium in nearby galaxies, providing empirical constraints on how dust-related carriers respond to local radiation fields, extinction, metallicity, and star-forming environments.

Acknowledgements
This work was supported by the Czech Ministry of Education, Youth and Sports, through the INTER-EXCELLENCE II program, project LUC24023 (MSMT-14950/2024-5). We also acknowledge support from the institutional project RVO:67985815.

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Circumstellar grain reactivity: A computational model based on dry montmorillonite with gaseous CO and CO/H_2

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Mineral surfaces are believed to play a fundamental role in molecular evolution in astrophysical and planetary environments. In particular, clay minerals such as montmorillonite provide reactive interfaces that adsorb, activate, and transform small molecules into more complex organic species [1]. In this study, we investigate the formation pathways of organic molecules on dry montmorillonite surfaces under elevated-temperature conditions relevant to early planetary environments and interstellar chemistry. Using molecular dynamics simulations, we explore how surface oxygen sites and interlayer cations influence molecular reactivity. Indeed, dry montmorillonite surfaces promote direct surface–molecule interactions and bond rearrangement to form new organic molecules. Our results reveal that the mineral surface acts not only as a physical support but also as a catalytic environment that stabilizes reactive intermediates and lowers barriers for bond formation. Distinct reaction channels are observed, leading to the formation of different classes of organic fragments. The interplay between confinement, surface charge distribution, and local coordination geometry is shown to be crucial in directing molecular evolution. These findings highlight the potential of clay minerals to drive prebiotic organic synthesis and contribute to the chemical complexity observed in space environments. The study provides mechanistic insight into surface-mediated molecular growth processes that may represent early steps toward the formation of carbon-based nanostructures and complex organic matter.

Acknowledgements
The authors thank Prof. Inga Kamp for insightful discussions. Y.Guermassi thanks the university of Groningen, the University of Carthage and Prof. Dr. Petra Rudolf for the travel grant to the University of Groningen for part of his project.

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Radiative stabilization of the first aromatic rings

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Aromaticity is ubiquitous in the universe, occurring in environments ranging from cold molecular clouds to irradiated planetary nebulae, and across cosmic history from the early universe to planetary atmospheres [1(a-d)]. However, the formation of the first aromatic ring, benzene, in astrophysical environments remains poorly understood. Extensive chemical networks have been proposed to explain its formation under different conditions, many of which identify dissociative recombination of $C_6H_7^+$ as the dominant pathway. Since $C_6H_7^+$ is thought to form through reactions of phenylium ($C_6H_5^+$) with H_2, these models highlight the central role of phenylium in benzene chemistry. However, the radiative association pathways proposed for phenylium formation have recently been questioned[2]. Moreover, chemical networks capable of reproducing benzene abundances in one environment, such as the protoplanetary nebula CRL 618[1a], fail in others, including the molecular cloud TMC-1[1b].

Here, we investigate the radiative stabilization of phenylium and benzene monocations in experiments using the cryogenic electrostatic ion-beam storage ring DESIREE The cryogenic extreme-high-vacuum conditions at DESIREE allow ions to be stored and studied in isolation over much longer timescales than in conventional mass spectrometers, enabling measurements under conditions directly comparable to astrophysical environments. Time-resolved dissociation rates for vibraitonally hot ions measured at DESIREE are interpreted using modelled radiative cooling and dissociation rate coefficients. We determine the critical energies below which the cations can be radiatively stabilized against dissociation. For phenylium, radiative stabilization is possible up to an internal energy of 5.0 eV, placing constraints on the exothermicity of proposed radiative association pathways. We also find that phenylium is stabilized four times faster than benzene cations. These results are discussed in the context of benzene formation and stability different astrophysical environments.

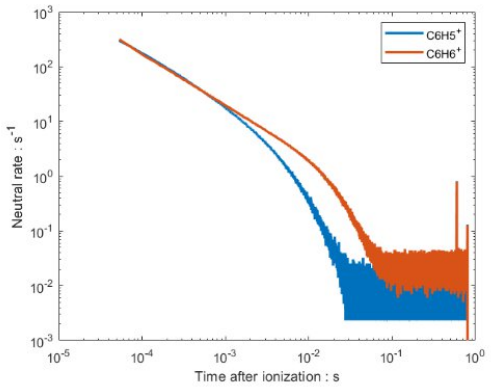


Figure 1: Absolute dissociation rates of benzene and phenyl cations

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NanoSpace Knowledge Hub: an interdisciplinary, tool-integrated Science 4.0 cosmic nanocarbon inventory database

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One of the main goals of the COST action NanoSpace, as described in the memorandum of understanding [1], is to deliver to the scientific community a structured database containing relevant information on nanocarbons for use in future projects. The identification of polycyclic aromatic hydrocarbons (PAHs) and fullerene-related species in astrophysical environments relies heavily on comparison with laboratory spectroscopic reference data. However, such data are frequently scattered across publications in heterogeneous formats, with full spectral curves often inaccessible beyond static figures, limiting reuse for spectral matching, machine learning, and cross-laboratory comparison. We present the NanoSpace Knowledge Hub, a relational database infrastructure primarily designed to consolidate infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopic data for PAHs, fullerenes, and related cations into a unified, queryable, and reproducible format.

The database architecture implements a three-tier schema for each spectroscopic modality, separating experimental metadata, complete spectral curves, and interpreted peak assignments into distinct relational tables linked by foreign-key constraints with cascading referential integrity. This design preserves full spectral fidelity—every measured data point—rather than reducing data to peak lists alone, while retaining structured fields for instrument parameters, measurement conditions, and literature provenance. Rather than serving as a static repository, the platform embeds scientific tools directly alongside data: a tool to fit and analyse PAH emissions from observational spectra, an embedded FITS viewer for spectroscopic inspection, a phonon band structure analyser, a molecular geometry viewer, and interactive plotting capabilities. Implemented features further include bulk data import and export, chemical validation services for molecular formulas, CAS numbers, SMILES, and InChI identifiers.

The Science 4.0 [2] philosophy is central to the platform's design. Community feedback gathered through surveys and workshops has directly shaped metadata standards and development priorities. This work establishes a scalable foundation for community-driven aggregation of molecular spectroscopic data relevant to interstellar and circumstellar chemistry, with planned extensions for computational spectra, API-based data access, and integration with existing astrochemical databases.

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A Lightweight PAH Spectral Analysis Tool For Online Astrophysical Diagnostics

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Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous in the Universe and serve as crucial tracers of the physical and chemical conditions within the interstellar medium (ISM). With the unprecedented sensitivity and spatial resolution of the James Webb Space Telescope (JWST), the volume of mid-infrared spectral data has grown exponentially, necessitating robust and automated analysis frameworks. In alignment with the scientific objectives of COST Action CA21126 (NanoSpace) Working Group 1, which focuses on the lifecycle and evolution of carbonaceous nanoparticles in space, we present practical web-tool designed to autonomously characterize astrophysical environments using PAH emission spectra. This tool systematically processes observational spectra to extract integrated fluxes of primary PAH emission features, specifically the 3.3, 6.2, 7.7, 8.6 and 11.3 μm bands. By calculating targeted band flux ratios—such as I6.2 / I11.3 to determine the ionization fraction (PAH+ / PAH0) and I11.3 / I3.3 to constrain the average molecular size and local ultraviolet radiation field intensity (G0) —the software automatically projects the observed data onto theoretical diagnostic diagrams based on established models [1][2].

This automated approach bridges the gap between raw spectral data and physical interpretation. It enables the rapid classification of distinct astrophysical regions, clearly distinguishing between the hard radiation fields of Active Galactic Nuclei (AGN) and the softer environments of star-forming regions. By integrating this diagnostic capability into a centralized database [3], the tool provides a dynamic mapping of PAH emission and size distribution across diverse galaxies. Ultimately, this work significantly enhances our capacity to track the chemical evolution of carbon dust in space, providing a scalable solution for the modern era of infrared astronomy.

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Benefits and challenges for public-private research collaborations in space science

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In this contribution we present lessons learned from participating as an service and R&D oriented SME to European research and innovation projects in the space domain.

We give insights from coordinating a Horizon 2020 space science project, participating to Research Infrastructures, Marie-Curie Training Networks, ANR common laboratories, and COST networking actions. What are the benefits, but also what are the respective expectations and challenges in public-private collaborations. We highlight particularities and differences we see for the space sciences and earth observation fields.

We conclude with some reflections on transitioning between academia and industry and how both "worlds" can support each other and build mutually beneficial relations.

Collaborations Between Academia and Thermo Fisher Scientific in Mass Spectrometry

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Mass spectrometry is a versatile analytical technology with applications spanning the life sciences, environmental and materials research, geochemistry, planetary science, and space exploration. Many advances in these fields have been driven by close interactions between academic researchers and technology developers.

Presented examples will include collaborations in life science and inorganic mass spectrometry, as well as the development of Orbitrap-based technologies for space research.

Particular emphasis will be placed on the factors that contribute to successful partnerships, including the alignment of scientific goals, complementary expertise, and the iterative exchange of ideas between researchers and instrument developers. The presentation aims to stimulate discussion on how academic–industry collaborations can drive innovation and advance analytical science across diverse research areas.

