



# AstroPAH

A Newsletter on Astronomical PAHs

Issue 110 • July 2024

**Evolution of the ionisation energy  
in chiral clusters of [4]helicene**





# Editorial

**Dear Colleagues,**

Welcome to our new 110<sup>th</sup> AstroPAH volume! We hope that you are all healthy and doing well!

Our cover picture features a montage showcasing the PEPICO (photoelectron photoion coincidence) spectroscopy experiments conducted at the SOLEIL synchrotron, which helped reveal the formation of [4]helicene clusters up to the heptamer (see the abstract section for more details).

Our In Focus features an interview with Dr. Sacha Foschino from the Observatoire des Baronnies Provençales (OBP) where he tells us all about his inspirations and science projects on transiting exoplanets and variable stars, as well as emerging citizen science programs to exploit astrophotographic data. Also... spiders!

We wish to thank you all for the diverse abstract contributions this month! They cover papers on the role of PAHs with edge defects to interpret IR emission observations, the growth of chiral clusters of [4]helicene, the photofragmentation of corannulene and sumanene cations, and the NIR absorption and radiative cooling of naphthalene dimers.

We will see you in September, after our annual break in August!

If you are on Instagram, be sure to check out our next [PAH of the Month!](#)

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us for a future In Focus or other ideas, feel free to use our [email](#).

**The Editorial Team**

**Next issue: 19 September 2024.  
Submission deadline: 6 September 2024.**

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## PAH Picture of the Month

Photoelectron spectroscopy experiments performed at synchrotron SOLEIL revealed the formation of [4]helicene clusters up to the heptamer. The experiments unveiled a trend in the ionisation energy of the smallest chiral PAH with increasing cluster size. Quantum chemistry calculations support these observations, and they predict an energetically favored homochiral aggregation route.

**Credits:** Sergio R. Domingos.



# In Focus

## An interview with Dr. Sacha Foschino

**Dr. Sacha Foschino**, is an astronomer currently working at the Observatoire des Baronnies Provençales (OBP). He did his PhD at the Institut de Recherche en Astrophysique et Planétologie (IRAP) in Toulouse after which he went back to his home in the south-east of France. He lives in a small village in the High Alps, close to where he spent a large part of his childhood and where you will find the darkest sky in France and maybe even in Europe. He also likes to study the connections between science and society. He is passionate about spiders, citizen sciences, and hikes. Sometimes he crochets and he is learning to play the Ukulele.



### What inspired you to become a scientist?

I've always been interested in science and mathematics. My parents offered me some illustrated books that fanned the flame of my curiosity on various subjects. At 7-8 years old I wanted to become an astrophysicist, just like this guy in TV documentaries, Hubert Reeves. Then I wanted to sell BMWs or to build them. . . It's really in high school that my physics teacher inspired me and made me love physics: my old dream came back. The same year I discovered the documentary series "Cosmos" of Carl Sagan, the public conferences of the French astronomer André Brahic, and the books of Hubert Reeves. At the end of high school I decided that I had to become an astrophysicist.

### How did you get into astrochemistry research?

During my physics studies, I discovered the wonders of spectrometry. This technique blew my mind. I wanted to do astrophysics using spectrometry (lucky me, it's one of the main tools!). During my master's degree at Toulouse, I met Paolo Pilleri and Christine Joblin who took me for an internship on the destruction of PAHs in photodissociation regions. It was spectrometry, nebulae and stardust; it was amazing. The following year, I worked with Christine and Olivier Berné for my master's thesis, and I had the chance to pursue PhD with them on the photophysics and evolution of PAHs in PDRs, in the era of *JWST*. It wasn't actual astrochemistry, but I studied PAHs from an astrophysical point of view: how do they evolve around massive stars, how to extract the representative spectrum of different PAH populations and how do PAHs contribute to gas heating.

## Can you tell us about your career path, the difficulties you have faced to stay in the field, and what guided your current choice?

At the end of my PhD, a researcher of my lab shared a job ad for an observatory in the French High Alps, the Observatoire des Baronnies Provençales (OBP). They wanted a young astrophysicist to do research, trainings and animations for the public. It was the description of my dream job, not far from my parents' place and close to where my grandparents lived. I also applied to two postdocs, without success. After few months of unemployment, I looked for jobs in space industry, data sciences, etc... I was still in the hiring process for the French observatory. Seven months after my PhD I was hired at the observatory where I am still working. If I do astrophysics, I want to do it in contact with the curious public and amateur astronomers. Public research does not allow for that but this private company, OBP, enabled it.

