

AstroPAH

A Newsletter on Astronomical PAHs

Issue 86 • March 2022



**Celebrating Women
in Science**



Editorial

Dear Colleagues,

Welcome to our new 86th AstroPAH volume! We hope all of you are healthy and doing well!

The AstroPAH Editorial board would like to congratulate Dr. Christine Joblin for **receiving the insignia** in the French National Order of Merit for her extensive contributions to the field of laboratory astrophysics. This award illustrates Christine Joblin's dedication to the field, emphasizing the contribution of multidisciplinary collaborations at her institution, at the national and international level. Congratulations!

We are happy to share with you two In Focus! The first celebrate the Women's History Month. We have put together a collection of inspirational words by women in the PAH community compiled from our previous newsletters and some new additions to highlight their work and challenges.

In the second In Focus, Prof. Melanie Schnell from the Christian-Albrechts-Universität zu Kiel writes about PAHs in the light of free-electron laser radiation, particularly the FLASH free-electron laser in Hamburg.

Finally, be sure to check out our meeting and job announcements. Two upcoming meetings (CPLT2022 and The life cycle of Cosmic PAHs) and a PhD/Postdoc position at Technische Universität Berlin are advertised at the end of this volume.

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**.

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**Next issue: 21 April 2022.
Submission deadline: 8 April 2022.**

AstroPAH Newsletter

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Contents

PAH Picture of the Month	1
Editorial	2
In Focus	4
In Focus	9
Recent Papers	16
Meetings	28
Announcements	31

PAH Picture of the Month

The diffuse interstellar bands (DIBs) are a set of ubiquitous absorption features seen in spectra of stars. They were observed for the first time by the American astronomer Mary Lea Heger in 1919. You can read more about the discovery of the DIBs in the publication by [Benjamin J. McCall and R. Elizabeth Griffin](#). With our AstroPAH cover, this month we would like to pay tribute to Mary Lea Heger and to all women in science.

Credits: Picture of the DIB spectrum by NASA. Picture of Mary Lea Heger from [UC Santa Cruz University library](#).

Women's History Month Special Celebrating the women in PAH research

March is Women's History Month with March 8th being celebrated as International Women's Day. The theme for this year is 'Break The Bias'. We've put together this collection of inspirational words by friendly advice from women active in the AstroPAH research from our previous newsletters and some new interviews to highlight the work done and the challenges faced by these researchers.

Dr. Christine Joblin

My advice to the young generation: There is not a single way in this life. Some of us have more opportunities to make choices. You have to catch yours and, maybe more importantly, you have to understand why you made these choices. That will give you enough resources to go through the stormy phases of life; not everything is going to be easy, not everything is going to be according to plan. A scientist is for me like an artist. He/she comes to science because he/she is looking for something more than a job.

AstroPAH #4



Dr. Xuejuan Yang

Q: How do you balance your professional and personal life? A: My job includes teaching, research, and administration. Teaching and administration parts break up time, which is not research-friendly. I have a 6-year-old boy, and I don't want to be absent from his life as he grows up. So it is not easy. I try to do time management better and priority setting more effectively. Say no to less important things. I think trying best to gather time is also very important, especially for doing research. Last, one needs to admit that nothing is perfect. Just do the right thing at the right time, and do our best.

AstroPAH #73



Dr. Melanie Schnell

I think it is important to find a research area that fascinates one, to find research questions that drive one's curiosity. This will ensure that research remains curiosity-driven which, to my opinion, is a good way to ensure unexpected new findings and insights. From a career-planning point of view, I think it would be optimal to change the area of research after the PhD to learn something new during the PostDoc period. These two research areas can then be naturally combined to form a new, unique research direction.

AstroPAH #17

Dr. Ewine van Dishoeck

Q: What was the most important advice somebody gave you?

A: Take the steepest route early in your career, since that determines where you end up. This was the advice that Martin Schwarzschild, Tim's mentor in Princeton, gave us. It meant that we spent some time living apart in two places during our first postdoc, Tim in Princeton and me in Harvard. Having strong CVs then helped us getting two positions in the same place later on.

Fortunately, the Princeton Institute for Advanced Study provided me with a visiting position in this period so that we could still spend considerable time together. Advice that I often give to students: make sure that you excel in at least one aspect of your work so that you get noticed. And be passionate about your work.

AstroPAH #52



Dr. Els Peeters

Q: Did you have a two-body problem and how did you deal with it? A: Yes, Jan and I graduated from the same program ('Licentiaat' in Physics) and were fortunate to both be given the opportunity to enroll in the European M.Sc. program in Astronomy. I left Porto earlier to start my Ph.D. research in Physics in Belgium while Jan moved to Leiden Observatory, The Netherlands, for his research project. Luckily, it's only a 2h drive between Leuven and Leiden and we spend most weekends together. Jan then started his Ph.D. research and

resided in Groningen, The Netherlands, for the first two years, doubling the travel time between us (not taking into account rush hour) but still doable for weekend travel. Note that for a typical Belgian (not working in Brussels), a one-hour drive is a long drive (FYI you can cross Belgium in 1.5 and 3 hours in respectively the shortest and longest distance). When I switched back to Astronomy, we "re-united" in Groningen. We had another bout of long-distance relationship when Jan moved to paradise (sunny California) 6 months before I did. Here as well, we were fortunate to both have a postdoc position at NASA Ames, thanks to Farid Salama and especially Lou Allamandola. Finally, we moved together to London, Canada, to take up a tenure-track and limited term faculty position at the University of Western Ontario and eventually both got tenure. The University of Western Ontario, as several other universities and organizations these days, has a system in place for

spousal/dual appointments and we negotiated a limited term faculty position when the offer was made for the tenure-track position. Thus we did not settle for the worst advice I was given in this respect near the end of my Ph.D. years. It was something like this: “You should be happy when you end up with 1 job for both of you”. While I did/do enjoy astronomy and PAHs a lot, I had zero intention to work full-time for half a salary. Overall, we were very fortunate regarding the distance and length of time we were separated. What helped us along the way is that we were lucky to work in compatible fields (and so both could get a job at NASA Ames for example), we were both competitive enough to be hired, we found jobs in ‘big’ institutions where several positions were available, and especially, met people along the way that were open to the two body problem and willing to help out where possible.

AstroPAH #29

Dr. Caterina Cocchi

Q: What is the best advice you can give to early career scientists?

A: Set your goals and follow them. Make them clear to yourself and to the people you work with. Avoid engaging yourself in activities that do not comply with your objectives and your interests. Instead, be open to any opportunity that is offered to you and think out of the box. You will find your way to whatever you want to achieve!



Dr. Ji Yeon Seok

Q: What is the most important advice someone gave to you/you give to your students? A: I am very fortunate in the sense that I have met and worked with a lot of respectable people. They always give me priceless advice and inspiration. One of the most important was “Do the most important task first”. I was a postdoc in ASIAA, Taiwan, and we had a regular chat with a director individually. At that time, I had just gotten married, and my husband went to US for his postdoc. Dr. Paul Ho (the former director of ASIAA) was a director, and I expressed difficulties about the “two-body” problem. He told me “Don’t give up your career and try your best to keep it”. Then, he mentioned that

time management would be very crucial. When there are several things to do, prioritize all tasks and do the most important part first. This is important because many people spend lots of time doing less important tasks. I realized that I was also one of these people and worked inefficiently. In particular, when I was involved in several projects at the same time, I sometimes lost my direction. On such occasions, I step back and consider what has the highest priority. This is very helpful for me to keep my pace.

