Issue 1 | October 2013

AstroPAH

A Newsletter on Astronomical PAHs

PAH Picture of the Month

Editorial

We are happy to introduce AstroPAH, a newsletter that acts as a bridge in the interdisciplinary and international community involved in astronomical Polycyclic Aromatic Hydrocarbons (PAHs) and related research. AstroPAH emerged as a defining result of the **Lorentz Center Workshop "The Molecular Physics of Interstellar PAHs"** that took place in Leiden,The Netherlands last summer. This workshop brought together an interdisciplinary and international community of scientists engaged in astronomical PAH and related research, with a high representation of the Dutch Astrochemistry Network (DAN; a program of NWO, the Netherlands Organisation for Scientific Research) and the Carbon in the Galaxy Consortium (C-in-G; NASA Ames Research Center). During the workshop, Dr. Isabel Aleman suggested the idea of a monthly newsletter to keep the PAH community informed of the latest developments in astronomical PAH research and as a tool to promote a constant communication between the different fields (Astronomy, Chemistry, and Physics) working with PAHs.

This first edition of AstroPAH is a special issue, where we have the pleasure to present the summary of the Lorentz Center Workshop "The Molecular Physics of Interstellar PAHs" and introduce the members of the editorial team. In its regular monthly editions, AstroPAH will post a collection of abstracts of accepted papers, theses, dissertations, job announcements, and important events of the astronomical PAH community. Each issue will also contain two special sections: the "PAH Picture of the Month", which name is self-explanatory, and "In Focus", an article covering an interesting PAH related topic (research, experimental facility, interview with a scientist, etc.). We emphasise that AstroPAH is made for the interdisciplinary community interested in the astronomical PAHs research and therefore scientists from all related areas (astronomy, astrophysics, quantum chemistry, spectroscopy, hydrocarbon chemistry, combustion, nanophysics, etc.) are encouraged to subscribe and contribute.

You can subscribe to the AstroPAH newsletter on our brand new website:

http://astropah-news.strw.leidenuniv.nl.

We would appreciate if you could circulate AstroPAH to people who may be interested. The success of this initiative relies strongly on the community involvement. We thus encourage scientists from all disciplines related to astronomical PAHs to submit abstracts of their recent work or send suggestions for the "Picture of the Month" and "In Focus" section to AstroPAH. You will find instructions on the website. The submission deadline for contributions for the next issue is November 12th 2013, 12:00 CET.

We take this opportunity to wish you a productive autumn.

THE EDITORIAL TEAM

WEBSITE:

http://astropah-news.strw.leidenuniv.nl

CONTACT:

astropah@strw.leidenuniv.nl

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PAH Picture of the Month

On the cover, the participants of the Workshop "The Molecular Physics of the Interstellar PAHs", the birthplace of the AstroPAH Newsletter.

Oort Workshop:
The Molecular Physics of Interstellar PAHs

29 July - 2 August 2013, Leiden, The Netherlands

Summary Paper

Lou Allamandola (NASA Ames)
Annemieke Petrignani (Leiden Observatory)
Xander Tielens (Leiden Observatory)