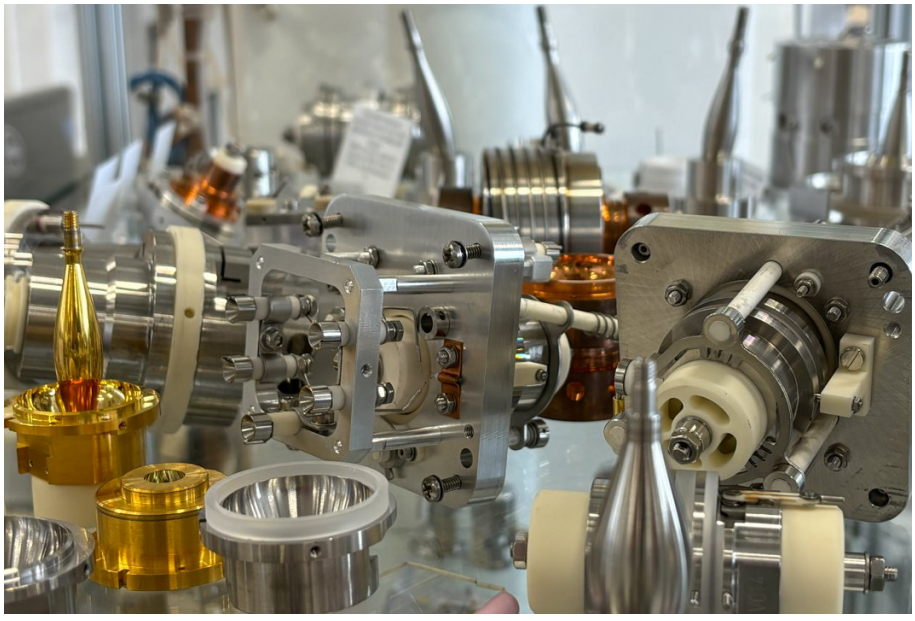


Figure 1: Historical hardware parts of Orbitrap mass spectrometers

Functionalization of Optical Fibers with Nanocarbons for Advanced Applications

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The functionalization of optical fibers with nanocarbon based materials has emerged as a promising strategy for the development of advanced photonic and sensing technologies. Nanocarbons, such as Carbon Dots exhibit exceptional optical, electrical, thermal, and mechanical properties that significantly enhance the performance of conventional optical fiber systems. This presentation explores the most relevant techniques for integrating nanocarbons onto optical fiber platforms, such as dip coating, chemical vapor deposition, layer by layer assembly, and laser assisted methods. Furthermore, the influence of nanocarbon functionalization on sensitivity, selectivity, signal stability, and light matter interaction is discussed. Special attention is given to applications in chemical and biological sensing, telecommunications, environmental monitoring, biomedical diagnostics, and nonlinear photonics. The presentation also highlights current challenges related to fabrication reproducibility, material stability, and large scale integration, as well as future perspectives for next-generation smart optical devices. The combination of optical fibers and nanocarbon materials represents a versatile and highly efficient approach for advancing modern photonic applications.

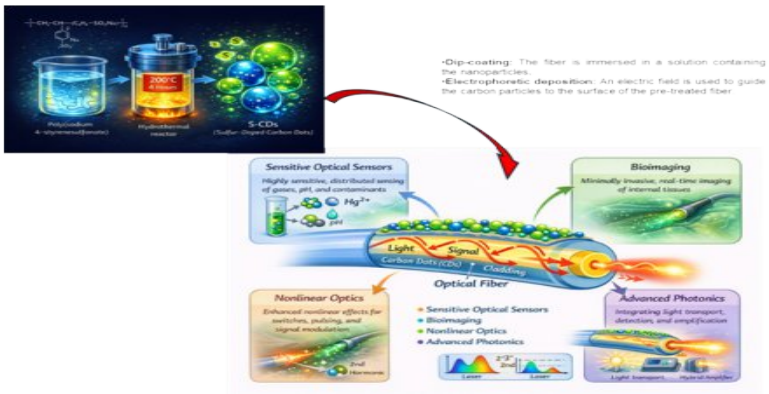


Figure 1. Schematic representation of optical fiber functionalization with carbon dots, highlighting integration techniques and representative applications.

Acknowledgements

It is grateful for financial support from the Spanish Ministry of Science and Innovation (MCIU/AEI/10.13039/501100011033/FEDER, UE) through projects PID2021-122613OB-I00 and COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology)

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Discharge-Pulse Synthesis and the Use of Carbon Nanostructures to Create Metal-Carbon Nanostructured Composites

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The results of targeted high-energy synthesis of various allotropic forms of nanocarbon (nanodiamonds, fullerenes, nanospheres, and nanotubes) are presented using high-voltage electric discharges of graphite and liquid hydrocarbons. The scientific originality of this work lies in the combination of the discharge-pulse method [1] for synthesizing carbon nanostructures with their subsequent use as active components for the synthesis of metal-carbon nanostructured composites using self-propagating high-temperature synthesis (SHS) and spark-plasma sintering (SPS). The results confirm the potential of using discharge-pulse nanocarbon for the energy-efficient production of nanostructured composites containing titanium carbides and MAX phases of the Ti-Al-C system. The practical significance of the work lies in the development of carbon nanopowders and composites [1, 2].

Acknowledgements
The research was performed with partial financial support from the Research Council of Lithuania and the Ministry of Education and Science of Ukraine in the framework of "Application of high-concentrated energy flows for producing nanostructured polyfunctional composite materials" joint project according to the results of joint Ukrainian–Lithuanian R&D projects for the period of 2022–2023 contest (Reg. No. P-LUP-22-5).
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The potential of nanocarbon in cancer research: C_{60} fullerene as "magic bullet" in the inhibition of tumour growth

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Fullerene C_{60} possesses 30 weakly conjugated double bonds. These double bonds are readily reactive with free radicals.[1] C, N, S, O centred radicals are able to add on the fullerene double bonds leading to neutral adducts.[1] For instance, up to 16 bulky benzyl radicals and up to 34 small methyl radicals can be added on a *single* C_{60} fullerene molecule.[2] For these unique properties the fullerenes and in particular C_{60} fullerene, has been defined as a "free radical sponge".[1,2] It was demonstrated experimentally that certain simple molecules which act as radical scavengers are able to inhibit the growth of tumours especially in the early stages.[4] However, all the radical scavengers commonly known as antineoplastic are able to accept just one or two free radicals per molecule. Instead, C_{60} fullerene is able to accept from 16 to 34 free radical per molecule. This may imply both the possibility to have fullerenes effective in the inhibition of tumour growth at very low dosages or to have a very powerful effect in tumour growth inhibition. The key problem is how to deliver the C_{60} molecule *in vivo* selectively where it is needed (the "magic bullet" concept). In fact, C_{60} is completely insoluble in water and aqueous solutions. We have discovered[4] and patented,[5] that fullerenes (either C_{60} or C_{70}) are strongly lipophilic and soluble in fatty acid esters including the common olive, soybean, sunflower, peanut, linseed and castor oils. This discovery has paved the way to use fats as a vehicle to deliver fullerenes *in vivo*.[6] As expected, the inhibition of tumour growth rate exerted by C_{60} has been experimentally observed,[7] as well as a significant prolongation of lifespan of rats under repeated administration *per os* of C_{60} vehicled in olive oil.[8] A recent review addresses the incredible pharmacological properties of pristine, chemically unmodified C_{60} fullerene, its protective effects in vivo and lack of toxicity.[9]

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From Astrochemistry to Prebiotic Chemistry: The Evolution of Organic Matter

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Some of the organic matter in our solar system may have originated in dense molecular clouds. These clouds are made up of silicate grains surrounded by ices including H_2O, CO_2, CO, CH_3OH and NH_3. In some areas, the cloud will collapse on itself to form a solar nebula that will potentially evolve into a planetary system such as our solar system. During this evolution, these ices will undergo numerous modifications leading to a complexification of the organic matrix. The agglomeration of these grains carrying more or less evolved organic matter have formed the small bodies of our solar system, from the asteroids to the comets far away. These small objects could have then served as a reservoir of organic matter for the development of prebiotic chemistry on the surface of a telluric planet such as the primitive Earth.

Using experimental approaches developed in our laboratory [1], we try to reproduce the conditions of formation of interstellar grains and to study their molecular composition. Following this strategy, we aim to determine the role of solid phases in the origin and evolution of organic matter (volatile and non-volatile) in these astrophysical environments [2]. Linked to the question of the origin of biochemical systems on Earth, our research could help determine how such organic matter may have served in the emergence of prebiotic chemical processes, representing the first stages towards the appearance of life [3].

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Formation of (cyano)polyynes in 1 keV electron irradiated hydrocarbon-rich ices

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The energetic processing of condensed hydrocarbons in space environments may result in the production of larger carbon-rich species. Of particular interest are the formation and chemistry of molecules that are relatively abundant in space and that could act as precursors to species directly relevant to biochemical and life-sustaining processes. Among such molecules are the straight-chain polyynes and cyanopolyynes, which have been observed in several astronomical environments across the interstellar medium. They are also believed to contribute to the tholin material in the atmosphere of Titan and may be present on the icy surface of Pluto (see references in [1]).

Solid-phase polyynes and cyanopolyynes (≤20 C atoms) exhibit distinct absorption bands below 350 nm [2], making ultraviolet spectroscopy a promising tool for studying their formation and chemistry in low-temperature environments. In addition, ultraviolet spectroscopy is becoming increasingly important due to its role in exploring the icy surfaces of outer Solar System bodies. Laboratory UV spectra provide essential reference data for interpreting observations from current and upcoming space missions, such as JUICE and Europa Clipper, thereby improving our understanding of the composition of extraterrestrial ices.

