



# AstropAH

A Newsletter on Astronomical PAHs

Issue 99 • June 2023



## Organic Molecules in the Early Universe



# Editorial

## Dear Colleagues,

Welcome to our new AstroPAH volume no. 99! We hope all of you are healthy and doing well! We thank you all for your contributions to AstroPAH!

Our cover showcases a breathtaking JWST observation of two galaxies almost perfectly lining up in JWST's field of view, one 12 billion light years away, the other 3 billion light years away. Complex organics molecules have been detected in the more distant galaxy!

Our In Focus entitled *Extraordinary Times* was kindly prepared by Christian Boersma and showcases how JWST will revolutionize how we explore the infrared universe and in particular PAHs, and how laboratory astrophysics and the PAH IR spectroscopic database play a key role in support of JWST observations.

In our abstract section, you can read about newly published papers on organic molecule synthesis through HI-catalyzed reactions, a model of interstellar dust, laboratory formation or hydrogenated and deuterated fullerene cations, a new analysis of ISO observations of star forming regions and late type stars, laboratory methane and acetylene ice irradiation experiments to simulate galactic cosmic ray processing of Kuiper Belt objects, and a study presenting the most distant detection of PAH feature from JWST observations of galaxy SPT0418-47. Many thanks again for all your contributions!

We draw your attention to two important announcements. First, the conference "Surveying the Milky Way: The Universe in Our Own Backyard" will be held October 23–27, 2023 in Pasadena, CA. Abstract deadline is June 30. Second, Prof. Otto Dopfer is proposing a PhD position in Molecular Physics/Laboratory Astrophysics at the Berlin Institute of Technology in Germany. Deadline for application is July 31st. Finally, two Postdoctoral positions are being advertised by Dr. Ralf Kaiser in the areas of gas phase reaction dynamics and combustion chemistry in the formation of PAHs. Deadline for applications is July 1st.

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: 20 July 2023.  
Submission deadline: 7 July 2023.**



## AstroPAH Newsletter Editorial Board:

Editor-in-Chief

**Prof. Alexander Tielens**

Leiden Observatory  
(The Netherlands)

Executive Editors

**Dr. Isabel Aleman**

University of São Paulo (Brazil)

**Dr. Ella Sciamma-O'Brien**

NASA Ames Research Center (USA)

Editors

**Dr. David Dubois**

NASA Ames Research Center  
BAER Institute (USA)

**Dr. Helgi Rafn Hróðmarsson**

Laboratoire Inter-Universitaire  
des Systèmes Atmosphériques  
(France)

**Dr. Rijutha Jaganathan**

Aarhus University  
(Denmark)

**Dr. Donatella Loru**

Deutsches Elektronen-Synchrotron  
(Germany)

**Dr. Julianna Palotás**

University of Edinburgh (UK)

**Dr. Ameek Sidhu**

University of Western Ontario  
(Canada)

**Dr. Sandra Wiersma**

Institute de Recherche en  
Astrophysique et Planétologie  
(France)

## Contact us:

[astropah@strw.leidenuniv.nl](mailto:astropah@strw.leidenuniv.nl)

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

[Click here to Subscribe to AstroPAH](#)

[Click here to Contribute to AstroPAH](#)

Follow us on:



## Contents

PAH Picture of the Month	1
Editorial	2
In Focus	4
Recent Papers	11
Meetings	17
Announcements	19

## PAH Picture of the Month

Astronomers using the Webb telescope discovered evidence of complex organic molecules similar to smoke or smog in the distant galaxy shown here. The galaxy, more than 12 billion light years away, happens to line up almost perfectly with a second galaxy only 3 billion light years away from our perspective on Earth. In this false-color Webb image, the foreground galaxy is shown in blue, while the background galaxy is red. The organic molecules are highlighted in orange.