## What are the different outreach activities that you perform?

I can do a lot of different outreach activities for all levels. The simplest one is the 1-3 hrs night sky observations in which we look at the greatest deep sky objects of the moment, we talk about the celestial mythology of all cultures while showing the (occidental) constellations. One of my favourite activities is to spend 2-3 hrs operating the 82 cm Cassegrain-Nasmyth telescope under the cupola, in which we can look in the eyepiece, with some (usually 10) members of the general public. During that time, another telescope (43 cm in diameter) is observing an exoplanetary transit using photometry. At around midnight we leave the cupola, go to the lab and analyse the still-ongoing transit observation. I show how we collect the data and how we interpret it. Then we use the Kepler's 3rd law to compute the exoplanet diameter! Also, I am very proud to propose a week-long training on spectrometry for amateur astronomers. During 60 hrs of training, I show them all the wonders of spectrometry, the instrument we use, how to use them and the science we can do. We do a lot of practice both on our instruments and theirs. Then, they can use this knowledge at home for their pleasure or come back to their club and develop their own spectrometry activities.

## How do you enjoy sharing your astronomy knowledge with the general public/amateur astronomers at the observatory?

I love to witness the evolution of the people coming at the observatory. They arrive on Sunday, sometimes not knowing how to use a telescope or even not knowing what a telescope is and they leave being fully operational, ready to discover the cosmos. Also, sometimes we witness something moving, like showing Saturn to a 102 year old women, seeing someone's wet eyes when they look at the moon for the first time in the 0.82 m telescope or all the kids' drawings after passing several days with them in a "discovery class".

## What is your current research about?

I reoriented my scientific interests towards transiting exoplanets and variable stars, eclipsing binary systems in particular. I am building a citizen science program exploiting the amateur data (astrophotography) to find as much eclipses as I can in the data of the maximum of different targets possible over the longest period possible. I call it "Photography

to Photometry”. Eclipsing binaries can have a flux variation of  $\approx 10$ -50 percent, very easy to detect even with a 9 cm telescope. I work on other applications like the search for asteroids, unknown planetary nebulae, solar-like star flares, supernovae, etc. Amateur data represent a huge, unexplored quantity of data.



*Figure 1: The astronomical image is the HII region NGC6188, and NGC 6164 (nebula around the massive spectroscopic binary HD148937), it has been obtained using one of our two telescopes located in Chile: a RASA 14", 81x120sec in the Johnson filters Rc, V and B. (RASA = Rowe-Ackermann Schmidt Astrograph, opened at f/2.2)*

**Which open question in Laboratory Astrophysics would you like to see answered in the near future? OR What are, in your opinion, the present forefronts of astrochemistry research?**

What is the exact true nature of the very small objects creating the Diffuse Interstellar Bands?

Can someone detect my favourite PAH, the *JWST*-shaped molecule Circumcoronene in the interstellar medium, please?

**Astrochemistry is a very multidisciplinary field. Can you comment on how you collaborate and communicate with different experts and what you like about such interactions?**

A very cool aspect of my PhD was to collaborate with my friend Dr. Gabi Wenzel. Among other parameters, she measured the ionization potential of some big PAHs in the obscure basements of IRAP. I used them to compute the photoelectric efficiency and gas heating rate inside the Iris nebula (NGC7023) and then I compared the theory to observations. From the lab to the sky, that is science!

**What was the most important advice somebody gave you?**

Make your decisions fully aware of the consequences.



## How do you balance your professional and personal life?

As we do our own scientific observations, we stay late at work very often. To dilute our working hours over the month, we have an organisation of 5 working days and 3 days of rest. It also allows the observatory to be opened all the time with at least one or two astrophysicists (out of 3). But work is work and life is life (thanks captain obvious). Even if I love my work, I will try not to work outside of work hours. However, sometimes I want my projects to progress so bad that I work a bit during weekends. It might sound trivial, but you are paid to do your work within work hours and research is. . . work. Life is too short to work for free.

## What do you do outside of work?

I live a few kilometres from the observatory, in a small medieval village (named Rosans) surrounded by mountains. Each weekend I take my walking sticks, my camera and go for a hike. I started to take macro photography of spiders and other small animals. When the weather is nice, I look for two nice trees, put my hammock in place and do nothing, maybe reading a manga while listening to music.



*Figure 2: My photograph of Thomisus Onustus*

## What advice would you give a grad student who wants a career in academia?

Research and studying the universe is very cool but also very competitive. Do your best but it's not the end of the world if you fail. You are not your work, and you will find another interesting job in which you will apply all your skills! It's not always a good idea to make your passion your work anyway (be careful with the indigestion of passion!).