AstroPAH #41





Dr. Heloisa M. Boechat-Roberty

Q: What difficulties have you faced in your career path and how have you overcome them? A: The biggest difficulty I had to face in my career was due to the necessity to manage my dedicated time, both at home and at work, to take care of my two children and carry out academic tasks at my university, such as teaching classes regularly and developing experimental work in laboratories. It is known that such at home or at work activities require a lot of dedication and daily physical presence. Another difficulty to be highlighted was caused by the lack of funding

for scientific research in developing countries. This fact prevented, for example, proposing new and sophisticated experimental setups that would allow reaching extremely relevant objectives. Early in my career, the feeling was that I was always in debt at home and at work. On one hand, I could not give the attention that my children deserved, and on the other hand, I felt that my work could not progress as I wanted, because I could not dedicate myself fully. Over time, after a lot of dedication, love, perseverance, and a lot of hard work, the feeling of guilt passed, and the difficulties were overcome. Today my children are successful adults and proud of their mother's scientific career. Professionally, I believe that I am respected for my academic and scientific career dedicated to the development of the area of Astrochemistry in my country.

Dr. Ir. Annemieke Petrignani

Q: Can you tell us about your career path, the difficulties you have faced as a scientist to stay in the field and how you overcame them? A: My journey has been a very multidisciplinary one, which has brought me from engineering to physics to astronomy and to chemistry or some combination thereof. This has kept the research always really interesting, and I have learned a lot from all disciplines along the way. It was very difficult from time to time though as I (not always voluntarily) changed fields a couple of times, and it felt like starting all over, especially as an experimentalist. Building up new experiments is - though often satisfyingly challenging - very difficult and time consuming. One



spends a lot of time trying to get things to work to only get results in the very end. To then have to move and leave it all behind, can be very frustrating. Getting enough funding to properly expand and/or build experiments is also not an easy task as few grants provide equipment funding. How to overcome these difficulties is not only about being an excellent scientist. It is also partly a matter of being in the right place at the right time. Over the years I have seen many good ideas and researchers being rewarded... or not. Like all scientists I know, you can only get over these barriers through passion, reflection, and perseverance.

AstroPAH #58



Dr. Dimitra Rigopoulou

Q: How do you balance your professional and your personal life? A: A number of colleagues have often said to me: 'I don't know how you do it'. And when I stop to think about how I do it I don't have a good recipe for success. Managing personal and professional life is an interesting balancing act. It is not an easy one but can be done. Often, although not solely, personal lives involve raising a young family or caring for elderly or disabled relatives. No matter the circumstances, the challenges are the same. I've got my partner and we have two children, my son is now 20 and at Uni (studying Physics) and my daughter is 11 and finishing primary school. Raising them alongside our careers in Astronomy has been challenging but also enormously

rewarding. My number one advice: accept that there will be moments (days/weeks) where you can't do it all. Choose what is important (a few things, a few tasks) and focus on those. Accept that you will fail at others. Set priorities but don't be afraid to reconsider them. Circumstances may change and so should our priorities. Whereas finishing that paper was important on Monday (or at the start of the week), staying by your child's bedside when they are not feeling well looks more important by Wednesday. Focus your energy on whatever you set as your priority. Be your best at those things that you chose as your top priorities/goals. The satisfaction you get from achieving your goals (when these are realistic) gives you the motivation you need to continue. Accept help when available and praise when offered. It is these moments of reward that makes the whole thing worthwhile and satisfying. With time you get better at juggling those balls up in the air and who knows one day you may be able to keep it up for a whole lot longer!

Sanjana Panchagnula

Q: What is the most important advice you've received? A: It's not exactly advice, but this is something I came across a while ago: "Great things are done by a series of small things brought together." Vincent van Gogh. It's easy to become enamoured by the bigger picture, particularly in science, but if you do what you do well things will always work out in the end.

AstroPAH #53



PAHs in the light of the free-electron laser FLASH

by **Melanie Schnell**

Polycyclic aromatic hydrocarbons (PAHs) are observed throughout the interstellar medium (ISM) and are thought to account for about 15% of the galactic carbon budget. They are expected to be present in a wide variety of interstellar environments and dominate the spectra of many objects. Even though, despite much spectroscopic efforts, the interstellar role of PAHs is not well understood yet (see for example Ref. [1-4] and references therein), they are assumed to be at the basis of a complex chemistry in the ISM of galaxies, for example by acting as catalysts [2,3].

Generally, chemical processes in interstellar space are manifold and strongly coupled with each other. Intense ionizing radiation is present in interstellar space, which makes it a particularly harsh environment, together with its inherently low temperatures and low particle densities. As a consequence, unimolecular reactions gain in importance compared to reactions taking place in a terrestrial environment [5]. Due to the constant interaction with the cosmic X-ray and UV photon field, a balance between build-up (bottom-up) and fragmentation processes (top-down approach) of the molecules can form, which strongly relies on the environment and the respective conditions. Detailed knowledge about how molecules, including PAHs, interact with (ionizing) high-energy photons and other types of energetic particles is still incomplete.

PAH molecules, including their substituted forms such as alkylated PAHs, are understood to play an important role in the energy balance of a galaxy. It is generally agreed that PAHs absorb stellar light followed by infrared (IR) fluorescence accounting for about 15-30% of the total galactic emission, although the detailed mechanisms are not known yet [2,3]. Related to that, it is assumed that astronomical PAHs exist in different charge and (de)hydrogenation states depending on the environment: Fully hydrogenated PAHs are injected into the ISM by stars. Near bright stars, photolysis will lead to complete loss of hydrogen atoms and fragmentation of graphene pieces. Further fragmentation may lead to the formation of rings and chains [1]. The interaction of the PAH molecules with energy-rich radiation will thus trigger the competing processes of ionization, dehydrogenation, fragmentation, and isomerization.