Lorentz Center Website

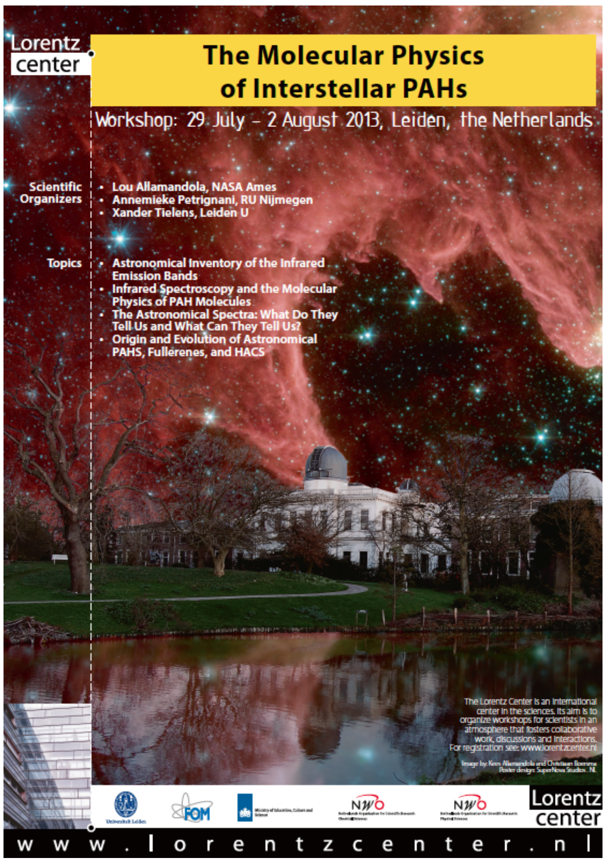
By all accounts, the Lorentz workshop "The Molecular Physics of Interstellar PAHs" (Polycyclic Aromatic Hydrocarbons) was an enormous success. It brought together experts from various fields involved in interstellar PAH research from around the world, identified key questions, and spawned new ideas and collaborations. World experts in PAH and related research in the fields of astronomy, astrophysics, quantum chemistry, spectroscopy, hydrocarbon chemistry, combustion, and nanophysics were brought together in an atmosphere that promoted lively discussions and devised new ways to attack long-standing problems. A total of 11 countries were represented, ranging from North and South America to Europe to China, with a high representation of the Netherlands Organisation for Scientific Research (NWO) Dutch Astrochemistry Network (DAN) and the NASA Ames Carbon in the Galaxy (C-in-G) Consortium.

The specific workshop goal was to chart the course to attain a state-of-the-art understanding of the characteristics of astronomical PAHs in galaxies, their emission spectra, and their origin and evolution in space. The overarching objective was to identify the areas of the PAH model that need to be improved for it to be up to the same level of details than the new observatories that will revolutionize astrophysics over the next decade: the Stratospheric Observatory For Infrared Astronomy (SOFIA), and the James Webb Space Telescope (JWST). The workshop aimed to maximize the scientific output of these missions through the analysis and interpretation of archival data obtained with the Spitzer and Herschel missions as well as to guide instrumental development for future missions.

Many workshop-wide and smaller-scale discussions took place to identify, refine, and sharpen the key outstanding questions hampering progress in astronomical PAH research and develop innovative ideas on how to tackle them. It is clear that although the PAH model is widely accepted and a consensus has been reached that PAHs are ubiquitous and dominate the mid-infrared spectral emission features of circumstellar and interstellar media, our understanding of the molecular physics involved, on which the PAH model rests, is rudimentary.

The participants pinpointed a number of key, high-priority, astronomical questions that must be addressed:

- How does the astronomical PAH spectrum vary across the universe and over cosmic time?
- What can we learn from the astronomical PAH spectra about the interaction of stars with their environment and the characteristics and evolution of galaxies?
- What is the molecular inventory of astronomical PAHs, where do they come from and go, and what is their role in the origin of life?



Workshop Webpage

The participants recommended the following strategy to tackle these questions:

- Increase spectral bandwidth for a diversity of astronomical objects
- Enhance guidance and prediction from laboratory and calculated data
- Develop an astronomer friendly toolbox that can be used to analyse astronomical observations at the detail level of the molecular physics that drives the emission
- Increase diversity and spatial decomposition of astronomical objects
- Encourage interdisciplinary collaboration through support of networks and teams

The participants concluded that significant progress will only be made through concerted interdisciplinary work spanning countries. As a first step, we endeavor to keep this community working together by structuring ourselves into a collaborative network, building upon the strong ties between the NWO DAN and the NASA C-in-G Consortium. A number of new cross-disciplinary projects between members of the different consortia were started at this meeting. The organizers are aware of several:

- Combining *theoretical* calculations on PAH formation with *experiments* on forming the simplest aromatics, benzene and naphthalene
- Combining *experimental* studies of anharmonicity with quantum chemical *calculations* to deepen our understanding of the PAH emission features in the 3μm region
- Applying the recently recognized dipole enhanced electron capture mechanism to re-evaluate the probability of finding interstellar PAH anions

- Comparing and contrasting existing spectroscopic analysis tools used in interstellar PAH research

Furthermore, a newsletter will be created to keep the astronomical PAH community abreast of new developments important to astronomical PAH research. The first edition will be released in October 2013 reviewing the workshop, as well as presenting the editorial team. The following editions will present relevant abstracts of new articles, scientific meetings, summer schools, and job opportunities in this field. In April 2014, another meeting between the NWO DAN and the NASA C-in-G team will take place at NASA Ames. Finally, we intend to have a follow-up meeting of this workshop in two years.