# Abstracts

## Role of Polycyclic Aromatic Hydrocarbons with Edge Defects in Explaining Astronomical Infrared Emission Observations

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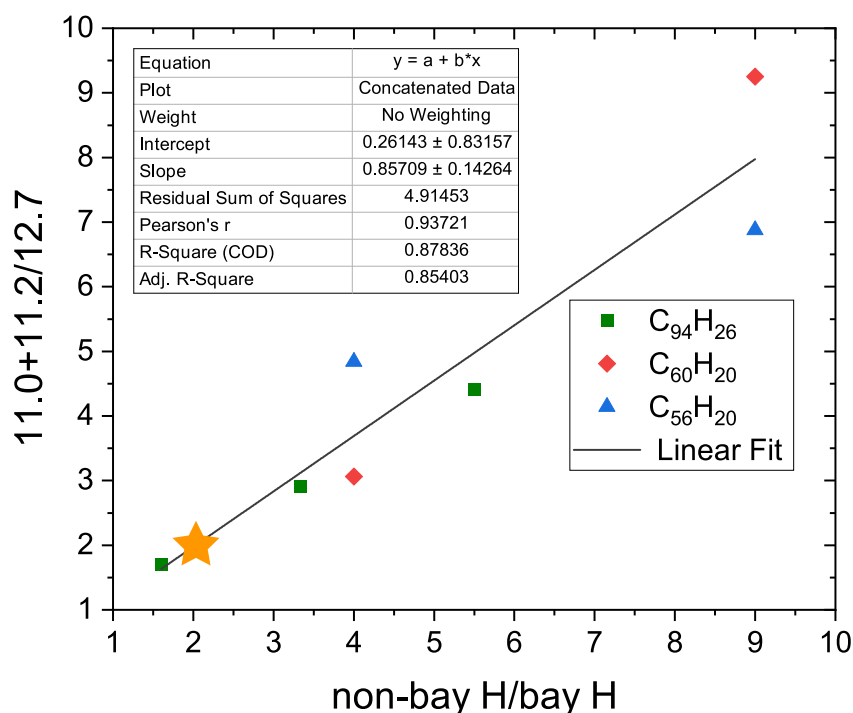
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A systematic study was performed on the spectral properties of polycyclic aromatic hydrocarbons (PAHs) with edge defects using harmonic density functional theory calculations. Their potential astronomical relevance was assessed through direct comparison with NIRSpec and MIRI-MRS spectra of the atomic PDR of the Orion Bar from the JWST Early Release Science PDRs4All program. It is found that the astronomical 6.2  $\mu\text{m}$  PAH emission band, including its blue side, is well reproduced by PAHs with edge defects, when taking into account effects of polarization in the computations, and without a need for PANHs. Small neutral PAHs with edge defects explain the blue wing of the 3.3  $\mu\text{m}$  band. A low number of edge defects is required to reproduce the 8.6 and 11.2  $\mu\text{m}$  band profiles, while the 11.0+11.2/12.7  $\mu\text{m}$  band intensity ratio is a measure for the number of edge defects. A blind database fit to the Orion Bar spectrum reproduces the 6–15  $\mu\text{m}$  region with an error of 9.9% and shows a clear delineation of charge, with the 6–10  $\mu\text{m}$  PAH bands being carried by PAH cations and the 10–15  $\mu\text{m}$  region by predominantly neutral PAHs. The contribution of anions is negligible. Armchair PAHs fit the 12.7  $\mu\text{m}$  band, simultaneously producing a very weak broad emission feature centered at 3.225  $\mu\text{m}$ . Zigzag PAHs fit the 11.2  $\mu\text{m}$  band. It is concluded that PAHs with a low number of edge defects, in addition to armchair and zigzag PAHs, all contribute to the observed interstellar infrared emission.





The  $11.0+11.2\mu\text{m}/12.7\mu\text{m}$  intensity ratio as a function of the ratio non-bay H/bay H using the following neutral and cation PAHs with edge defects:  $\text{C}_{56}\text{H}_{20}$ ,  $\text{C}_{60}\text{H}_{20}$ , and  $\text{C}_{94}\text{H}_{26}$ . Each point corresponds to the average for all the structures having a given non-bay H/bay H ratio. The linear fitting curve is shown in black and the fitting parameters are shown in the inset. The orange star shows the  $11.0+11.2/12.7\mu\text{m}$  intensity ratio found for the Orion Bar.