We have used vacuum-ultraviolet photoabsorption spectroscopy to characterise the production of polyynes and cyanopolyynes as a result of the 1 keV electron irradiation of neat CH_4, C_2H_4, C_2H_6, C_3H_8, C_6H_{14}, and C_8H_{18}astrophysical ice analogues as well as their binary mixtures with $N_2$and NH_3. Our results suggest that the radiolytic synthesis of (cyano)polyynes in hydrocarbon- and nitrogen-rich icy space environments is plausible [1].

Acknowledgements
EU Horizon 2020 RI CALIPSOplus (No. 730872), COST Actions TD1308, CM1401, CA20129, Europlanet 2024 RI, Danish National Research Foundation through the Centre of Excellence ‘InterCat’ (No. DNRF150), Slovak Grant Agency for Science (grant No. 2/0059/22)

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From simple hydrocarbons to complex organics: the role of acetyleneinice chemistry

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The detection of complex organic molecules (COMs) in star-forming regions reveals that rich physical and chemical processes occur even under the harsh conditions of interstellar space, characterized by cryogenic temperatures, low densities, and intense radiation fields. One important top-down chemical pathway transforms large polycyclic aromatic hydrocarbons (PAHs) into fullerenes while releasing a variety of hydrocarbon fragments. Among these, acetylene (C_2H_2), the simplest alkyne, is among the most abundant dissociation products and has been proposed to serve as a fundamental molecular backbone for incorporating oxygen-, nitrogen-, and sulfur-bearing functional groups, ultimately contributing to the chemical inventory from which planetary systems emerge.

In early star-forming regions, cosmic dust grains provide catalytic surfaces where gas-phase species accrete, diffuse, and react, facilitating the underlying chemistry. This presentation highlights a series of laboratory studies investigating the versatile role of C_2H_2 on dust-grain surfaces and within interstellar ice mantles. UV photolysis of pure C_2H_2 ice efficiently produces polyynes ($C2_nH_2$) and, under intense irradiation, refractory organic residues containing aromatic structures.[1] In contrast, when solid C_2H_2 reacts with H and OH radicals, precursors to H_2O ice formation in translucent clouds, a variety of O-bearing COMs, including vinyl alcohol, acetaldehyde, and ethanol, are formed. This chemistry is further extended by investigating analogous reactions involving NH_2 and SH radicals. The corresponding N- and S-bearing COMs have been unambiguously identified, demonstrating an efficient low-temperature radical-addition mechanism in interstellar ices.[3] The temporal evolution of these products over astrophysically relevant timescales enables quantitative comparison with molecular abundances observed at different stages of star formation. A comprehensive solid-state reaction network linking these laboratory results to interstellar chemical evolution will be presented.

Acknowledgements

This work has been supported by the Danish NationalResearch Foundation through the Center of Excellence InterCat (Grant Agreement No. DNRF150). It has also been funded by DANII and NOVA.G.F. acknowledges the Xinjiang Tianchi Talent Program (2024).Thispresentationis made possible by theCOST Action NanoSpace, CA21126, supported by COST (European Cooperation in Science and Technology).

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Heavy Ion Irradiation of Propionitrile Ice as an Analogue for Titan's Stratospheric Chemistry

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Titan, Saturn's largest moon, hosts a dense nitrogen- and carbon-rich atmosphere often regarded as a natural laboratory for prebiotic chemistry [1]. In the stratosphere, nitrile-bearing molecules such as propionitrile (C2H5CN) condense onto aerosol particles forming icy mantles, where they are subjected to energetic particle radiation from cosmic rays and Saturn's magnetosphere [2], driving complex chemistry that contributes to the molecular complexity of Titan's organic haze.

Propionitrile ice was irradiated with heavy ion beams (MeV energies) at the IRRSUD beamline at CIMAP-GANIL, using the IGLIAS setup with in-situ FTIR spectroscopy. Irradiation-induced spectral changes were monitored as a function of fluence, allowing identification of radiolysis products formed within the ice phase.

Several new species were identified, including acrylonitrile (C2H3CN), hydrogen cyanide (HCN), and cyanoacetylene (HC3N) - all detected in Titan's atmosphere by Cassini/CIRS. Their formation points to a sequential fragmentation and recombination chemistry driven by electronic energy deposition along the ion track, supporting the role of ion processing of stratospheric ices in Titan's atmospheric molecular inventory.

Acknowledgements

This work benefits from state aid managed by the French National Research Agency under France 2030 investment plan (reference ANR MIRRPLA; ANR-22-EXOR-0012) within PEPR Origins framework (https://pepr-origins.fr/en/the-pepr/). R.S acknowledges support from Normandie Region.

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Large-scale dusty nebulae around symbiotic binaries

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Symbiotic stars (SySts) are interacting binary systems composed of a cold, dust-producing red giant, losing material to a hot white dwarf (WD), and embedded in a surrounding nebula as a result. Interactions between the stellar components, such as mass transfer via Bondi–Hoyle–Lyttleton accretion or Roche-lobe overflow, can trigger outbursts, jet formation, and nova-like explosions. Such events can significantly affect the circumstellar environment. As a result, dusty filaments can form in the immediate vicinity of the system or on a larger scale. To date, BI Cru, R Aquarii, and Omi Ceti are the only known symbiotic systems clearly exhibiting these dusty features.

While large-scale gaseous nebulae around SySts have extensively been studied, the dusty material surrounding these systems has not yet been systematically investigated. In this contribution, we present new results on the detection of extended dust emission from all Galactic symbiotic stars (284 sources) using archival imaging data from various IR telescopes. Our initial results reveal only a small number of detections of extended dust emission. The identified systems studied in more detail using hydrodynamic simulations to explore the role of binary interaction and outburst evolution. In addition, we discuss possible reasons for the apparent lack of detectable dust nebulae around the majority of symbiotic stars.

Acknowledgements
This work is based upon work from COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology).

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Curvatures of fullerene graphs

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A fullerene graph is a 3-regular, 3-connected, plane graph with only pentagonal and hexagonal faces. Among the main driving forces behind the study of fullerene graphs has been a desire to find graph-theoretical invariants which could be used as predictors of stability of the corresponding fullerene species. Many invariants have been examined, with only a moderate success so far. In this work, we consider some recently introduced graph curvatures and investigate whether they could be used as stability predictors.

Acknowledgements
This work was partially supported by the Croatian Science Foundation under the project number HRZZ-IP-2024-05-2130.

Effects of Gamma Irradiation on the Optical Properties of GO and GO-Based Nanocomposites

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Graphene oxide (GO) and GO-based nanocomposites have become among the most extensively studied materials in recent years due to their unique structural and functional properties. In particular, understanding the influence of various technological and environmental factors on their physical characteristics remains an important research topic. One of the most significant external factors is gamma irradiation, which can considerably modify the physical properties of GO and GO-based nanocomposites. In this study, the effects of gamma irradiation on the optical properties of GO nanosheets, GO–PVA, and GO–PVA–AgNWs nanocomposites exposed to different radiation doses were investigated. GO nanosheets were synthesized using a modified Hummers method, while the nanocomposites were prepared by the solution-casting technique [1]. To evaluate their radiation stability and the degree of structural modification, the samples were irradiated with a 60Co gamma source at doses ranging from 10 to 1500 kGy.

The results revealed that gamma irradiation induces a red shift of the absorption edge toward longer wavelengths in both GO nanosheets and GO-based nanocomposites. Furthermore, the optical band gap values determined using the Tauc method decreased with increasing irradiation dose [1], as summarized in Table 1. The reduction of the band gap in GO is attributed to the partial reduction of graphene oxide under gamma irradiation. In the GO–PVA and GO–PVA–AgNWs nanocomposites, gamma exposure promotes the aggregation of GO sheets and generates additional structural defects within the polymer matrix. These irradiation-induced defects introduce new localized energy states in the electronic structure, thereby reducing the energy required for optical transitions and leading to a decrease in the optical band gap.

Table 1. Band gap values of GO and GO-based nanocomposites.

γ irradiation	0 kGy	10 kGy	250 kGy	500 kGy	1500 kGy
Band gap E_g (eV)					
GO	-	2.00	1.60	1.44	1.33
GO-PVA	5.26	-	4.96	4.85	3.86
GO-PVA-AgNW	5.07	-	4.94	4.84	3.82

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A Spectral View of Extremal Nullity Carbon Molecules

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Our aim is to discuss the singular graph models of Carbon molecules and their classifications based on the number of non–bonding orbitals according to the tight binding theory. Three subclasses, namely, nut graphs, nuciferous graphs and uniform core graphs, are presented as mathematical structures modelling molecular conductivity in chemical physics, within the Hu¨ckel theory for Π-conjugated carbon frameworks.

The Hamiltonian of a molecule is the 0–1–adjacency matrix A of the Carbon atom framework (called a graph G) where the edges of the graph represent the sigma–bonds between pairs of Carbon atoms. For a device (G, y, z), which is a connected graph G, with two pre–identified vertices y and z, the zero–nonzero pattern of a basis for the nullspace of A reveals the nullity signature $\{\eta(G), \eta(G - y), \eta(G - z), \eta(G - y - z)\}$. Mathematical constraints restrict the number of realizable nullity signatures to 11.

We focus on three structures, the nut graph, the nuciferous graph and the uniform core graph, all extremal with respect to the nullspace Ker(A) of A.

For a nut graph, every vector in Ker(A) is full, (that is, it contains no zero entries). Hence nut graphs have nullity one and turn out to be the only omni–conductors among core graphs of nullity one. A nuciferous graph H has nullity signature $\{\eta(H), \eta(H) + 1, \eta(H) + 1, \eta(H)\}$ for each pair of vertices x and y. It follows that H is non–singular and each vertex–deleted subgraph $H - v$ is a nut graph. A uniform core graph (UCG) U has nullity signature $\{\eta(U), \eta(U) - 1, \eta(U) - 1, \eta(U) - 2\}$ for each pair of vertices y and
z. Consequently, $\eta(U) \geq 2$. Nut graphs are found as induced subgraphs of certain UCGs.