Key Astronomical Questions

How does the astronomical PAH spectrum vary across the universe and over cosmic time?

JWST will provide astronomical spectra covering the complete mid-IR molecular region (0.8-28μm) from objects spanning the universe. The resolution will be sufficient to track detailed spectral variations over 0.07 arcsec scale-sizes. Interpreting these spectra will require a much more detailed astronomical PAH model than we have today.

What can we learn from the astronomical PAH spectra about the interaction of stars with their environment and the characteristics and evolution of galaxies?

PAH composition and evolution is tied to variations of local physical conditions. Differing conditions lead to changes in the observed bands, plateaux, and continuum. Today, we do not fully understand the molecular physics behind the emission. Once this is achieved, we will be able to use the spectroscopic details of the emission spectra as astronomical templates that probe the physical conditions and temporal evolution of astronomical objects spanning the universe.

What is the molecular inventory of astronomical PAHs, where do they come from and go and what is their role in the origin of life?

A full evaluation of the astronomical PAH population and their place on the overall organic inventory of space, will require spectroscopic signatures over the full wavelength range. This holds not only for the full mid-IR molecular signature range (2-25μm), but includes the optical (UV-Vis), far-IR and radio ranges as well. This will provide information essential to characterize the astronomical PAH species and link them with local conditions. Laboratory and theoretical spectra of PAH species are required to understand the astronomical inventory. PAH formation, destruction, protection, and repair mechanisms need to be studied to understand the evolution of carbon from its birthplace in circumstellar shells through its evolution in the interstellar matter to its incorporation into star and planet forming systems and finally as building blocks of life.

Strategies

Increase spectral bandwidth for a diversity of astronomical objects

There is a need for high-quality, pan-spectral PAH signatures to constrain the species and their microphysical properties, ranging from the UV, optical (electronic), and FIR (rotational) to the radio. The IR emission bands need to be treated as a family of bands, not individual features. Constraints on the PAH model may be identified through the simultaneous detection of UV and IR spectra, of the 3.3μm band (CH stretch) along with the other mid-IR bands and/or the possible overtone detection at 1.68μm with JWST. Intensity correlations such as in dust producing sources and along lines of sight with well-characterized extinction curves will provide additional insights. This strategy may involve innovative instrumental design, such as in the X-ray region where non carbon-based designs would be required.

Enhance guidance and prediction from laboratory and calculated data

Sophisticated and high-resolution laboratory studies and quantum chemical calculations are essential to link observational spectra to local conditions and the other way around. Increased spectral bandwidth demands an important expansion of databases. And PAH formation, survival (repair and protection), and destruction pathway mechanisms have to be identified to understand the temporal evolution and PAH inventory and chemistry.

Some examples of data needs are: detailed consideration of intrinsic molecular properties such as size, anharmonicity, and level of excitation; the poorly understood role of large PAHs emphasized by The Virtual Atomic & Molecular Data Centre VAMDC “Big PAH data needs”; the need for a coherent HAC (Hydrogenated Amorphous Carbon) candidate family; the 3 vs 1.68μm CH stretch as key to energy flow; measuring a class A emitter in the lab as proposed end product of UV processing; spectroscopy in the 15-20μm range for closed-shell PAHs or aliphatic side bands, and in the 3.4μm band for small molecule hot bands or aliphatic carbons; understanding of the ring-formation rate, the role of heteroatoms and reaction selectivity in PAH formation, (de)hydrogenation, linearization, clustering (including soot formation) and their possible reversibility; particle and UV destruction pathways; and the connection to PAH related species such as heterocyclic PAHs, fullerenes and HACs.

Develop an astronomer friendly toolbox

An “astronomer friendly” toolbox is desired to analyze astronomical observations at the detail level of the molecular physics that drives the emission. This toolbox should allow the use of PAHs as tracers/probes. This requires the development of standard methods and spectra for the interpretation of observations, molecular benchmark prototypes and sensitivity analysis, and PAH spectral decomposition (dust continuum, plateaux, extinction).