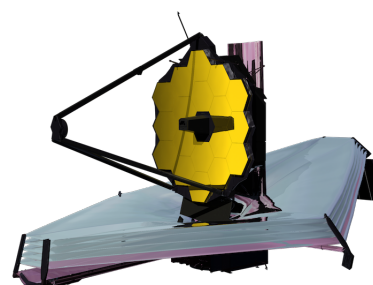
**Credits:** J. Spilker / S. Doyle, NASA, ESA, CSA.

## Extraordinary Times

Christiaan Boersma

### Introduction

We truly live in extraordinary times. The James Webb Space Telescope (JWST; Figure 1) has started unraveling the infrared (IR) Universe like never before with its unprecedented spatial- and spectral resolution and unrivaled sensitivity. While it is still early in its run, JWST is already showing us, once again, that PAHs are omnipresent and that they, likely, entered the Cosmic stage not long after the first galaxies formed (Spilker et al., 2023; Woods, 2023). Furthermore, the detection of fullerenes in the IR (Cami et al., 2010; Sellgren et al., 2010) and cyano-PAHs in the radio (McGuire et al., 2018, 2021) have been major milestones in the development of the PAH model. Also, the strong connection between Laboratory Astrophysics and Astronomy, so crucial to the field of PAH research, is now well established in the US with both the American Astronomical Society and American Chemical Society having dedicated subdivisions fostering this synergy; the [Laboratory Astrophysics Division](#) and [Astrochemistry Subdivision](#), respectively.



**Figure 1** – *Maya-3D rendering of the James Webb Space Telescope.*

Laboratory Astrophysics now has the capability to perform astrophysically-relevant gas-phase PAH absorption, and in some cases even emission, experiments (Maltseva et al., 2015; Lacinbala et al., 2022). Computational chemistry has also seen extraordinary progress, with the year-over-year increase in computational power and improved techniques *full-cascade anharmonic PAH emission* spectra are now, somewhat, readily computed (Mackie et al., 2015, 2016, 2018, 2022). Moreover, the [Decadal Survey on Astronomy and Astrophysics 2020](#) that guides the US's research direction on Astronomy and Astrophysics has spotlighted Laboratory Astrophysics and, in particular, databases.

The NASA Ames PAH IR Spectroscopic Database<sup>1</sup> (PAHdb; Bauschlicher et al., 2010; Boersma et al., 2014; Bauschlicher et al., 2018; Mattioda et al., 2020), which after 15 years still holds the world's foremost collection of laboratory-measured and theoretically computed PAH spectra, is poised to capitalize on these extraordinary times.

<sup>1</sup>[www.astrochemistry.org/pahdb/](http://www.astrochemistry.org/pahdb/)



# The NASA Ames PAH IR Spectroscopic Database



**Figure 2** – The NASA Ames PAH IR Spectroscopic Database (PAHdb) Patch.

NASA Ames has a long history with the astronomical PAH field, going all the way back to the early days of the Kuiper Airborne Observatory's (KAO) pioneering observations of some of the first PAH emission (see [AstroPAH 27](#)). Looking ahead, the Astrophysics & Astrochemistry Laboratory at NASA Ames Research Center remains focused on unlocking and mining the treasure trove of information hidden in the astronomical PAH signature utilizing data, models and (software) tools<sup>2</sup> made available through PAHdb (Figure 2).

After a very successful four-year Round 1 Laboratory Astrophysics NASA Directed Work Package (LADWP) that came about in direct support of PAHdb, last year a Round-2 successor was selected and funded that continuous supporting PAHdb efforts. These efforts revolve around the strong synergy between the astronomers, laboratory and computational chemists that are part of the Astrophysics &

Astrochemistry Laboratory at NASA Ames. As a result, PAHdb has seen significant additions and improvements since the reporting in [AstroPAH 27](#).