In the context of the Hu¨ckel tight-binding theory, graphs model Π–conjugated carbon frameworks. Nut graphs emerged as the molecules of nullity one with no core–forbidden vertices, which allow the transfer of elec-trons for all pairs of connecting vertices across a small bias voltage. As a result they were characterized as the class of strong omni–conductors of nullity one in source-and-sink models of ballistic molecular conduction. Nu-ciferous graphs and UCGs were designed to meet the needs of specific re-search in molecular conductivity. Nuciferous graphs were identified as the non–singular molecular graphs that are ipso omni–insulating (for y = z) but distinct omni–conducting molecules (for $y \neq z$). UCGs turned out to be the distinct omni–insulating molecules among core graphs. We explore the in-terplay among these three subclasses of singular graphs. The predictions of molecular conductivity in singular graphs are currently being investigated through experimental electrical circuit models using coaxial cables at the Physics and Astronomy School of Mathematical Sciences of the University of Sheffield, UK.

NanoSpace: a four years trip

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Over the past four years, the COST Action NanoSpace has grown into a multidisciplinary European network dedicated to understanding the formation, processing, and spectral signatures of carbonaceous nanomaterials in space. This talk looks back on that journey, from the Action's initial goals to the collaborations and results it has fostered along the way. The timing could hardly have been better: NanoSpace developed in step with the*James Webb Space Telescope*(JWST), whose transformative infrared observations are revealing dust and molecules across diverse astronomical environments, ranging from the interstellar medium (ISM) and protoplanetary disks to high-redshift galaxies. Interpreting the rich molecular and solid-state features uncovered by JWST demands close interaction between astronomical observations, laboratory astrophysics, theoretical chemistry, and materials science, precisely the expertise that NanoSpace set out to connect. By bringing these disciplines together, the Action has promoted laboratory measurements, modelling efforts, and collaborative analyses that directly support the interpretation of JWST data. Here, I revisit the goals and main activities of NanoSpace, share some highlights from its four years of work, and reflect on how coordinated multidisciplinary collaboration can maximize the scientific return of JWST observations in diverse cosmic environments, as well as on the legacy the Action leaves behind.

List of Posters

Counting Geodesic Paths on Nanotubes

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We investigate geodetic paths on (p,0)-nanotubes using a coordinate-based framework. We define minimal parallelogram patches containing all shortest paths between two vertices, and classify them according to the vertex type. We provide explicit combinatorial formulas for the number of geodetic paths, expressed as sums of binomial coefficients over all periodic lifts of a vertex. Our results also identify regions where nanotube distances coincide with planar distances and where the cylindrical identification yields shorter paths.

Oxygenated Helicenes: Beyond the archetypal PAHs

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PAHs have been predicted by the astrophysical community as one of the most abundant carbon-containing species in space[1]. Archetypal PAHs encompass a family of molecules which characterizes by a structure of fused-hexagon rings, producing linear/branched planar or helical geometries. The former describes a PAH known as helicene whose helix structure allow them to possess chiral properties. However, there are few studies related to helicenes and their implications to the astrophysical/astrochemistry community in spite to have unique properties that could ease its detection. This work is focused in the anharmonic-DFT study of pristine and oxidized/hydroxylated helicenes using the 4-, 5- and 6-helicene molecules to compare with analogous archetypal PAHs. In addition, all the helicenes species have been studied under different charged states (neutral, cation and anion). Our results reveal that helicenes can exhibit large values of permanent dipole moment (*D*), unlike typical PAHs where $D \approx 0$ or very low, especially in the case of charged species. This trend improved for the anions of oxidized helicenes while for the case of the hydroxylated ones it depended on the helix length in the structure, as consequence of an improvement in the intramolecular interactions. On the other hand, our calculations indicated that helicenes vibrational modes had a strong contribution in regions assigned to duo and trio C-H of PAHs. In general, the infrared spectra of helicenes were as richer as those obtained for large PAHs, without the need of a large molecular size.

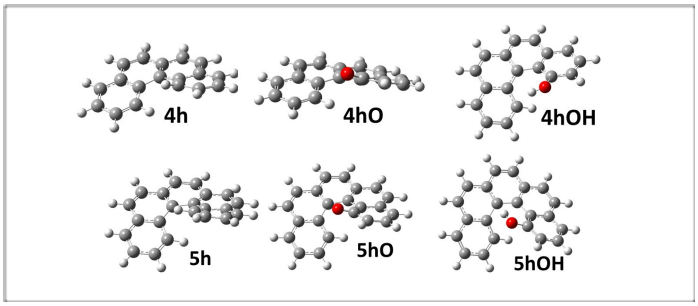


Figure 1: Models of the 4- and 5 helicenes: pristine, oxidized (O) and hydroxylated (OH).

Acknowledgements
We would like to acknowledge the generous allocation time received from the LaPalma Supercomputer, Teide HPC and the IAC-HPC facilities.

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Molecular Topology Governs Resonances in PAH Anions: Implications for Interstellar Molecules

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Negatively charged polycyclic aromatic hydrocarbons (PAHs) are believed to play a crucial role in the chemistry of the interstellar medium (ISM) [1], yet their formation mechanisms, abundances and reactivities remain poorly understood [2]. Anion formation is thought to proceed via capture of a low-energy electron into a metastable state lying above the ionization threshold: if this species is sufficiently long-lived, it can seed further chemical complexity. These transient states are difficult to study: experimentally, their short lifetimes limit spectroscopic access; computationally, they evade standard bound state description. Additionally, experimental data for PAH anions resonances are scarce and exhibit significant variability that may reflect sensitivity to molecular geometry [3]. In this work, we use extended multiconfigurational quasidegenerate perturbation theory (XMCQDPT2) to probe how changes in molecular structure affect resonance energies and autodetachment lifetimes. Our results demonstrate that even modest changes in geometry produce marked shifts in the resonance landscape, with implied consequences for the electron capture cross-section and anion stability. As these states control the branching between autodetachment and other chemical channels leading to changes in the molecular inventory, structure emerges as a previously overlooked determinant of PAH anion abundances in the ISM.

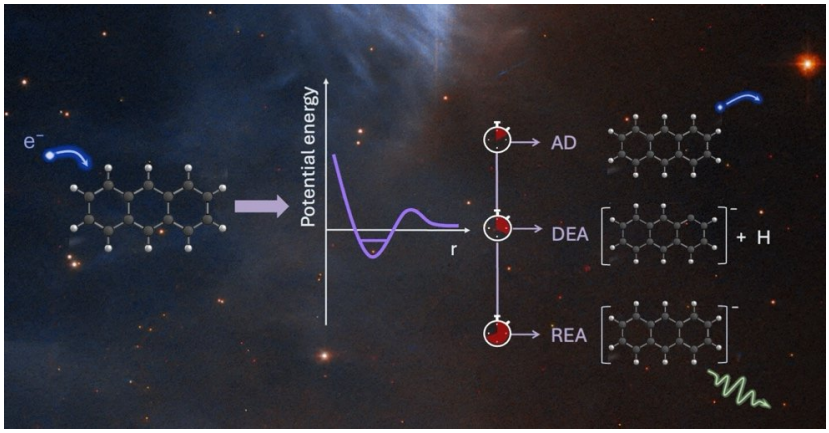


Figure 1: A schematic of electron attachment to neutral anthracene, leading to three different products depending on the lifetime of the metastable state.

Acknowledgements
We are grateful to Etienne Garand for fruitful discussion around unpublished experimental data.

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MOST. The Molecular & Optical Science and Technology Beamline. A tool for in-depth investigations in astrochemistry and physics @Elettra2.0

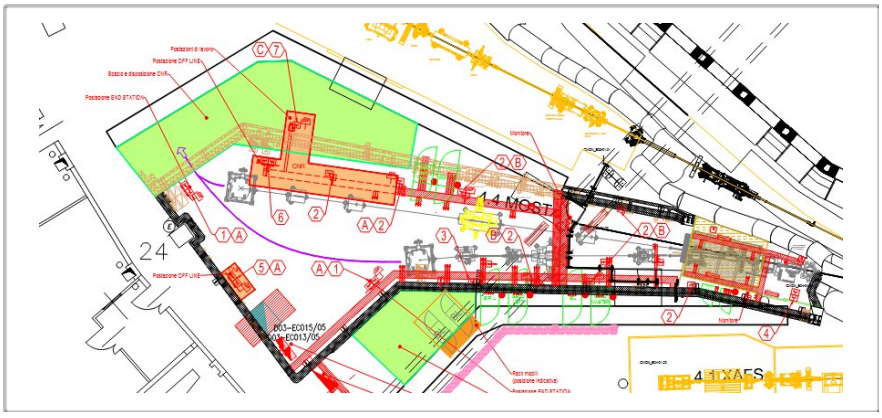
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The MOST project combines the scientific interests of the community used to work at the Gas Phase Photoemission beamline [1] and the Circular Polarization beamline [2] (CiPo) for studies of isolated species (atoms, molecules, clusters and nanoparticles), chirality, liquids and magnetic adsorbate systems.

MOST will address topics in basic and applied science, as well as contributing to the development of novel methodologies for state-of-the-art synchrotron radiation spectroscopy.