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*The Astrophysical Journal*, **968**, 128 (2024)

<https://ui.adsabs.harvard.edu/abs/2024ApJ...968..128R>

# Evolution of the ionisation energy with the stepwise growth of chiral clusters of [4]helicene

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Polycyclic aromatic hydrocarbons (PAHs) are widely established as ubiquitous in the interstellar medium (ISM), but considering their prevalence in harsh vacuum environments, the role of ionisation in the formation of PAH clusters is poorly understood, particularly if a chirality-dependent aggregation route is considered. Here we report on photoelectron spectroscopy experiments on [4]helicene clusters performed with a vacuum ultraviolet synchrotron beamline. Aggregates (up to the heptamer) of [4]helicene, the smallest PAH with helical chirality, were produced and investigated with a combined experimental and theoretical approach using several state-of-the-art quantum-chemical methodologies. The ionisation onsets are extracted for each cluster size from the mass-selected photoelectron spectra and compared with calculations of vertical ionisation energies. We explore the complex aggregation topologies emerging from the multitude of isomers formed through clustering of P and M, the two enantiomers of [4]helicene. The very satisfactory benchmarking between experimental ionisation onsets vs. predicted ionisation energies allows the identification of theoretically predicted potential aggregation motifs and corresponding energetic ordering of chiral clusters. Our structural models suggest that a homochiral aggregation route is energetically favoured over heterochiral arrangements with increasing cluster size, hinting at potential symmetry breaking in PAH cluster formation at the scale of small grains.

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*Nature Communications*, **15**, 4928 (2024)

<https://www.nature.com/articles/s41467-024-48778-0>



# Photofragmentation of Corannulene ( $C_{20}H_{10}$ ) and Sumanene ( $C_{21}H_{12}$ ) cations in gas phase and its Astrophysical implications

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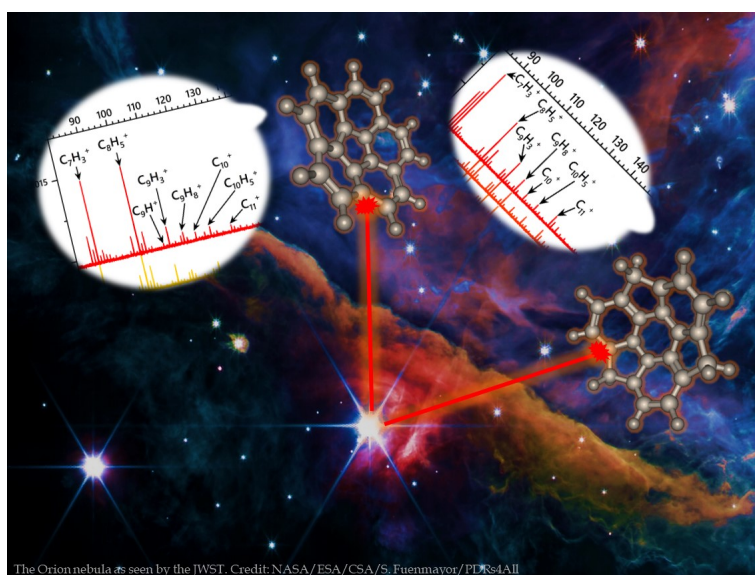
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The aromatic infrared Bands (AIBs) dominate the mid-infrared spectra of many galactic and extragalactic sources. These AIBs are generally attributed to fluorescent emission from aromatic molecules. Unified efforts from experimentalists and theoreticians to assign these AIB features have recently gotten additional impetus with the launch of the James Webb Space Telescope (JWST) as the Mid-InfraRed Instrument (MIRI) delivers mid-IR spectrum with greatly increased sensitivity and spectral resolution. PAHs in space can exist in either neutral or ionic forms, absorb UV photons and undergo fragmentation, becoming a rich source of small hydrocarbons. This top-down mechanism of larger PAHs fragmenting into smaller species is of utmost importance in photo-dissociation regions (PDR) in space. In this work, we experimentally and theoretically investigate the photo-fragmentation pathways of two astronomically significant PAH cations – corannulene ( $C_{20}H_{10}$ ) and sumanene ( $C_{21}H_{12}$ ) that are structural motifs of fullerene  $C_{60}$ , to understand their sequential fragmentation pathways. The photo-fragmentation experiments exhibit channels that are much different from planar PAHs. The breakdown of carbon skeleton is found to have different pathways for  $C_{20}H_{10}$  and  $C_{21}H_{12}$  because of the number and positioning of pentagon rings; yet the most abundant low mass cations produced by these two species are found to be similar. The low mass cations showcased in this work could be of interest for their astronomical detections. For completeness, the qualitative photo fragmentation behaviour of the dicationic corannulene and sumanene have also been experimented, but the potential energy surface of these dications are beyond the scope of this paper.