Increase diversity and spatial decomposition of astronomical objects

The variation of the PAH spectrum throughout the universe is best understood if a larger variety of astronomical objects and environments are studied. In particular, observations focusing on measuring the IR spectrum of the “true” diffuse gas (JWST, SPICA) and others directed to resolving chemical frontiers (spatial resolution $<$ 1”) will add significantly to our understanding of the astronomical PAH population.

Encourage Interdisciplinary collaboration

Predictions and laboratory data are required to validate, interpret, guide, and develop observations and future missions. Understanding the molecular physics behind PAH emission is essential to using PAHs as a probe of local conditions. Astronomical PAH research can benefit greatly from the fields of combustion chemistry and nanophysics to better understand formation and destruction routes of PAH species and the transition to nanoparticles.

Introducing Our Editors

by Xander Tielens

Astrochemistry is a highly interdisciplinary field where astronomers, molecular physicists, spectroscopists, and quantum chemists meet. As no single scientist, no single institute, not even a single country can be expected to be on top of all aspects of these fields by themselves, the community will have to organize itself to ensure progress. This newsletter is one way to build an active and involved community. The editorial team, introduced below, is in itself an example of how interdisciplinarity and internationality can enrich the astronomical PAH community.

Dr. Isabel Aleman

"I am a postdoctoral researcher in the Interstellar Medium group at the Leiden Observatory (University of Leiden, Netherlands). I have a doctoral degree in Astrophysics from the Institute of Astronomy, Geophysics and Atmospheric Sciences of the University of São Paulo (IAG-USP, Brazil) where I developed my thesis on modeling the molecular hydrogen infrared emission from planetary nebulae. As part of that work, I implemented the molecular hydrogen microphysics in the photoionisation code AANGABA.

Isabel's Webpage

Since then I have worked as a postdoctoral fellow in wonderful places: the University of São Paulo, the University of Manchester (UK), the University of Rio Grande do Sul (Brazil), and now at the University of Leiden. My main interests are models of photoionised nebulae with special focus on the study of chemical and physical processes and their effects in the emission spectra.

In my work, I see the importance of having molecular data to use in our models to better interpret the astronomical observations. I am sure the AstroPAH Newsletter will contribute to bridge the gap between different fields that have this same goal. I am happy to be part of it."

Dr. Alessandra Candian

"I am a post-doctoral research scientist at the Leiden Observatory (The Netherlands).

Alessandra's Webpage

I come from Italy and I obtained my Master in Astrophysics from Universitá di Padova, which is the university where Galileo Galilei taught astronomy and performed his observations of the phases of Venus. Fascinated by the interplay between chemistry and astronomy I moved to the United Kingdom, where last year I obtained a PhD in Astrophysical Chemistry from the University of Nottingham. My primary interest lies in the spectroscopy and photoprocessing of Polycyclic Aromatic Hydrocarbons (PAHs) and the characterization of their observational signatures. My approach is mostly theoretical and I use quantum chemistry tools, such as Density Functional Theory. Other interests are infrared astronomy and the physics of the interstellar medium.

I have joined the editorial board of the AstroPAH newsletter because I believe that communication between scientists is the only way an interdisciplinary topic such as the study of astronomical PAHs can advance."

Dr. Elisabetta Micelotta

"I obtained my PhD in Astronomy & Astrophysics in 2009 from Leiden University (The Netherlands). After a postdoc at NASA Goddard Space Flight Center (USA) and at the University of Western Ontario (Canada), I am currently a Marie Curie postdoctoral fellow at the Institut d'Astrophysique Spatiale in Orsay (France), working in the Interstellar Matter and Cosmology group (MIC).

Elisabetta's
Publications List
and LinkedIn

My expertise lies at the intersection of theoretical molecular astrophysics, infrared astronomy, high-energy astrophysics and atomic and molecular physics, with a strong inter- and multidisciplinary approach and an emphasis on connecting theory to observations. During my PhD I developed the first models for the interaction of interstellar PAHs with energetic ions and electrons (collisional processing). My research interests include the analysis of cosmic rays, the study of the stability of interstellar fullerenes and hydrocarbon grains against photo- and collisional processing, and the physical processing of supernova-condensed dust grains. My current research focuses on the physical characterization of the carbonaceous nanoparticles that populate the interstellar dust, to establish the connection between PAHs, fullerenes and such nanoparticles in the astrophysical context.