Here we present the main features of the new beamline: an open structure whose characteristics also make it interesting for astrochemical and astrophysical research.



Layout of MOST beamline @Elettra 2.0

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Scanning tunnelling microscopy studies of fullerenes

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Ultrahigh vacuum, low temperature scanning tunnel microscopy is a powerful method for probing the fundamental properties of molecules deposited on conducting substrates. Here we present the result of two different studies involving fullerene molecules, specifically $C_{60}$and Li@C_{60}.

The presence of Li inside the carbon cage lifts the icosahedral symmetry of the $C_{60}$and introduces a pseudo-Jahn-Teller distortion of the cage. This can be clearly identified by manipulating the position of the Li inside the cage using a high tunneling current and imaging the resulting occupied and unoccupied molecular orbitals, comparing the observed images with Hückel Molecular Orbital calculations. The position of the Li inside the cage determines the JT distortion axis. Different positions of Li produce different tunneling currents, mainly due to the interaction of the diffuse S-SAMO (SuperAtomMolecularOrbital) with the metal substrate, thus producing a multi-position single molecule switch [1]. The Li stabilises the JT distortion giving stable switch positions that require an additional high current pulse to return to the lowest energy position with the Li at the top of the cage. Evidence for JT distortion can also be seen for pure $C_{60,}$as expected when there is a sufficiently high electron transfer to the cage, but is unstable and rapidly returns to the initial state thus being unsuitable as a nanoelectronic switch.

A high tunnel current applied to an individual C_{60}molecule in a 2D monolayer can selectively fragment the individual molecule. We have shown that the fragmentation of C_{60}deposited on a metal at low temperature (4 K) follows a sequential C_2emission [2], similar to the fragmentation mechanism observed for isolated molecules in the gas phase. This could provide a mechanism for producing relatively large amounts of C_2as well as a broad range of smaller fullerene species under conditions relevant for astrochemistry.

Acknowledgements
Some of the work reported is based upon work from COST Action CA 21126 Carbon molecular nanostructures in space (NanoSpace*)*, supported by COST (European Cooperation in Science and Technology). RS and ESS acknowledge support from EPSRC through grant EP/T518062/1.

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Synthesis and characterization of hybrid Fe@Melanin catalysts

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In a global context where climate change, the reduction of natural resources and environmentalpollution represent urgent challenges, it has become essential to rethink chemical processesfrom a sustainable and environmentally friendly perspective. Based on these premises, thecatalysis sector has recently undergone a real renewal with the development of new types ofcatalysts that meet the requirements of sustainability. In this framework is set the workaimed at the development of new heterogeneous melanin-based catalysts.

Melanin are a class of pigments widely diffused in nature characterized by a unique set ofchemical-physical properties that have stimulated the application of the pigments as innovativebiomaterials in different sectors. [1]

Exploiting their known insolubility, robustness and ability to chelate metal ions thanks to thepresence of catechol, phenol and carboxyl moieties, we have carried out the synthesis of a setof iron-melanin hybrid materials by treating synthetic melanin polymers with $FeCl_3$. To thisaim, four different types of synthetic melanin have been prepared via the oxidativepolymerization of 1,8-dihydroxynaphthalene (DHN), the monomer precursor of fungalallomelanin, and L-3,4-dihydroxyphenylalanine (L-DOPA), 5,6-dihydroxyindole (DHI) and5,6-dihydroxyindole-2-carboxylic acid (DHICA), the precursors of eumelanin. [2][3]

A set of Fe@melanin hybrids have been prepared by treating the melanin polymers with $FeCl_3$in water at 90 °C for 3 h. The solids have been recovered by centrifugation, extensively washedwith water and then freeze-dried.The hybrids have been characterized by ATR-FTIR and EPR spectroscopy and their antioxidantpower has been assessed via the DPPH assay.

Overall, the data collected suggest that after the treatment with $FeCl_3$, the electronic asset of themelanin polymer is changed with a more or less evident increase of the quinone moieties vsthecatechol ones (ATR-FTIR evidence) that correspond to a significant reduction of the spinconcentration (EPR evidence) and of the antioxidant power (DPPH assay). This may beascribed to the well reported ability of melanin to interact with metal ions promoting theirreduction via the oxidation of the many catechol/phenol sites.

A preliminary investigation of the catalytic activity of the hybrids has been carried out byperforming the pyrogallol spectrophotometric assay. The data show that all the hybrids exhibit
a peroxidase-like activity, being able to promote the hydrogen peroxide mediated conversion of pyrogallol into purpurogallin.

These preliminary results open to a new concept of melaninas active support for transition metal-based catalysts.

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Fe@melanin hybrids: synthesis, characterization and possible implications in prebiotic chemistry

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In recent decades we have assisted to an evolution of the concept of catalysis, opening up from one side to the definition of new methodological approaches, such as photo and electrocatalysis, and technologies such as mechanochemistry and flow-chemistry, and from another side to the development of new types of catalysts, such as artificial enzymes, single-atom catalysts and metal organic frameworks.

In the frame of a research project focused on the investigation of the chemical processes that may have led to the emergence of life on the early Earth, we decided to explore a new aspect of catalysis still poorly studied, that is its role in prebiotic chemistry.[1]We know that metal-based catalysis was likely essential on the early Earth, where different minerals and metals such as Fe, Cu, Mn, and Mg facilitated the conversion of simple inorganic molecules such as $NH_3$and CO_2into organic molecules and, ultimately, into the building blocks of life.[2]Based on this background, we have undertaken a study aimed at assessing the possible role of the organic dark matter as support for the formation of metal-based hybrid materials. In particular, we have focused our attention on the melanin, a class of pigments widely diffused in nature, characterized by a set of physical-chemical properties including the ability to chelate metal ions through catechol, phenolic, and carboxylic functional groups.

In this connection, we have prepared a set of Fe@melanin hybrids starting from $FeCl_3$ and DHN-melanin obtained from the oxidative polymerization of 1,8-dihydroxynaphthalene (DHN) and resembling the dark matter found in meteorites. For comparative purposes, other melanin polymers, that is the ones obtained starting from L-3,4-dihydroxyphenylalanine (L-DOPA), 5,6-dihydroxyindole (DHI) and 5,6-dihydroxyindole-2-carboxylic acid (DHICA), have been used to prepare the corresponding hybrid materials. Data collected from spectroscopic analyses revealed that, after $FeCl_3$ treatment, the electronic properties of the melanin polymers were modified, with a more or less pronounced increase in quinone moieties with respect to catechol ones (ATR-FTIR evidence), leading to a significant decrease in spin concentration (EPR evidence) and in antioxidant power (DPPH assay evidence). A preliminary investigation of the catalytic activity of these materials suggested their role as nanozymes with peroxidase-like and catalase-like activities that in some cases proved to be comparable with those of the native enzymes, so providing useful insights for the definition of the possible role of the organic matter in promoting key prebiotic processes.

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A computational investigation of low-range hydrogenated fullerenes C_{60}

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Hydrogenated fullerenes (fulleranes) represent an important class of functionalized carbon nanostructures whose properties are governed by a balance between strain relief and disruption of π-conjugation.[1]Despite extensive studies of highly hydrogenated species, the structures and energetics of low- to moderately hydrogenated fullerene derivatives remain poorly understood due to the large number of possible isomers and complex reaction pathways. In this work, we employ modern computational methods to investigate hydrogenation patterns of $C_{60}$for compositions $C_{60}H_x$(x = 2–10). Using a graph-theoretical framework to efficiently explore the vast configurational space, we identify energetically favorable isomers, characterize preferred hydrogen addition motifs, and analyze the competing effects of cage strain relief and loss of aromatic stabilization. The results provide new insights into the structural evolution of fullerene cages during the early stages of hydrogenation and establish trends governing the stability of partially hydrogenated C_{60}species.

Acknowledgements
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Hydrated PAH clusters and the “magic” water tetramer

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Polycyclic aromatic hydrocarbons (PAHs) are a ubiquitous class of carbonaceous molecules found in a variety of astrophysical environments, from protoplanetary discs and planetary atmospheres to icy mantles coating dust grains in the interstellar medium, where they are believed to become incorporated.. The latter served as an inspiration for our current study [1], in which we prepare mixed water and PAH clusters in a supersonic expansion (PAH = naphthalene, cyanonaphthalene, anthracene and phenanthrene). Subsequently, the clusters were subjected to electron ionization to produce positively and negatively charged fragments, which were probed by time-of-flight mass spectrometry. The mass spectra unambiguously reveal high signal intensities of $[(PAH)_m(H_2O)_4]^{+/-}$cluster ions. We further discuss these findings and support them with theoretical calculations.