PAHs, with their extended electron systems, provide an interesting framework to explore ultrafast dynamics and beyond-Born-Oppenheimer effects. Within the Born-Oppenheimer approximation, electrons are assumed to move much faster than the nuclei, and the electronic and nuclear frameworks can therefore be treated separately. If the electronic and nuclear motion are instead strongly coupled, this can result in the ultrafast energy transfer

from electronic excitation into nuclear motion, and the Born-Oppenheimer approximation breaks down [6-10]. Non-adiabatic electronic relaxation has been demonstrated in recent ultrafast time-resolved studies on a series of small PAHs revealing electronic lifetimes of the monocation in the range 30–55 fs [11]. Theoretical calculations suggest the presence of conical intersections facilitating rapid electronic relaxation. Further experiments indicate that the electronic lifetimes increase with both the molecular size and the cationic excitation energy, and that multi- electronic and non-Born-Oppenheimer effects must be accounted for to provide accurate theoretical calculations [12-14]. With their rich structural variability and photochemistry, PAH molecules are thus proposed to contribute to many key physical processes that affect the basic structure and evolution of the interstellar medium of galaxies. As such, there is the need for detailed experimental and theoretical studies of PAHs of different structures and in different charge and dehydrogenation states. Answers to these fundamental questions can be given by performing both time-independent and time-resolved laboratory spectroscopy experiments, aiming at mimicking the conditions in interstellar space. In laboratory astrophysics experiments, harsh radiation is provided by different light sources depending on the experiments to be performed and the scientific question to be answered, ranging from lamps, high-power LEDs, and lasers in table-top experiments to synchrotrons and free-electron lasers (FELs) at dedicated facilities. There is a wealth of experimental and theoretical studies to unravel the photochemistry of PAH molecules, see for example Ref. [15] and references therein, and it will be beyond this In-Focus article to provide a good overview here. In the following, the discussion will thus be restricted to FEL experiments on PAHs, with a special focus on recent experiments that we performed at the free-electron laser in Hamburg FLASH [16]. In the following, there will first be a short introduction to FELs using the example of FLASH, the world's first XUV and soft-X-ray FEL [16], followed by a discussion of our time-resolved studies on a series of medium-sized PAHs using FLASH [17].

The Free-Electron Laser in Hamburg, FLASH

FLASH is in operation since 2005 and provides intense, short pulses of radiation in the VUV to soft X-ray regime (tunable from 14-310 eV with 10-220 fs photon pulse duration and a spectral width of 0.5-2%) [16]. An FEL is basically a device that transforms the kinetic energy of a relativistic electron beam into electromagnetic radiation [18]. In analogy to an optical laser, the electrons are the active medium. The term “free” in FEL describes the state of the electrons, which are not bound as in atomic or molecular lasers. However, the electrons are also not really “free” in FELs because they are confined and accelerated by the periodic magnetic field, as explained below.

FLASH's home is a several hundred meters long tunnel on the DESY campus, equipped with two experimental halls where the experiments are performed (Figure 1). At the beginning of the tunnel, electrons are generated by an electron gun. They are subsequently accelerated using seven supraconducting niobium resonators with a total length of 84 m in a linear arrangement. The electron accelerators are followed by undulators consisting of periodic magnetic fields. Here, the electron beam passes through this transverse periodic magnetic field, which makes the electron beam oscillate in a direction perpendicular to the magnetic field and its propagation direction. As a result, the electrons emit radiation confined in a narrow cone along the propagation direction. The wavelength of the emitted radiation depends on the undulator period, the strength of the magnetic field, and the electron energy,

so that FELs for different wavelength regions can be realized, ranging from microwaves (cm) to X-rays (Å).

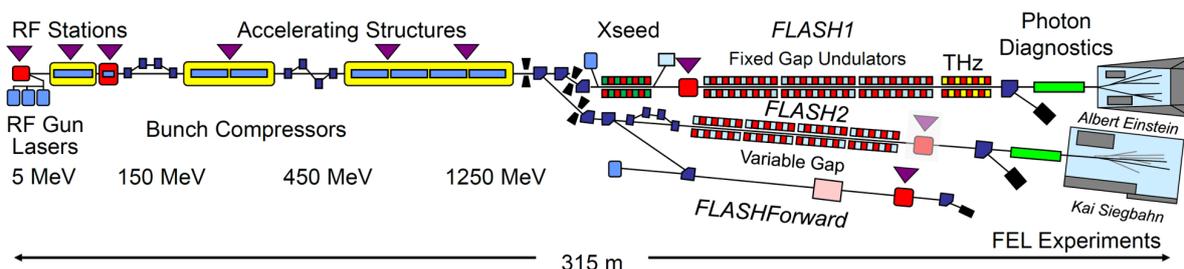


Figure 1 – FLASH – schematic layout of the facility (not to scale) (taken from Ref. [16]). The two main SASE beamlines FLASH1 and FLASH2 are in operation for user experiments.

In general, the FEL radiation can be of two different kinds: basic spontaneous emission, i.e., synchrotron radiation, which comes from the direct interaction of the electron beam with the undulator magnetic field with no injected field, which is also described as self-amplification of spontaneous emission (SASE), while stimulated emission occurs when a seeded radiation field copropagates with the electron beam (so-called seeded FELs) [18] FLASH is based on the SASE principle, with an upgrade to seeded operation currently ongoing [16]. FLASH consists of two FEL parts, FLASH1 and FLASH2, which share the accelerator part, but differ in the undulators. FLASH2's undulators have tunable gaps, so that wavelength tuning is straightforward. For FLASH1, the older setup, the radiation wavelength is tuned by changing the electron beam energy. Intense pulses with just a few 10s of femtosecond widths can be generated and used for time-resolved experiments. As such, FELs such as FLASH are well-suited machines for time-resolved laboratory astrophysics experiments.

Time-resolved relaxation and fragmentation of PAHs investigated in the ultrafast XUV-IR regime

To investigate the processes occurring in PAHs upon interaction with harsh radiation in a time-resolved manner with a time resolution in the 10-100 femtoseconds range, we performed XUV-IR pump-probe experiments with ultrafast pulses provided by FLASH and by an IR fs laser at 800 nm [17]. For this, we used the CAMP endstation at beamline 1 at FLASH1 [19]. We focused on the ultrafast photoinduced dynamics of fluorene (FLU), phenanthrene (PHE), and pyrene (PYR), and the experiments are supported by quantum-chemical calculations. The structures of these molecules are included in Figure 2. This comparative study of three medium-sized PAHs uses 30.3 nm (40.9 eV) XUV photons, which correspond to the He II emission line that is a dominant spectral line in the interstellar environment. It thus provides valuable insight into the stability and the accessible reaction pathways of these complex molecules [20] and nicely complements previous work. Figure 2 provides a scheme of the experimental setup together with TOF mass spectra for the three PAHs fluorene, phenanthrene, and pyrene. The time-resolved photodynamics of the PAHs are investigated by concurrently recording the photoelectrons using velocity-map imaging (VMI) and the photoions by VMI and time-of-flight (TOF) mass spectrometry. Simultaneous measurements of the ion yields, ion momenta, and electron momenta as a function of time

delay between the two ultrafast lasers allow a detailed insight into the various molecular processes.