To make progresses in the field of astronomical PAHs, a better communication between scientists from different fields is necessary. I have joined the editorial board of AstroPAH with the firm belief that this newsletter will greatly promote and facilitate the exchange of knowledge and ideas among researchers."

Dr. Annemieke Petrignani

" I am a research scientist working with Prof. Tielens at the Leiden Observatory. I am of Dutch and French origin and live with my family near Amsterdam in a small historic town. Over the years I have performed many experiments of interest to planetary atmospheres, astrophysics, and astrochemistry. I have a strong background and interest in interdisciplinary and international work, being involved in experimental molecular quantum dynamics, quantum chemistry, and spectroscopy in collaboration with theoretical astrophysical modellers, planetary atmospheric modellers, and theoretical quantum physicists and chemists.

Annemieke's Webpage, ResearchGate, and LinkedIn

I obtained my PhD in 2005 from the FOM Institute AMOLF in Amsterdam on ion-electron recombination reactions relevant to planetary airglows. In 2006, I went to Germany for experiments of astrophysical interest with a high focus on H_3^+ spectroscopy at the Max-Planck Institute for Nuclear Physics in Heidelberg, where I lived for 5 years. I have gained experience in (cold) ion-electron collisions, high-sensitivity and high-resolution spectroscopy from the infrared to the ultraviolet, ion traps, ion storage rings (CRYRING and TSR), fast-beam setups, and in acceleration, RF, cryogenic, and imaging techniques. Currently, I study neutral and ionic PAH species in the gas-phase using mass spectroscopy and UV/IR spectroscopic techniques in collaboration with members of the Dutch Astrochemistry Network; Prof. Oomens at the FELIX Facility and Prof. Buma at the University of Amsterdam.

After a successful and fantastic experience in the organisation of the Lorentz workshop on the Molecular Physics of Interstellar PAHs, I have joined the editorial team of AstroPAH to stimulate further interaction and the exchange of knowledge about astronomical PAHs research. I am looking forward to playing an active role in supporting the knowledge exchange within this community."

Dr. Ella Sciamma-O'Brien

"I am currently a research scientist working with Dr. Farid Salama in the Astrophysics & Astrochemistry Laboratory group at NASA Ames Research Center.

I received my PhD in experimental plasma physics from the University of Texas at Austin in December 2007, working on a propulsion system concept for future manned missions to Mars. At the end of my PhD though I realized that I would rather be the one exploring our solar system than the one designing the rocket for someone else to go... so I applied to the ESA astronaut program in 2008. I passed three selections, but was not one of the lucky four to be chosen. I then looked for a postdoc that would allow me to make a link between my plasma physics background and planetary science, and found a postdoc at the Laboratoire Atmospheres Milieux Observations Spatiales (LATMOS) in France to work on a plasma experiment, called PAMPRE. This experiment simulates Titan's atmosphere in order to study the complex organic chemistry between its two main constituents, N_2 and CH_4. I started my postdoc at NASA Ames in April 2011, working on the Titan Haze Simulation (THS) experiment developed at the NASA Ames COSmIC facility to study the chemical pathways that link the simple molecules resulting from the first steps of the N_2-CH_4 chemistry to benzene, and to PAHs and nitrogen-containing PAHs (PANHs) as precursors to the production of solid aerosols. My research goals are to study the chemical and physical properties of both the gas and solid phases using mass spectrometry, IR absorption spectroscopy, nuclear magnetic resonance and scanning electron microscopy imaging.

Ella's Webpage and LinkedIn

Being part of the Astrophysics and Astrochemistry Laboratory group at Ames, I started to be more involved in the Carbon in the Galaxy project. After seeing how successful the Workshop on the Molecular Physics of Interstellar PAHs was, I am certain that the AstroPAH newsletter will be very helpful in connecting the different pieces of the puzzle to advance this pluridisciplinary field. I am looking forward to being part of the AstroPAH editorial team."

AstroPAH Newsletter

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astropah@strw.leidenuniv.nl

Next issue: 19 November 2013
Submission deadline: 12 November 2013