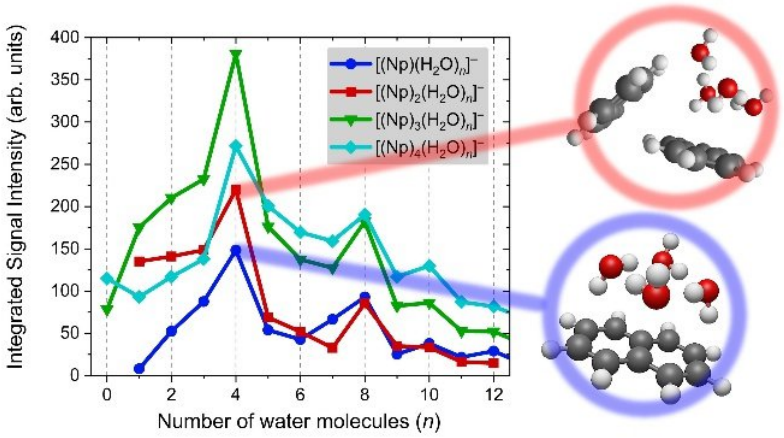


Figure 1: Signal intensities of $[(PAH)_m(H_2O)_n]^-$cluster anions as a function of number of water molecules (n)

Acknowledgements
The work has been funded by Czech Science Foundation (GAČR) Project No.: 24-11390S and partially funded by a grant from the Programme Johannes Amos Comenius under the Ministry of Education, Youth and Sports of the Czech Republic CZ.02.01.01/00/22_008/0004558 Advanced MUltiscaLe materials for key Enabling Technologies, AMULET

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fUV-Visible spectroscopy of gas-phase benzonitrile in various charge states

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Polycyclic aromatic hydrocarbons (PAHs) have been detected in various astrophysical environments. Since neutral gas-phase benzonitrile was detected in TMC-1 in 2018,[1]a number of nitrogen-bearing aromatic molecules have been detected.[2]Following these observations, many new laboratory and computational studies have been conducted to better constrain the spectroscopy and energetics of thesearomatic molecules. By exploring the photo-physics and fragmentation pathways of these molecules we aim to understand the photo-stability of such systems.

We use two experimental setups to study the interaction of UV-visible light with aromatic molecules in the gas-phase. One setup is equipped with a supersonic jet to probe neutral molecules by multiphoton ionisation (MPI) spectroscopy. This setup can be coupled with a plasma discharge source that produces singly-hydrogenated neutral radicals. The second setup is a cryogenically cooled ion trap, where photofragmentation spectroscopy can be performed on ionic species, such as protonated molecules[3]and radical cations. In both cryogenic setups, mass-selected aggregates with small molecules such as water can be studied.[4]Experiments can provide information on the spectroscopy of aromatics and thus their geometries and electronic structures, as well as other properties such as photo-detachment onsets or fragmentation patterns.

Here, we will show various recent studies of different charge states of benzonitrile, including the neutral molecule and the protonated molecular ion. In particular, we show results of an extensive study on the ionisation potentials of small aggregates with water and first results for the neutral hydrogenated radical. This study of the aromatic molecule benzonitrile in varying charge and hydration states shows variations in the measured spectroscopy, ionisation energies and fragmentation. By comparing these we aim to explore how charge state and/or hydration impacts photostability, with an aim to estimating the photophysical behaviour of these species in various astrophysical environments subject to different radiation fields, and ultimately assess their potential observability.

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Size-Dependent Stability of Charged Diamondoids

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Diamondoids are cage-like, saturated hydrocarbons whose carbon framework represents the smallest molecular fragments of the diamond lattice. Owing to their exceptional thermal and chemical stability, they have attracted considerable interest in physical chemistry, materials science, and astrochemistry. In astrophysical environments, where ultraviolet radiation and energetic particles readily induce ionization, diamondoids are expected to occur in charged states. Their stability toward ionization and fragmentation is therefore expected to play a key role in determining their abundance, chemical evolution, and potential contribution to interstellar carbon chemistry.

The geometric structure, vibrational (IR and Raman), electronic, and photoelectron spectra of neutral diamondoids have been extensively investigated experimentally and theoretically over the past two decades [1,2]. In contrast, systematic investigations of how molecular size influences the stability of charged diamondoids remain scarce, despite their relevance to ionizing environments such as combustion plasmas and the interstellar medium. In particular, it is unclear how increasing cage size affects charge localization, ionization-induced structural changes, and the energetic preference for fragmentation versus charge retention.

This work presents a theoretical investigation of the size-dependent stability of positively charged diamondoids using benchmark of quantum chemical calculations. Particular attention is given to the effect of increasing cage size on ionization energies, charge distribution, and the relative stability of the resulting radical cations. Furthermore, fragmentation pathways and their associated energetic barriers are examined to assess the resistance of charged diamondoids to dissociation following ionization. The relationship between molecular size, electronic structure, and thermodynamic stability is analyzed to provide insight into their potential survival under energetic conditions relevant to laboratory and astrophysical environments. These findings are anticipated to contribute to a better understanding of the chemical evolution of diamondoids and their potential role as molecular precursors in the formation of larger diamond-like carbon nanostructures.

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Modelling CH_3 bombardment of small hydrocarbon mixtures: a machine-learning assisted approach

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The presence of methyl radicals (CH_3) and small hydrocarbon species such as benzene in diverse astrophysical environments is now well established [1,2]. The CH_3 species can be very reactive towards benzene through molecule-radical reactions, depending on the temperature. However, our knowledge concerning the evolution of these radical species in astrophysical environments is scarce. In this work, we explored the CH_3 bombardment of small hydrocarbon mixtures (e.g., formed by benzene $C_6H_6$and other hydrocarbons), using molecular dynamics (MD) simulations. Machine-learning potentials have been used to describe the C-H and C-C interactions as implemented in the atomistic simulation code TurboGAP. Molecule mixtures were designed according to astronomical data in order to retain the abundance ratio between species [3,4,5]. Initial configurations were generated by random distributions of the molecules within a spherical region inside a simulation box, which was subsequently relaxed to improve molecule-molecule interactions (see Figure 1). This was followed by MD simulations at the NVT ensemble applying different temperatures (180, 240, and 300 K) to thermalize the models. Finally, CH_3 bombardment was performed in four random directions with respect to the simulation box, allowing to reduce the bias in the evolution of the molecule mixtures. Radial distribution functions were explored searching for combined species like C_6H_6-CH_3, C_6H_6-C_2H_5, among others. Our findings may shed light on the complex hydrocarbon chemistry in space, but also will help to improve the atomistic simulations of carbon materials in the astrochemical and astrophysical contexts.

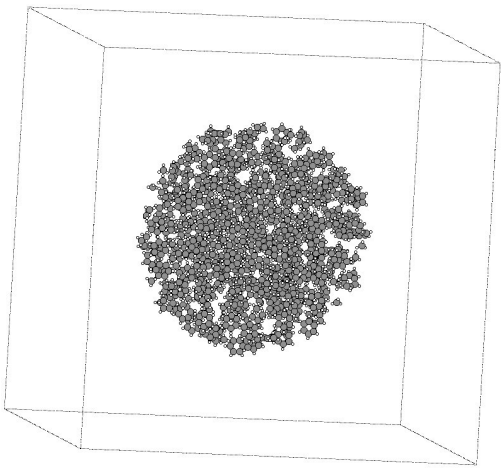


Figure 1: Example of a random distribution of C_6H_6 and CH_3 within a spherical region inside a simulation box, before relaxation.

Acknowledgements
We acknowledge the CPU allocation time granted by LaPalma supercomputer and the IAC-HPC facilities. We also acknowledge support from the State Research Agency (AEI) of the Spanish Ministry of Science, Innovation, and Universities (MICIU) of the Government of Spain, and the European Regional Development fund (ERDF), under grant PID2023-147325NB-I00/AEI/10.13039/501100011033.

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Ion irradiation of benzene (C6H6) ices, relevant to Titan's Stratosphere

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Since the first observations of Saturn's rings and moons, the Saturnian system has remained a central target for planetary exploration. Successive missions, including Pioneer 11, Voyager 1 and 2, and most notably the Cassini-Huygens mission, have significantly advanced our understanding of Saturn and its complex moon system. Among Cassini-Huygens' most impactful achievements was the detailed investigation of Titan, Saturn's largest moon, whose dense, hazy atmosphere continues to intrigue researchers.

During its descent at 10° S, the Huygens probe measured Titan's atmospheric structure, revealing variations in molecular composition, temperature, and pressure [[1](https://www.iac.es/es/responsabilidad-legal)]. While these measurements provided unprecedented insight into Titan's lower atmosphere and surface, the processes governing the formation and evolution of Titan's haze remain poorly understood. Current models suggest that nitrogen and methane in the ionosphere interact with high-energy photons to form ions and complex organic molecules, which eventually contribute to haze layers [2]. As these organics descend, they are predicted to condense onto haze particles in the lower atmosphere. Benzene and is one among the first molecules expected to condense, potentially altering haze properties [3-5].

At these lower altitudes, long-wavelength UV photons and cosmic-ray are the primary energy sources capable of modifying condensed ices. However, the effects of cosmic-ray irradiation on benzene have not been experimentally explored, leaving a key gap in our understanding of Titan's atmospheric chemistry. This poster addresses this gap by investigating how cosmic-ray analogue ion processing under Titan-like conditions alters the benzene ices and influences haze formation pathways.

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Atomistic machine learning models for predicting solvation free energies of drug-like compounds

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Atomistic machine learning methods provide a framework to accurately and with a low computational cost predict the energies of organic compounds. I will present three different machine learning methods: Gaussian approximation potential (GAP), multi-atomic cluster expansion (MACE) [2] and chemically interpretable graph interaction network (CIGIN) [3]. The work focuses committee models, which are models that themselves consist of several models. The models in the committees were varying in either the data used in the training of them or the changing of hyperparameters between the models.

Committee models provide two benefits compared to singular models: lower prediction error and the capability to estimate the prediction error itself. Lower prediction error of committee models arises due to the average of several models mitigating the errors of singular models and different models in the committee capturing different interactions between molecules. The variance of the predictions of the committee members acts as the error estimate of the committee. Both the error estimates and committee predictions can be modified to yield even better results.

My work aims to answer if atomistic machine learning models can be used in predicting solvation free energies for drug-like molecules. Solvation free energy is of great interest in pharmaceutical research, especially in the screening for potential new drug molecules. It correlates with several important quantities for drugs, such as the blood-brain barrier permeability, which is crucial for effective drug action. The experimental determination of solvation free energies for molecules is labour-intensive. Accurate and efficient machine learning methods allow for faster screening of potential drug molecules.