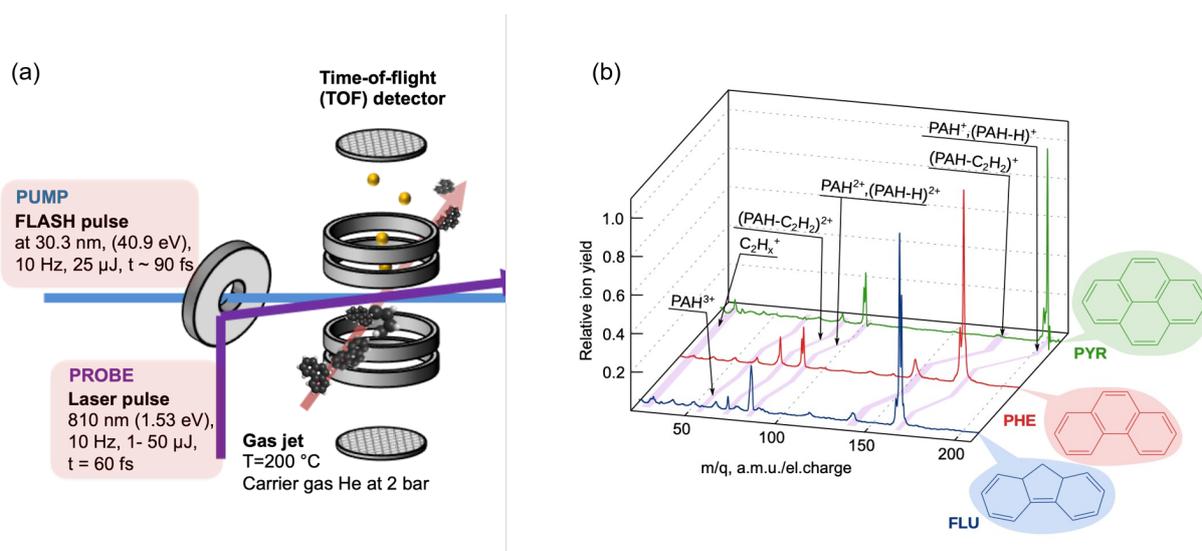


Figure 2 – (a) Scheme of the experimental setup at the CAMP endstation consisting of a pulsed valve with an option to heat the samples, the two lasers, and the double-sided VMI setup allowing for simultaneous detection of photoelectrons and photoions. The ion side (top) is equipped with the Pixel Imaging Mass Spectrometer (PImMS) camera [23] (not indicated) for parallel acquisition of the ion kinetic energy release and angular distribution of different fragments. (b) Time-of-flight mass spectra of the three PAHs fluorene, phenanthrene, and pyrene, averaged over all time delays between the two lasers (adapted from Ref. [17]).

As can be seen from Figure 2b, both the parent cation and dication are formed in these experiments (XUV pulse only), and even small signals of the trication are observed. Furthermore, ions resulting from loss of individual hydrogen atoms are observed. The masses corresponding to losses of C_2H_2 units are pronounced for both the series of monocations and dications, in agreement with earlier studies on the photochemistry of PAHs [21,22]. The ion side (top) is equipped with the Pixel Imaging Mass Spectrometer (PImMS) camera [23] for parallel acquisition of the ion kinetic energy release and angular distribution of different fragments. These parallel measurements allow the application of recoil-frame covariance analysis to the ion images, which provides a detailed mechanistic insight into the fragmentation pathways of the PAH^{2+} ions. An overview of the full recoil-frame covariance map images for FLU is given in Figure 3a. The axis labels refer to the number of carbons in the monocationic species and omit the number of hydrogen atoms. The black arrow in the inset indicates the direction of the reference ion in all covariance maps. For example, in $cov(C_{10}H_x^+, C_3H_y^+)$, $C_{10}H_x^+$ is the ion of interest, while $C_3H_y^+$ is the reference ion. In short, a blue spot in a cell indicates that the two respective ions, ion of interest and reference ion, are formed from the same event and recoil against each other. Fragment ion parts that have a total number of carbons greater than that of the parent ion, $C_{13}H_{10}^{2+}$, show no covariance as they cannot be formed as partners from the parent molecule; these have been omitted for clarity. Any ion species will also show covariance with itself (autocovariance), and these entries have been omitted as well. Notably, signal in the cells along the main diagonal of the matrix (highlighted in black) corresponds to the two-body dissociation pathways from the FLU^{2+} ion, which provide a significant recoil signal. In addition, we also observe recoiling for ions where two and four carbons atoms, respectively, are lost in form of neutral co-

fragments, which are given by the cells highlighted in blue and red. The effect of this loss is further highlighted in the inset that shows expansions of the maps. Increased blurring is visible as more carbon atoms are lost in neutral co-fragments. From a deeper covariance analysis of these recoil frame images, the fragmentation pathways upon interaction with the different fs pulses can thus be investigated. We observe a strong preference for dissociation into two monocations, where neutral co-fragments contain an even number of carbon atoms.

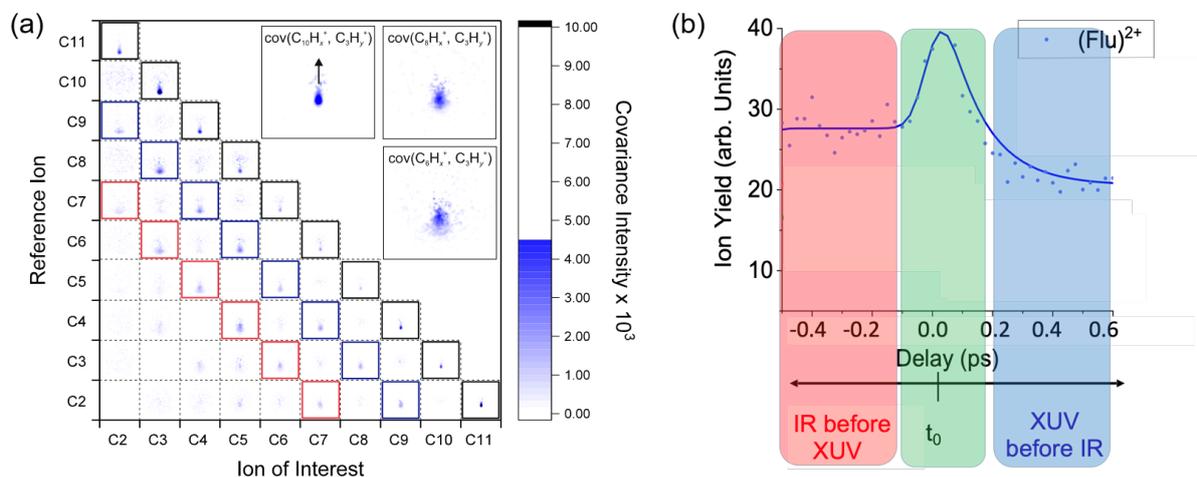


Figure 3 – (a) Full recoil-frame covariance map images for FLU. The axis labels refer to the number of carbons in the monocationic species and omit the number of hydrogen atoms. The inset shows expansions of the maps showing increased blurring as more carbon atoms are lost in neutral co-fragments. The black arrow indicates the direction of the reference ion in all covariance maps (see text for more detail; adapted from Ref. [17]). (b) Example for the dependence of the ion yield for the FLU^{2+} ion as a function of pump-probe delay between the XUV and the IR pulse.