The continuously expanding contents of PAHdb now includes the laboratory-measured spectra of 84 PAHs ([Mattioda et al., 2020](#)), density-functional-theory (DFT) computed spectra of 4,233 PAHs ([Ricca et al., 2019](#)), and the laboratory-measured ([Roser and Allamandola, 2010](#); [Roser et al., 2014](#); [Roser and Ricca, 2015](#)) and DFT computed ([Ricca et al., 2013](#)) spectra of a number of PAH clusters.

PAHdb models and software have matured considerably over the past few years, with the IDL<sup>3</sup> Suite of tools<sup>4</sup> having seen many optimizations, e.g., caching of applied emission model results, which is necessary to be able to deal with the ever-increasing number of spectra in PAHdb's libraries. Given IDL's non-free and proprietary nature, software development has been moved to Python<sup>5</sup>. Most recently, all PAH emission models have been ported from IDL to Python. Furthermore, the rudimentary set of online tools, which are implemented using a backend written in C++<sup>6</sup>, have been expanded to now allow a PAH emission model to be applied to the laboratory-measured data. This is achieved through the use of an empirical approximation for the PAH cooling rate (see [Bakes et al., 2001](#)).

For the astronomical (PAH) community to be able to effectively use PAHdb data, models and (software) tools, complete and up-to-date documentation is paramount. Documentation on using the PAHdb website, software, and a cookbook with data analyzes recipes can be found via the PAHdb Documentation Portal<sup>7</sup>. In addition a dedicated YouTube channel<sup>8</sup> offers a number of background and tutorial videos. The number of available videos will be expanded over time.

A paper is being prepared for publication in The Astrophysical Journal Supplement Series

<sup>2</sup>[github.com/PAHdb](https://github.com/PAHdb)

<sup>3</sup>[www.l3harrisgeospatial.com/Software-Technology/IDL](http://www.l3harrisgeospatial.com/Software-Technology/IDL)

<sup>4</sup>[github.com/pahdb/AmesPAHdbIDLSuite](https://github.com/pahdb/AmesPAHdbIDLSuite)

<sup>5</sup>[github.com/pahdb/AmesPAHdbPythonSuite](https://github.com/pahdb/AmesPAHdbPythonSuite)

<sup>6</sup>[github.com/PAHdb/PAHdb/Backend](https://github.com/PAHdb/PAHdb/Backend)