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Theoretical Predictions of Spectral Properties of Multilayer Boron Nitride Introduced by Point Defects

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The optical fingerprints of point defects in hexagonal boron nitride (hBN) are usually interpreted on the basis of monolayer models, whereas experiments are almost invariably performed on multilayer samples. Here we examine systematically how the layer structure surrounding a defect modifies its photophysics. A doped hBN sheet and its neighbors are represented by finite hydrogen-capped clusters (typically 102 atoms, $B_{40}H_{22}N_{40}$) stacked one over another, with the defect placed at the geometric center of the doped layer and an interlayer separation fixed at the experimental value of 3.3 Å [1]. Geometries were obtained with the semiempirical GFN2-xTB method [2], benchmarked against ωB97X-D3 [3]/SVP [4] density-functional calculations, while absorption spectra were simulated with ZINDO/S [5], validated for small test clusters against TD-DFT with the CAM-B3LYP functional [6] and the jun-cc-pVDZ basis set [7]. The character of each excitation was resolved through natural transition orbitals (NTOs) [8] and charge-transfer numbers [9].

Twenty-six defect structures were considered, spanning boron and nitrogen vacancies, single- and double-atom substitutions involving C, Si and Al, antisite B_N and N_B defects, and their combinations with vacancies and with one to three hydrogen atoms. Each defect was studied for AA, AA’ and AB bilayers, for AAA, AA’A, ABA and ABC trilayers, and for an AA’AA’A pentalayer. Additional layers shift excitation energies by up to about 1 eV and, in several instances, reverse the energetic order and the character of the lowest excited states. The largest effects arise when a defect breaks the planarity of the doped sheet, so that the dopant approaches an adjacent layer and part of the excitation leaks into it, as observed for silicon-containing defects, for Al_N, and for the nitrogen void filled with two hydrogen atoms. For the widely studied C_BC_N center responsible for the 4 eV emission line, stacking lowers the first excitation energy relative to the monolayer while raising the second one for most trilayers. Additionally, two further effects were quantified for this defect: isotopic substitution ($^{10}B/^{11}B$, $^{14}N/^{15}N$, $^{12}C/^{13}C$) and a scan of the interlayer distance from 3.0 to 3.8 Å, mimicking applied pressure. Overall, stacking sequence emerges as a key design parameter alongside defect type.

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Insight in the reaction path of C_{60} and acetylene

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The interaction between C60 fullerene and acetylene was investigated using density functional theory (DFT) calculations at the B3LYP/6–31G(d,p) level to elucidate the reaction mechanisms and pathways.

Unlike larger fullerenes, the high symmetry of C60 limits the number of non-equivalent reactive sites enabling a systematic analysis of the regioselectivity of acetylene addition. Three non-equivalent reactive sites of the C60 cage were examined, considering both [2 + 1] and [2 + 2] cycloaddition routes.

The optimized geometries, formation energies and reaction rates of the resulting cycloadducts were analyzed. In addition, hydrogen migration and dissociation reactions were investigated through single and double detachment of acetylene H atoms.

The calculations reveal a clear preference for acetylene addition at 6–6 (hexagon–hexagon) bonds over 5–6 (pentagon–hexagon) bonds, highlighting the crucial role of the local bonding environment in governing fullerene reactivity. Thermodynamic analysis indicates that the [2 + 2] cycloadducts are the most stable reaction products, followed by the [2 + 1] cycloadducts.

These results elucidate the multi-step reaction mechanisms and reaction pathways associated with acetylene addition to C60, providing theoretical insight into the regioselectivity, reactivity, and stability of fullerene derivatives. Furthermore, they offer a fundamental understanding of carbon-based nanostructure functionalization processes and contribute to the rational comprehension of fullerene-derivatives formation.

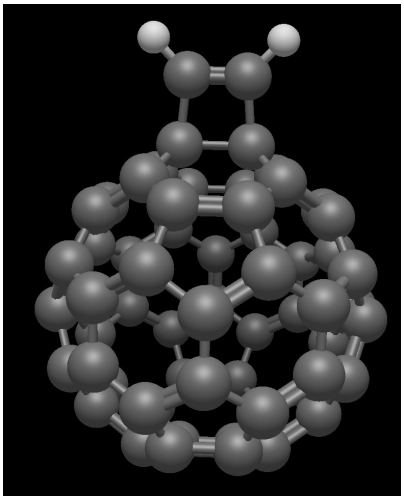


Figure 1: adduct [2+2]_hexagon-hexagon

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Interstellar Carbon Reactivity: A Theoretical Study of Carbon-Polyyne Collisions

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Recent advancements in spectroscopy continue to uncover new astrochemical species. Small molecules, ions, and radicals play a central role in reaction networks that lead to the formation of more complex compounds in space. In dense interstellar clouds, extremely low temperatures favor barrierless processes, such as reactions between atomic carbon and unsaturated hydrocarbons. [1]. In this work, we investigate the formation of cyclic hydrocarbons initiated by collisions of ground-state atomic carbon with acetylene (HC_2H) and the smallest polyynes—diacetylene (HC_4H) and triacetylene (HC_6H). These processes proceed via cyclic intermediates followed by atomic hydrogen elimination:

$$C + HC_{2n}H \rightarrow c\text{-}C_3HC_{2(n-1)}H \rightarrow c\text{-}C_3C_{2(n-1)}H + H \ (n = 1, 2, 3)$$

Hydrogen loss is considered exclusively on the lowest triplet potential energy surface. To better resolve the reaction pathway, we additionally performed nudged elastic band (NEB) calculations to characterize the reaction coordinate. The energetics of cyclic intermediate formation are analyzed using QTAIM-based IQA methodology, while reaction dynamics are explored through DFT-based molecular dynamics simulations. Our main findings include: (1) non-classical interactions dominate along the reaction pathway; (2) reaction coordinate analysis shows that $C(^3P)$ is consistently attracted to highly polarizable triple bonds; and (3) alkynes undergo rotational motion that enables an almost perpendicular ("vertical") approach, largely independent of initial conditions. An open question that remains is the determination of hydrogen elimination rate constants for reactions involving polyynes and triplet carbon.

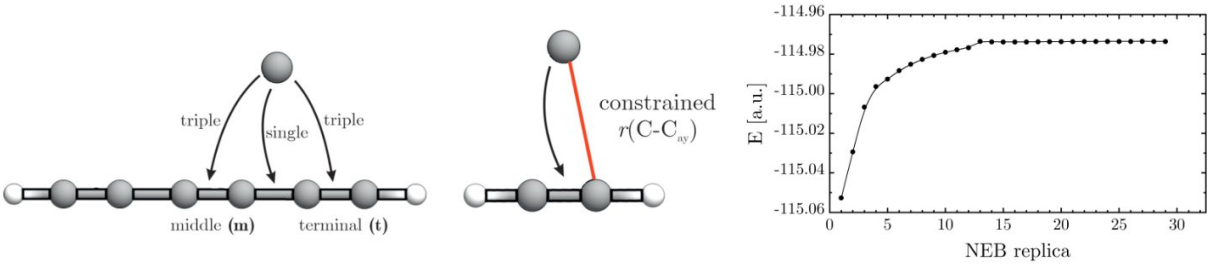


Figure 1: Model system for the studied reactions, highlighting the constrained geometrical parameters used in the IQA analysis and the targeted bond type. The figure also includes the corresponding NEB energy profile for atomic carbon addition on HC_2H.

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Detection of organic matter on Mars: an experimental approach to simulate transformation pathways of polycyclic aromatic hydrocarbons (PAHs)

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The detection of Raman Spectral features potentially due to polycyclic aromatic hydrocarbons (PAHs) in sulfate-bearing rocks within Jezero Crater by SHERLOC (Scanning Habitable Environments with Raman and Luminescence for Organics and Chemicals) instrument onboard NASA's Perseverance rover has renewed interest in the role of aromatic organic compounds as potential tracers of prebiotic chemistry and possible biosignatures on Mars[1]. Recent investigations of samples collected from the crater floor and fan-top deposits revealed spectral features in the 1300-1700cm^{-1}region spatially associated with magnesium and calcium sulfates. Comparison with laboratory analogues suggest that some of these signatures may be coherent with presence of PAH-like compounds preserved through interactions with sulfate minerals, highlighting the potential importance of mineral matrices in the long-term stabilization of organic matter under Martian conditions[2]. Within this framework, the present thesis project aims to investigate the transformation pathways and the spectroscopic evolution of selected aromatic organic compounds subjected to environmental stresses relevant to Mars and other planetary bodies. The experimental work will focus on a set of reference compounds representative of polycyclic aromatic and heteroaromatic molecular systems of astrochemical interest. These compounds will be tested as they are or in association with epsomite and calcium sulphate, minerals selected as representative of the Martian soil. To simulate processes potentially experienced by the organic matter during planetary evolution, all the samples will be subjected to thermal treatments to reproduce extreme thermal events, UV irradiation to investigate the photochemical evolution over controlled exposure times, and mechanochemical treatments by using a ball mill to simulate high pressure shock events associated with asteroid impacts and regolith processing. After each treatment, all the samples will be characterized by using ATR-IR, UV-visible and fluorescence spectroscopies to evaluate molecular alterations, degradation pathways, and the possible formation of new species. The most interesting samples will be selected for complementary Raman analyses to be carried out by using a SHERLOC-like instrument available at the laboratory of Prof. Fornaro (INAF, Arcetri).