Insight into the corresponding time scales and lifetimes of excited states can be provided by an analysis of the observed ion yields as a function of the pump-probe delay between the two pulses. Here, the XUV FLASH pulse acts as a pump, while the result is probed by the fs IR pulse. Figure 3b shows an example of the ion yield of the FLU^{2+} ion as a function of the pump-probe delay. A transient increase is observed where both lasers overlap in time. A sophisticated fitting procedure provides the excited state life times of the respective species. In short, three different excitation regimes occur, as indicated by the color code in Figure 3b. At negative time delays, the IR pulse interacts with the molecules first, followed by the XUV pulse. Here, IR excitation mostly results in excitation of the neutral FLU molecule, with some ion formation due to multi-photon absorption. The XUV pulse, hitting second, has sufficient energy to double ionize the molecule to form FLU^{2+} . The FLU^{2+} ion yield undergoes a transient increase around t_0 , where both pulses are close in time. For positive time delays, the XUV pulse interacts with the molecules first, followed by the IR pulse. Here, the XUV pulse will lead to formation of a variety of parent cations again (see also the mass spectra in Figure 2b), including FLU^+ , which is relevant for the analysis of the ion-yield curve shown in Figure 3b. If the time delay between the two laser pulses is short, the incoming IR laser pulse can further ionize FLU^+ , leading to an increased formation of FLU^{2+} , as seen in Figure 3b. For longer time delays between the XUV and the IR pulses, the initial excitation caused by the XUV pulse will have partially decayed, so that with increasing time delays, the energy provided by the IR pulse will not be sufficient for the formation of FLU^{2+} anymore, explaining the decrease in FLU^{2+} ion yield at longer positive delay values. A more detailed

discussion is given in Ref. [17]. Such analysis provided the electronic decay lifetimes of the electronically excited (indicated by *) species FLU*, FLU⁺⁺, FLU²⁺⁺, which are 35±8 fs, 57±13 fs, and 17±5 fs, respectively, with the given errors referring to the fit errors. Similar values have been determined for phenanthrene and pyrene.

This work showcases the potential for the novel technique of recoil-frame covariance map imaging to unravel the dynamics of large molecules with multiple competing fragmentation channels. Furthermore, in addition to the excited state lifetimes obtained in a recent study using high-harmonic generation [11], the ultrafast relaxation times determined experimentally and theoretically indicates that electronically excited PAHs are short lived. A working hypothesis might thus be that such molecules are populating mostly the electronic ground state in the ISM, which would greatly simplify astrochemical modelling. An extension of such time-resolved studies to PAHs with increasing size and of larger structural flexibility as well as the usage of different probe wavelength, such as energies in the UV and Vis range, will be relevant to further test this hypothesis.

Acknowledgements

Such experiments require a large team of people with different expertise, so that these studies are the result of intense and fruitful collaborations before, during, and after the beamtimes, which is greatly acknowledged here. This work was supported by the ERC Starting Grant ASTROROT, grant number 638027.



Prof. Melanie Schnell is a professor for physical chemistry at the Christian-Albrechts-Universität zu Kiel and head of the research group "Spectroscopy of molecular processes" at DESY since 2017. After her chemistry studies at the Universities of Hannover and Bonn, she joined the group of Jens-Uwe Grabow for her PhD research in microwave spectroscopy. That's when she first studied a PAH, namely corannulene, of which she experimentally determined the permanent electric dipole moment with a newly developed Stark setup. After her PhD research, she performed a research stay with Jon T. Hougen at NIST in Gaithersburg to work on permutation-inversion group theory. In 2005, she joined the Department of Molecular Physics at the Fritz-Haber-Institut in Berlin with Gerard Meijer, first as a postdoc, then heading her own small group, working on manipulating the motion of polar molecules using microwave radiation. During the Berlin time, her two daughters were born. In 2010, she moved to Hamburg to build up her own group in broadband rotational spectroscopy. Support by the 2014 ERC Starting grant "ASTROROT" helped her group to intensify research on astrochemically relevant molecules, including PAHs. Her group also works on fundamental questions of chirality and intermolecular interactions of gas-phase molecules, which nicely connects to astrochemistry as well.

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Abstracts

Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts

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It has been experimentally observed that water-ice-embedded polycyclic aromatic hydrocarbons (PAHs) form radical cations when exposed to vacuum UV irradiation, whereas ammonia-embedded PAHs lead to the formation of radical anions. In this study, we explain this phenomenon by investigating the fundamental electronic differences between water and ammonia, the implications of these differences on the PAH-water and PAH-ammonia interaction, and the possible ionization pathways in these complexes using density functional theory (DFT) computations. In the framework of the Kohn-Sham molecular orbital (MO) theory, we show that the ionic state of the PAH photoproducts results from the degree of occupied-occupied MO mixing between the PAHs and the matrix molecules. When interacting with the PAH, the lone pair-type highest occupied molecular orbital (HOMO) of water has poor orbital overlap and is too low in energy to mix with the filled π -orbitals of the PAH. As the lone-pair HOMO of ammonia is significantly higher in energy and has better overlap with filled π -orbitals of the PAH, the subsequent Pauli repulsion leads to mixed MOs with both PAH and ammonia character. By time-dependent DFT calculations, we demonstrate that the formation of mixed PAH-ammonia MOs opens alternative charge-transfer excitation pathways as now electronic density from ammonia can be transferred to unoccupied PAH levels, yielding anionic PAHs. As this pathway is much less available for water-embedded PAHs, charge transfer mainly occurs from localized PAH MOs to mixed PAH-water virtual levels, leading to cationic PAHs.

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A dusty veil shading Betelgeuse during its Great Dimming

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Red supergiants are the most common final evolutionary stage of stars that have initial masses between 8 and 35 times that of the Sun. During this stage, which lasts roughly 100,000 years, red supergiants experience substantial mass loss. However, the mechanism for this mass loss is unknown. Mass loss may affect the evolutionary path, collapse and future supernova light curve of a red supergiant, and its ultimate fate as either a neutron star or a black hole. From November 2019 to March 2020, Betelgeuse — the second-closest red supergiant to Earth (roughly 220 parsecs, or 724 light years, away) — experienced a historic dimming of its visible brightness. Usually having an apparent magnitude between 0.1 and 1.0, its visual brightness decreased to 1.614 ± 0.008 magnitudes around 7–13 February 2020 — an event referred to as Betelgeuse's Great Dimming. Here we report high-angular-resolution observations showing that the southern hemisphere of Betelgeuse was ten times darker than usual in the visible spectrum during its Great Dimming. Observations and modelling support a scenario in which a dust clump formed recently in the vicinity of the star, owing to a local temperature decrease in a cool patch that appeared on the photosphere. The directly imaged brightness variations of Betelgeuse evolved on a timescale of weeks. Our findings suggest that a component of mass loss from red supergiants is inhomogeneous, linked to a very contrasted and rapidly changing photosphere.

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Photochemical Synthesis and Spectroscopy of Covalent PAH Dimers

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Laser photochemistry of pressed-pellet samples of polycyclic aromatic hydrocarbons (PAHs) produces covalently bonded dimers and some higher polymers. This chemistry was discovered initially via laser desorption time-of-flight mass spectrometry experiments, which produced masses (m/z) of $2M-2$ and $2M-4$ (where M is the monomer parent mass). Dimers are believed to be formed from photochemical dehydrogenation and radical polymerization chemistry in the desorption plume. Replication of these ablation conditions at higher throughput allowed PAH dimers of pyrene, perylene and coronene to be produced and collected in milligram quantities. Differential sublimation provided purification of the dimers and elimination of residual monomers. The purified dimers were investigated with UV-visible, IR and Raman spectroscopy, complemented by computational studies using density functional theory at the CAM-B3LYP/def2-TZV level. Calculations and predicted spectra were calibrated by comparison with the corresponding monomers and used to determine the lowest energy dimer structures. Infrared and Raman spectroscopy provided few distinctive signatures, but UV-visible spectra detected new transitions for each dimer. The comparison of simulated and experimental spectra allows determination of the most prevalent structures for the PAH dimers. The work presented here provides interesting insights into the spectroscopy of extended aromatic systems and a new strategy for the photochemical synthesis of large PAH dimers.