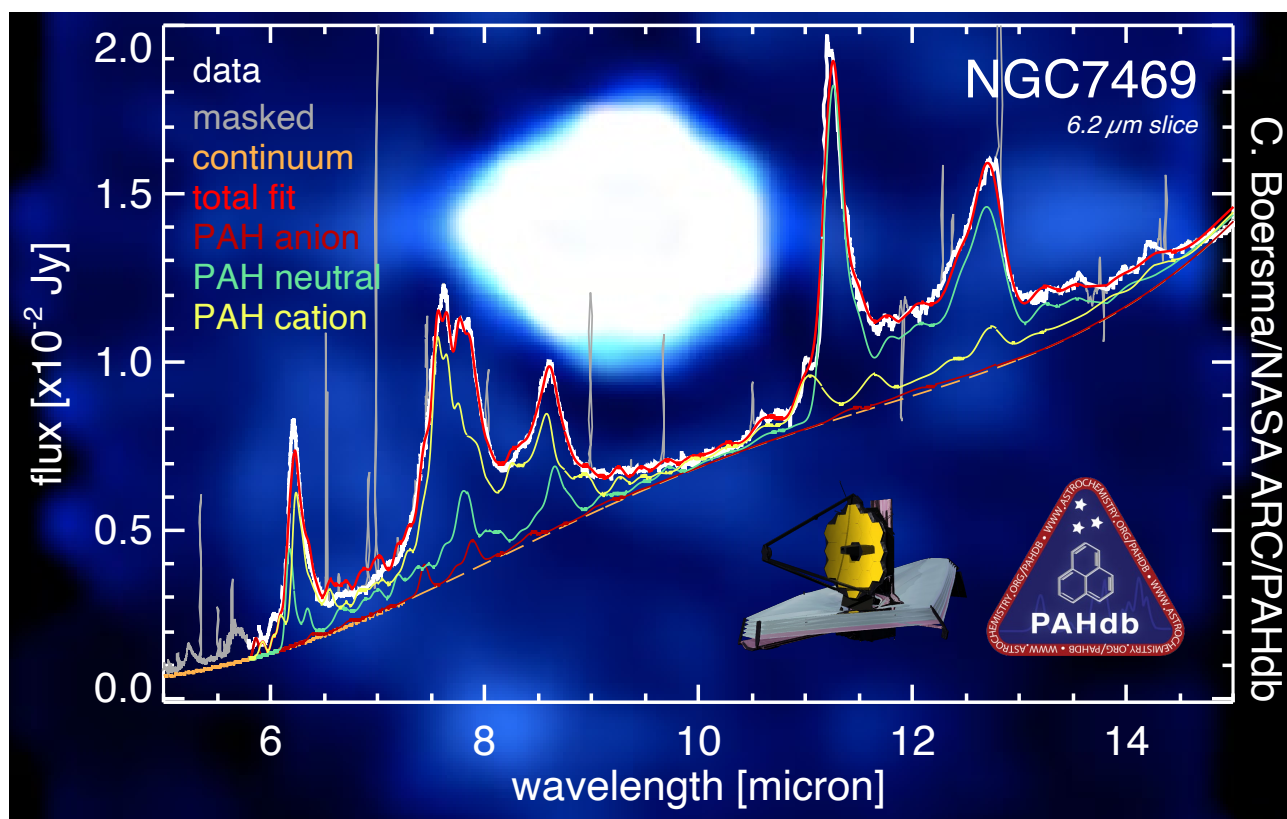
<sup>7</sup>[pahdb.github.io](https://pahdb.github.io)

<sup>8</sup>[www.youtube.com/@pahdb](https://www.youtube.com/@pahdb)

describing the latest updates and improvements to PAHdb (Ricca et al. in prep.).

## JWST and PAHdb

The JWST Early Release Science (ERS) PDRs4All<sup>9</sup> program (Berné et al., 2022) has observed the famous Orion Bar in exquisite detail (see also AstroPAH 49). One of the deliverables of the ERS PDRs4All program is the pyPAHdb<sup>10</sup> tool. PyPAHdb can readily fit the PAH component of a spectrum and break the emission down in terms of PAH charge and size. It is written in Python and uses a pre-computed matrix of PAH emission spectra. This matrix is based on data from version 3.00 of PAHdb's library of theoretically computed PAH spectra and has an emission model with fixed parameters applied. For more control over the choice of emission model and its parameters, the suite of IDL or Python tools can be used. PyPAHdb has been developed with the need to deal with large spectral mosaics in mind. As such, pyPAHdb was able to process the Orion Bar MIRI-MRS spectral cube consisting of some 4,000 spaxels with an actual spectrum, each holding  $\sim 20,000$  wavelength elements, in less than 90 minutes (Maragkoudakis et al. in prep.). PyPAHdb was presented and described at the 2018 SciPy conference (Shannon and Boersma, 2018).



**Figure 3** – PAHdb-fit to the PAH component of a MIRI-MRS spectrum of the interacting galaxy NGC7469 from JWST ERS program 1328, broken down in terms of PAH charge. The backdrop shows the 6.2  $\mu\text{m}$  slice of the spectral cube.