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*Physical Chemistry Chemical Physics*, **28**, 19332 (2024)

<https://doi.org/10.1039/D4CP01247J>

<https://pubs.rsc.org/en/content/articlepdf/2024/CP/D4CP01247J>



# Near-infrared absorption and radiative cooling of naphthalene dimers $(C_{10}H_8)_2^+$

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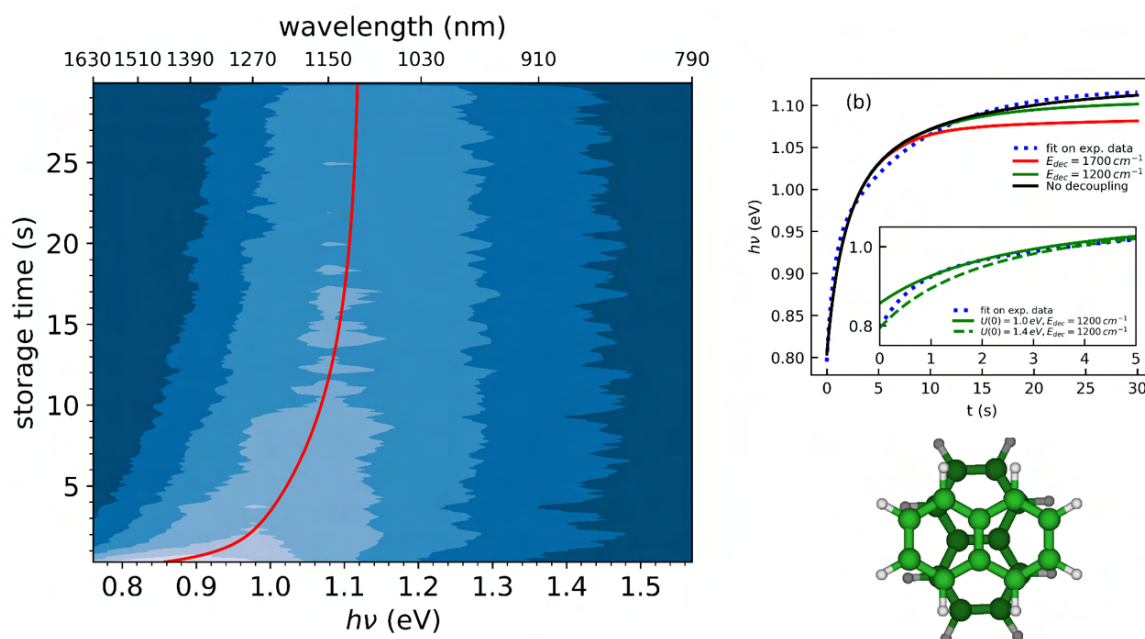
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The radiative cooling of naphthalene dimer cations,  $(C_{10}H_8)_2^+$  was studied experimentally through action spectroscopy using two different electrostatic ion-beam storage rings, DESIREE in Stockholm and Mini-Ring in Lyon. The spectral characteristics of the charge resonance (CR) band were observed to vary significantly with storage time of up to 30 seconds in DESIREE. In particular, the position of the CR band shifts to the blue, with specific times (inverse of rates) of 0.64 s and 8.0 s in the 0-5 s and 5-30 s storage time ranges, respectively. Such long-time scales evoke that the internal energy distribution of the stored ions evolves by vibrational radiative cooling, which is consistent with the absence of fast radiative cooling via recurrent fluorescence for  $(C_{10}H_8)_2^+$ . Density Functional based Tight Binding calculations with local excitations and Configuration Interactions (DFTB-EXCI) were used to simulate the absorption spectrum for ion temperatures between 10 and 500 K. The evolution of the band width and position with temperature is in qualitative agreement with the experimental findings. Furthermore, these calculations yielded linear temperature dependencies for both the shift and the broadening. Combining the relation between the CR band position and the ion temperature with the results of the statistical model, we demonstrate that the observed blue shift can be used to determine the radiative cooling rate of  $(C_{10}H_8)_2^+$ .



Left: Action spectra of laser-induced naphthalene-dimer dissociation,  $(C_{10}H_8)_2^+ \rightarrow C_{10}H_8^+ + C_{10}H_8$  recorded at different storage times in DESIREE. Top right : Time evolution of the center of the charge resonance band (dotted line: experiment, plain lines: model). Bottom right: parallel twisted geometry of the naphthalene dimer cation.

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*Physical Chemistry Chemical Physics*, **26**, 18571 (2024)

<https://doi.org/10.1039/D4CP01200C>

<https://pubs.rsc.org/en/content/articlelanding/2024/cp/d4cp01200c>

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Next issue: 19 September 2024

Submission deadline: 6 September 2024