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Multiply charged naphthalene and its C₁₀H₈ isomers: bonding, spectroscopy and implications in AGN environments

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Naphthalene (C₁₀H₈) is the simplest polycyclic aromatic hydrocarbon (PAH) and an important component in a series of astrochemical reactions involving hydrocarbons. Its molecular charge state affects the stability of its isomeric structures, which is specially relevant in ionised astrophysical environments. We thus perform an extensive computational search for low-energy molecular structures of neutral, singly, and multiply charged naphthalene and its isomers with charge states $+q = 0-4$ and investigate their geometric properties and bonding situations. We find that isomerisation reactions should be frequent for higher charged states and that open chains dominate their low-energy structures. We compute both the scaled-harmonic and anharmonic infrared spectra of selected low-energy species and provide the calculated scaling factors for the naphthalene neutral, cation, and dication global minima. All simulated spectra reproduce satisfactorily the experimental data and, thus, are adequate for aiding observations. Moreover, the potential presence of these species in the emission spectra of the circumnuclear regions of active galactic nuclei (AGNs), with high energetic X-ray photon fluxes, is explored using the experimental value of the naphthalene photodissociation cross-section, σ_{ph-d} , to determine its half-life, $t_{1/2}$, at a photon energy of 2.5 keV in a set of relevant sources. Finally, we show that the computed IR bands of the triply and quadruply charged species are able to reproduce some features of the selected AGN sources.

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The EDIBLES survey V: Line profile variations in the $\lambda\lambda 5797, 6379,$ and 6614 diffuse interstellar bands as a tool to constrain carrier sizes.

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Context. Several diffuse interstellar bands (DIBs) have profiles with resolved sub-peaks that resemble rotational bands of large molecules. Analysis of these profiles can constrain the sizes and geometries of the DIB carriers, especially if the profiles exhibit clear variations along lines of sight probing different physical conditions.

Aims. Using the extensive data set from the ESO Diffuse Interstellar Bands Large Exploration Survey (EDIBLES) we searched for systematic variations in the peak-to-peak separation of these sub-peaks for three well-known DIBs in lines of sight with a single dominant interstellar cloud.

Methods. We used the spectra of twelve single-cloud sight lines to examine the $\lambda\lambda 5797, 6379,$ and 6614 DIB profiles. We measured the peak-to-peak separation in the band profile substructures for these DIBs. We adopted the rotational contour formalism for linear or spherical top molecules to infer the rotational constant for each DIB carrier and the rotational excitation temperature in the sight lines. We compared these to experimentally or theoretically obtained rotational constants for linear and spherical molecules to estimate the DIB carrier sizes.

Results. All three DIBs have peak separations that vary systematically between lines of sight, indicating correlated changes in the rotational excitation temperatures. The rotational constant B of the $\lambda 6614$ DIB was determined independently of the rotational excitation temperature; we derived $B_{6614} = (22.2 \pm 8.9) \times 10^{-3} \text{ cm}^{-1}$, consistent with previous estimates. Assuming a similar rotational temperature for the $\lambda 6614$ DIB carrier and assuming a linear carrier, we found $B_{5797}^{\text{linear}} = (5.1 \pm 2.0) \times 10^{-3} \text{ cm}^{-1}$ and $B_{6379}^{\text{linear}} = (2.3 \pm 0.9) \times 10^{-3} \text{ cm}^{-1}$. If the carriers of those DIBs are spherical species, on the other hand, their rotational constants are half that value, $B_{5797}^{\text{spherical}} = (2.6 \pm 1.0) \times 10^{-3} \text{ cm}^{-1}$ and $B_{6379}^{\text{spherical}} = (1.1 \pm 0.4) \times 10^{-3} \text{ cm}^{-1}$.

Conclusions. Systematic variations in the DIB profiles provide the means to constrain the molecular properties. We estimate molecule sizes that range from 7–9 carbon atoms ($\lambda 6614$ carrier, linear) to 77–114 carbon atoms ($\lambda 6379$, spherical).

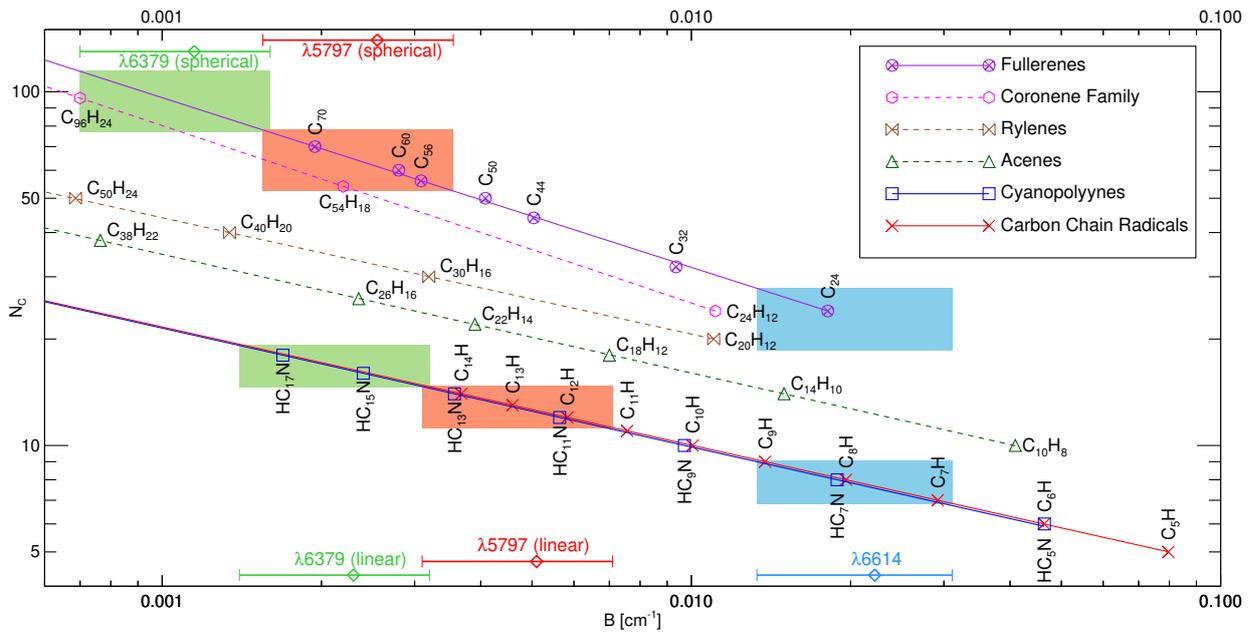


Figure 4 – Sizes of various molecules (expressed as equivalent number of carbon atoms N_c) as a function of their rotational constants B for experimentally measured or theoretically calculated values from the literature (see main text for details). The lines are linear models fitted to these values for individual molecular families and extrapolated to larger sizes. We used the solid lines to determine DIB carrier sizes for linear and spherical species; the dashed lines for PAHs are for illustrative purposes only. The shaded areas represent our results for the $\lambda\lambda 6379$ (green), 5797 (red) and 6614 (blue) DIBs assuming either a spherical geometry (top) or linear species (bottom). The width of these shaded areas indicate our nominal $1-\sigma$ confidence intervals for the derived B values (also indicated at the top and bottom of the figure, with the nominal value indicated by the \diamond symbols) while the height of these shaded areas represents the corresponding confidence interval for the derived N_c values. We note that the B -value for the $\lambda 6614$ DIB is independent of the assumed geometry. Copyright: H. Maclsaac et al., forthcoming in *A&A*, 2022, reproduced with permission © ESO