This thesis attempts to reconstruct the possible evolutionary pathways of aromatic organic matter under Martian-like conditions. Such investigations are expected to contribute to the broader search for organic matter beyond Earth and provide new insights into the identification and interpretation of potential biosignatures in future planetary exploration missions.

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The Carbon Budget in the Milky Way

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Carbon, in its various forms (C^+, C^0, and CO), is a fundamental coolant of the interstellar medium (ISM) and a key tracer of its physical conditions and energetics. Photodissociation regions (PDRs), shaped by ultraviolet (UV) radiation from massive OB stars, host the transition between ionized, atomic, and molecular carbon phases, making them ideal environments for studying the ISM as show in Figure 1 (Wolfire et al. 2022[1]). Large-scale surveys such as the Herschel Open Time Key Project Galactic Observations of Terahertz C+ (GOTC+)(Pineda et al. 2013[2]) have provided velocity-resolved observations of the [CII] 158 μm line along ∼452 line of sights, revealing the structure of Galactic gas and the presence of a significant CO-dark molecular gas (Grenier et al. 2005[3];Wolfire et al. 2010[4]); however, the neutral atomic carbon ([CI]) component remains poorly constrained in Galaxy-wide studies due to observational limitations and its relatively faint emission compared to CO. Observations (Shimajiri et al. 2013[5]; Frerking et al. 1989[6]) show that [CI] emission is widespread throughout molecular clouds, challenging classical PDR models in which atomic carbon is confined to cloud surfaces. To address this gap, we complement the (GOTC+) survey by combining already existing datasets with Galaxy-wide [CI] observations using the Atacama Pathfinder Experiment (APEX) telescope equipped with the nFLASH receiver, enabling simultaneous observations of the [CI] $^3P_1 \rightarrow {}^3P_0$transition at 492 GHz and multiple CO isotopologues at high angular resolution. The goals of this study are to incorporate for the first time the atomic carbon component into a Galaxy-wide survey, assess the role of [CI] as a tracer of CO-dark molecular gas through comparisons of velocity resolved column densities of C^+, C^0, CO and quantify the contribution of [CI] emission in diffuse gas.

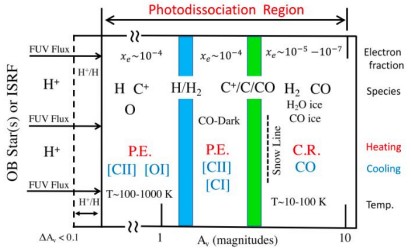


Figure 1: Schematic of a PDR as a function of visual extinction, AV , into the cloud. CO-dark molecular gas lies between the H2 and CO layers, where [CII] and [CI] dominate the cooling.

Acknowledgements
I would like to thank the Max Plank Society and my supervisors for this opportunity.

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Theoretical modeling of experimental EELS data for van der Waals heterostructures involving two-dimensional materials

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Electron energy loss spectroscopy (EELS) is a commonly used experimental technique for investigating electronic and plasmonic properties of two-dimensional (2D) materials and van der Waals heterostructures (vdWHs) [1,2]. We have extensive experience in the theoretical modeling of the experimental EELS data for free-standing (single and multilayer) graphene sheets obtained by scanning transmission electron microscope [3,4], as well as in the theoretical modeling of the experimental EELS data for monolayer graphene supported by different substrates [5-7].

In this publication [8], we derive an analytical expression for the surface response function (SRF) of vdWHs involving 2D materials. Our theory is primarily designed for EELS with non-penetrating trajectories. Furthermore, our SRF is applicable to tip-based scattering-type scanning near-field optical microscopy.

Acknowledgements
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H_2 promotes the formation of silicon carbide in evolved stars

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Asymptotic Giant Branch stars (AGBs) are the main source of cosmic dust in space. In carbon rich stars (C-rich), the dust is mainly composed of amorphous carbon and silicon carbide grains, although the physical and chemical processes governing their formation remain insufficiently understood. In the case of silicon carbide several molecular precursors have been proposed.

We will present our latest results on the formation of silicon carbide dust grains using laboratory astrochemistry and kinetic modelling [1]. We observe that molecular hydrogen, the most abundant gaseous species in the circumstellar envelopes of AGBs, plays a crucial role in the formation of silicon carbide dust and identify SiC_2as its molecular precursor. In particular, we only observe SiC_2formation when the ratio of $H_2$to atomic C/atomic Si is comparable to that of C-rich AGBs whereas in the absence of $H_2$$SiC_2$is not detected. We also observe that in the presence of $H_2$the production of silicon carbide dust is very highly enhanced. Finally, the dust analogues are composed of three populations of nanograins, namely, aliphatic amorphous carbon, partially crystalline hydrogenated silicon, and amorphous silicon carbide (both hydrogenated and non-hydrogenated), reflecting the competition between different chemical pathways. We rationalize the experimental results on the basis of thermochemical calculations and chemical kinetics modelling.

Our findings reveal the central role of molecular hydrogen in the formation of SiC_2 and silicon carbide dust and contribute to a deeper understanding of dust formation processes in evolved stars, from atoms to molecules, clusters, and ultimately dust grains.

Acknowledgements
Support from the European Research Council under the European Union's Seventh Framework Programme ERC-2013-SyG (Grant Agreement No. 610256, NANOCOSMOS and from the Severo Ochoa Centres of Excellence programme (Grant No. CEX2024-001445-S) are acknowledged.

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VUV Photoionization Study of Nitrogen-Substituted Polycyclic Aromatic Hydrocarbons (NPAHs)

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One of the most challenging aspects of chemistry is understanding and characterizing reactive intermediates. Radicals and cations, fundamental yet highly demanding species, have garnered widespread attention. However, the study of nitrogen-centered radicals (NCRs), Nitrogen-Substituted Polycyclic Aromatic Hydrocarbons (NPAHs) and their corresponding nitrenium ions remains limited compared to their carbon counterparts, with their synthetic potential largely unappreciated and unexplored in the context of astrochemistry.[1]

This work describes the VUV photoionization of the *N*-carbazolyl radical, using a combination of synchrotron radiation, photoelectron photoion coincidence spectroscopy, and supporting ab initio calculations. Through these methods, the adiabatic ionization energy of the *N*-carbazolyl radical to both the singlet and triplet state of its corresponding nitrenium ion is directly determined using photoion mass-selected threshold photoelectron spectroscopy. The *N*-carbazolyl radical is characterized as a highly delocalized σ-radical, which leads to the generation of an extremely unstable antiaromatic nitrenium ion.[2]

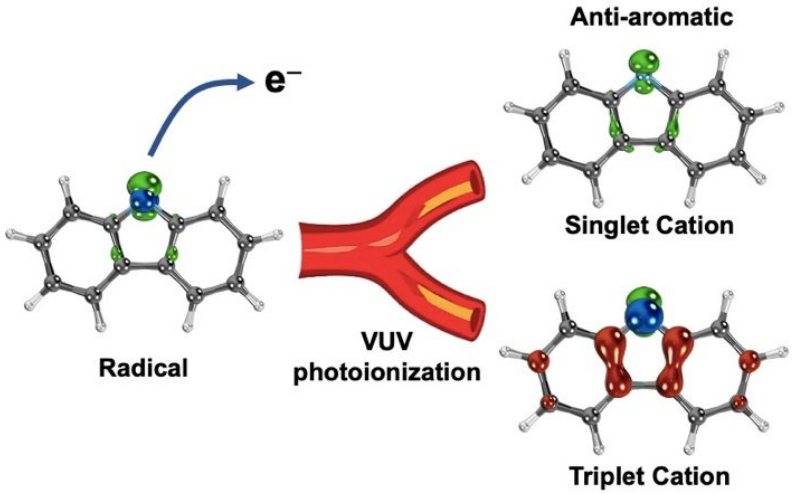


Figure 1: Photoionization of *N*-carbazolyl radical.

Acknowledgements
This project received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 801459-FP-RESOMUS and was funded by the Deutsche Forschungsgemeinschaft (DFG) under Germany's Excellence Strategy–EXC 2033-390677874-RESOLV.

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Computational Investigation of Confined Dye–Carbon Interactions in Graphene-Based Model Systems

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Understanding the molecular interactions governing adsorption is essential for the rational design of sustainable carbon-based materials. In this work, computational modeling was employed to investigate the adsorption of the azo dye Reactive Black 5 (RB5) on lignocellulosic and graphene-based models representing non-carbonized and carbonized hemp-derived biosorbents. Conformational sampling of the supramolecular complexes was performed using CREST with the GFN-FF force field, followed by geometry optimization at the GFN2-xTB level with implicit solvation. Four adsorption models were examined: RB5 adsorbed on two cellulose chains, confined by three cellulose chains, adsorbed on a graphene sheet, and confined between two graphene layers. The calculations showed that lignocellulosic systems are stabilized primarily by cooperative hydrogen bonding and dispersion interactions, whereas graphene-based models are dominated by π–π stacking. The strongest stabilization was observed for the confined bigraphene model, in which two graphene-like layers form a supramolecular adsorption pocket around RB5. These findings demonstrate that adsorption affinity depends not only on surface chemistry but also on nanoscale confinement, structural flexibility, and graphitic domain organization, highlighting the potential of computational modeling to elucidate adsorption mechanisms and guide the rational design of sustainable carbon-based adsorbents.

Acknowledgements
This work was supported by the CEI KEP project *European Bridges of Science and Knowledge: Capacity Building in Computational Approaches for Young Scientists (EuroSciComp-Bridge)*Project Number 304.4.2025.040.

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