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Mixed Quantum/Classical Theory for Collisional Quenching of PAHs in the Interstellar Media

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Computationally affordable methodology is developed to predict cross sections and rate coefficients for collisional quenching and excitation of large molecules in space, such as PAHs. Mixed quantum/classical theory of inelastic scattering (MQCT) is applied, in which quantum state-to-state transitions between the internal states of the molecule are described using time-dependent Schrodinger equation, while the scattering of collision partners is described classically using mean-field trajectories. To boost numerical performance even further, a decoupling scheme for the equations of motion, and a Monte-Carlo sampling of the initial conditions, are implemented. The method is applied to compute cross sections for rotational excitation and quenching of benzene molecule C_6H_6 by collisions with He atoms in a broad range of energies, using a very large basis set of rotational eigenstates up to $j = 60$, and close to one million non-zero matrix elements for state-to-state transitions. The properties of collision cross sections for $C_6H_6 + He$ are reported and discussed. The accuracy of approximations is rigorously tested and is found to be suitable for astrophysical/astrochemical simulations. The method and code developed here can be employed to generate a database of collisional quenching rate coefficients for PAHs and other large molecules, such as iCOMs, or for molecule-molecule collisions in cometary comas.

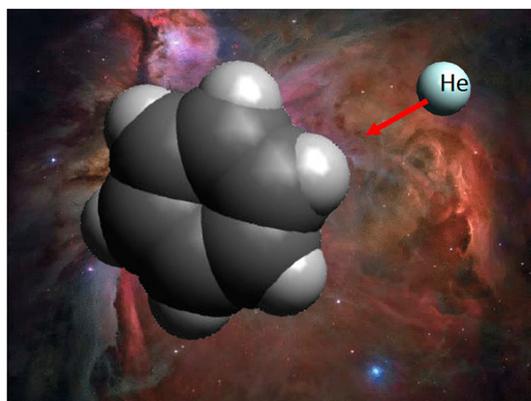


Figure 5 – Collisional quenching of benzene rotations by He atom in the interstellar medium.

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Effect of surface H₂ on molecular hydrogen formation on interstellar grains

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We investigate how the existence of hydrogen molecules on grain surfaces may affect H₂ formation efficiency in diffuse and translucent clouds. Hydrogen molecules are able to reduce the desorption energy of H atoms on grain surfaces in models. The detailed microscopic Monte Carlo method is used to perform model simulations. We found that the impact of the existence of H₂ on H₂ formation efficiency strongly depends on the diffusion barriers of H₂ on grain surfaces. Diffuse cloud models that do not consider surface H₂ predict that H atom recombination efficiency is above 0.5 over a grain temperature (T) range 10 K and 14 K. The adopted H₂ diffusion barriers in diffuse cloud models that consider surface H₂ are 80% H₂ desorption energies so that H₂ can be trapped in stronger binding sites. Depending on model parameters, these diffuse cloud models predict that the recombination efficiency is between nearly 0 and 0.5 at $10 \text{ K} \leq T \leq 14 \text{ K}$. Translucent cloud model results show that H₂ formation efficiency is not affected by the existence of surface H₂ if the adopted average H₂ diffusion barrier on grain surfaces is low (194 K) so that H₂ can diffuse rapidly on grain surfaces. However, the recombination efficiency can drop to below 0.002 at $T \geq 10 \text{ K}$ if higher average H₂ diffusion barrier is used (255 K) in translucent cloud models.

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Relations between mid-IR dust emission and UV extinction

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We analyze low resolution *Spitzer* infrared (IR) 5-14 μm spectra of the diffuse emission toward a carefully selected sample of stars. The sample is composed of sight lines toward stars that have well determined ultraviolet (UV) extinction curves and which are shown to lie beyond effectively all of the extinguishing and emitting dust along their lines of sight. Our sample includes sight lines whose UV curve extinction curves exhibit a wide range of curve morphology and which sample a variety of interstellar environments. As a result, this unique sample enabled us to study the connection between the extinction and emission properties of the same grains, and to examine their response to different physical environments. We quantify the emission features in terms of the PAH model given by Draine & Li (2007) and a set on additional features, not known to be related to PAH emission. We compare the intensities of the different features in the *Spitzer* mid-IR spectra with the Fitzpatrick & Massa (2007) parameters which describe the shapes of UV to near-IR extinction curves. Our primary result is that there is a strong correlation between the area of the 2175 Å UV bump in the extinction curves of the program stars and the strengths of the major PAH emission features in the mid-IR spectra for the same lines of sight.

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<https://iopscience.iop.org/article/10.3847/1538-4357/ac3825/pdf>

<https://arxiv.org/pdf/2112.02631.pdf>

Polycyclic Aromatic Hydrocarbons, the Anomalous Microwave Emission, and Their Connection to the Cold Neutral Medium

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Using new large area maps of the cold neutral medium (CNM) fraction, f_{CNM} , we investigate the relationship between the CNM, the abundance of polycyclic aromatic hydrocarbons (PAHs), and the anomalous microwave emission (AME). We first present our f_{CNM} map based on full-sky HI4PI data, using a convolutional neural network to convert the spectroscopic HI data to f_{CNM} . We demonstrate that f_{CNM} is strongly correlated with the fraction of dust in PAHs as estimated from mid- and far-infrared dust emission. In contrast, we find no correlation between f_{CNM} and the amount of AME per dust emission and no to weakly negative correlation between f_{CNM} and the AME peak frequency. These results suggest PAHs preferentially reside in cold, relatively dense gas, perhaps owing to enhanced destruction in more diffuse media. The lack of positive correlation between f_{CNM} and AME peak frequency is in tension with expectations from theoretical models positing different spectral energy distributions of AME in the cold versus warm neutral medium. We suggest that different PAH abundances and emission physics in different interstellar environments may explain the weaker than expected correlation between 12 μm PAH emission and AME even if PAHs are the AME carriers.

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The Astrophysical Journal, in press

<https://ui.adsabs.harvard.edu/abs/2021arXiv211103067H/abstract>

Similarities and dissimilarities in the fragmentation of polycyclic aromatic hydrocarbon cations: A case study involving three dibenzopyrene isomers

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The photon induced fragmentation behavior of the cations of three dibenzopyrene ($C_{24}H_{14}$) isomers (DPBae, DPBah and DPBal) is studied in a series of systematic mass spectrometric experiments. The ions are collected in an ion trap system and irradiated with different numbers of photons before being released into a time-of-flight mass spectrometer. The resulting mass spectra show a number of remarkable similarities, despite the structural differences between the three precursor species. Differences in the fragmentation patterns are found as well. Whereas it is not straight forward to explain the molecular origin of these findings, it is clear that the observed fragmentation patterns are relevant to further interpret the molecular composition of the interstellar medium (ISM), in which PAHs are omnipresent and subject to intense radiation. The main conclusion of this work is that PAHs comparable to the one studied here, may enrich the ISM with pure carbon species, C_n^+ , with n values roughly between 11 and 15, following a top-down approach.

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<https://doi.org/10.1016/j.ijms.2022.116834>



Meetings

Chemistry and Physics at Low Temperatures CPLT2022

Visegrád, Hungary
3–8 July, 2022

<http://www.cplt2022.elte.hu>

The CPLT Conference 2020 has been postponed to 3–8 July 2022 due to the COVID-19 outbreak.

Topics:

- Reactive and unstable species, radicals, intermediates
- Photochemistry
- Atmospheric & astrochemical species, astrochemical ices
- Biomolecules in matrices and jet-cooled beams
- Quantum hosts
- New methods and applications
- Tunneling & dynamics
- Ultracold molecules
- Cryosynthesis, materials, clathrates
- Theory helping cryogenic studies

Oral contribution are expected by April 11, 2022. Poster abstracts before June 6, 2022. Late registration (at increased fee) is from June 1, 2022.

Organizing Committee:

György Tarczay (Hungary)

Gábor Magyarfalvi (Hungary)

Mrs. Klara Biszkupne Nanasi (Altagra Agency, Hungary)

E-mail for contact: cplt@altagra.hu

The life cycle of cosmic PAHs

Aarhus University, Denmark
5–9 September, 2022

<https://conferences.au.dk/cosmicpah2022>

Dear Colleagues,

The aim of this symposium is to bring together observational astronomers, theorists and experimentalists working on PAH observations, formation, fragmentation, photo-physics, spectroscopy, surface science and chemistry to shed light on the lifecycle of cosmic PAHs and to explore the future opportunities for PAH research provided by novel theoretical and experimental methods and future observational missions, with focus on JWST and ELT. This is the third installment in a series of meetings on interstellar polycyclic aromatic hydrocarbons (PAHs) with previous meetings held in Toulouse in 2010 and in Noordwijk in 2016.

Registration and abstract submission are now open. We are limited to a maximum of 80 participants.

Abstract submission for contributed talks and posters closes on 2nd May 2022.

Invited speakers include:

Kathrin Altwegg, University of Bern
José Ángel Martín Gago, CSIC
Partha P. Bera, NASA Ames Research Center
Christiaan Boersma, NASA Ames Research Center
Sandra Brünken, Radboud University

Wybren Jan Buma, Universiteit van Amsterdam
Jan Cami, University of Western Ontario
Ewen K. Campbell, University of Edinburgh
Jérémy Chastenot, University of California San Diego
Leen Decin, University of Leuven

Francois Dulieu, Université de Cergy-Pontoise
Michael Duncan, University of Georgia
M. Samy El-Shall, Virginia Commonwealth University
Christine Joblin, Université Toulouse III - Paul Sabatier
Stefanie N. Milam, NASA Goddard Space Flight Center

Giacomo Mulas, INAF
Conor A. Nixon, NASA Goddard Space Flight Center
Els Peeters, University of Western Ontario
Mathias Rapacioli, Université Paul Sabatier

Melanie Schnell, Christian-Albrechts-Universität zu Kiel
Alan Tokunaga, University of Hawaii
Henning Zettergren, Stockholm University
Xander Tielens, Leiden University.

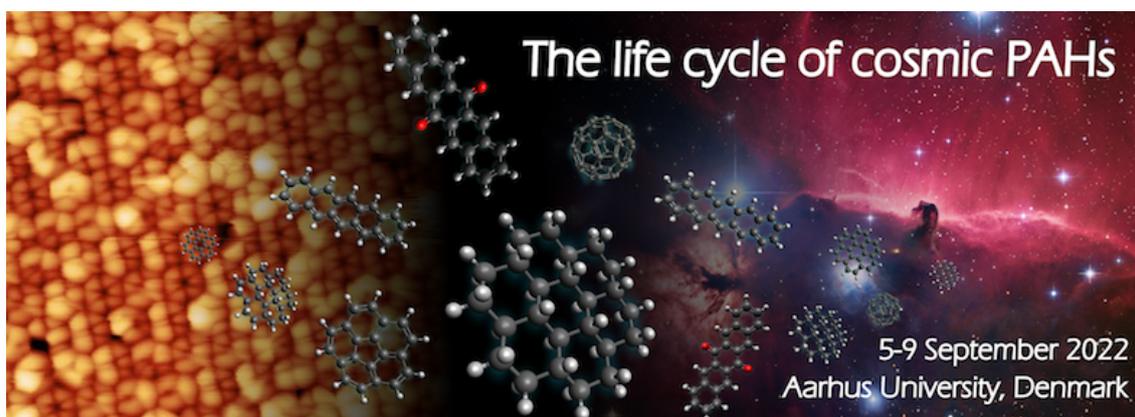
Scientific Organising Committee: Liv Hornekær; Els Peeters; Olivier Berné; Xander Tielens; Annemieke Petrignani.

We look forward to welcoming you in Aarhus.

On behalf of the organizing committees,

Liv Hornekær

E-mail for contact: cosmicPAH@phys.au.dk



Credit: Horsehead Nebula - Robert Gendler; STM image of coronene - SDL laboratory, Aarhus University.



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PhD or Postdoc position Molecular Physics / Physical Chemistry Laboratory Astrophysics

Advertised by Otto Dopfer

A PhD position (3 years) or postdoc position (2 years), funded by the German Science Foundation (DFG), is available in the laser molecular spectroscopy group of Otto Dopfer at Technische Universität Berlin, Germany. This project deals with the laser spectroscopic and quantum chemical characterization of the geometric, electronic, optical and chemical properties of aromatic cluster cations and their microsolvated solvated clusters in the context of intermolecular forces, solvation effects, interstellar chemistry, combustion, and materials science. Further information about the group and its projects (and recent publications) is available at: https://www.ioap.tu-berlin.de/menue/arbeitsgruppen/ag_dopfer/ A key paper for this particular project is: Aromatic Charge Resonance Interaction Probed by Infrared Spectroscopy, K. Chatterjee, Y. Matsumoto, O. Dopfer, *Angew. Chem. Int. Ed.* 58, 3351 (2019), DOI: 10.1002/anie.201811432.

Interested candidates can send their application to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de). Evaluation of the applications will begin March 31 (2022) and continue until the position is filled. Desired starting date is as soon as possible (but negotiable to some extent). Being an European capital, Berlin offers an exciting international scientific and cultural environment.

Deadline: March 31, 2022

E-mail for contact: dopfer@physik.tu-berlin.de

Webpage: https://www.ioap.tu-berlin.de/menue/arbeitsgruppen/ag_dopfer/

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Submission deadline: 8 April 2022