Figure 3 shows the fit to a 5.8-15  $\mu\text{m}$  JWST MIRI-MRS spectrum of the interacting galaxy NGC7469 from ERS program 1328. The fit was performed using the suite of PAHdb tools written in IDL and spectra from an upcoming release of PAHdb's library of computed

<sup>9</sup>[pdrs4all.org](http://pdrs4all.org)

<sup>10</sup>[github.com/PAHdb/pyPAHdb](https://github.com/PAHdb/pyPAHdb)



spectra that includes spectra from PAHs with varying edge structures (Ricca et al. in prep.). Compared to that presented in [AstroPAH 27](#), the quality of the fit here has significantly improved. Notably, the 6.2  $\mu\text{m}$  PAH band is now well-matched, as is the 10-15  $\mu\text{m}$  emission, and the need for PAH anions has been drastically reduced. The fit demonstrates how the 6-9  $\mu\text{m}$  PAH emission is carried predominantly by cations and that between 10-15  $\mu\text{m}$  by neutrals.

JWST General Observer (GO) Cycle 1 program 1591 titled “NIRSpec IFU: Deuterated PAHs, PAH-nitriles, and PAH Overtone and Combination Bands” observed 7 objects along the low-mass stellar life cycle with PAH emission. Many unique, but weak, PAH features are predicted in the 1-5  $\mu\text{m}$  region ([Allamandola et al., 2021](#), and references therein). However, due to its low intrinsic intensity, this region of the spectrum has been often overlooked. The NIRSpec Integral Field Unit (IFU) onboard JWST changes this. The first observations of GO program 1591 were taken September, 2022 and the final in May, 2023. The data show a wealth of features in the spectra, including the 3  $\mu\text{m}$  PAH complex, a PAH-continuum, and atomic and molecular emission lines from H I, He, H<sub>2</sub> and other species. CO<sub>2</sub>-ice absorption and CO emission is also seen. Multi-component decomposition reveals a possible aliphatic deuterated PAH feature. Clear signs of the overtone of the 3.3  $\mu\text{m}$  PAH band, aromatic deuterated PAH feature, and cyano-PAH emission appear to be absent. A paper taking a first look at these data has been submitted to *The Astrophysical Journal* for publication (Boersma et al. submitted).

Anharmonic effects particularly influence the 1-5  $\mu\text{m}$  PAH spectrum, but also impact shoulders, wings, and relative strengths of longer wavelength bands. DFT computed PAH spectra that take into account the effects of anharmonicity provide the only means for properly interpreting the NIRSpec data and longer wavelength PAH band profiles. Pure, deuterated-, and cyano-PAH *full-cascade emission* spectra are being computed to meet this need and are to be eventually included into a PAHdb library (Esposito et al. submitted).

In conclusion, astronomical PAH research, PAHdb, and JWST go hand-in-hand to get the most out of these exciting times.



**Dr. Christiaan Boersma** is a Sr. Research Scientist at NASA Ames Research Center, California, USA. Dr. Boersma is Lead of the NASA Ames PAH IR Spectroscopic Database and Deputy Lead of the Laboratory Astrophysics Directed Work Package at NASA Ames. He is involved with various initiatives for making Laboratory Astrophysics and Planetary Science data, including associated tools, available to the community. This encompasses the NASA Ames PAH IR Spectroscopic Database ([PAHdb](#)), the Optical Constants Database ([OCdb](#)) and the NASA Raman Database ([Ramdb](#)). Dr. Boersma has been Treasurer of the Laboratory Astrophysics Divisions (LAD) of the American Astronomical Society (AAS) since 2019.

**Email:** [Christiaan.Boersma@nasa.gov](mailto:Christiaan.Boersma@nasa.gov)

## References

- J.S. Spilker, K. A. Phadke, M. Aravena, M. Archipley, M.B. Bayliss, J.E. Birkin, M. Béthermin, J. Burgoyne, J. Cathey, S.C. Chapman, H. Dahle, A.H. Gonzalez, G. Gururajan, C.C. Hayward, Y.D. Hezaveh, R. Hill, T.A. Hutchison, K.J. Kim, S. Kim, D. Law, R. Legin, M.A. Malkan, D.P. Marrone, E.J. Murphy, D. Narayanan, A. Navarre, G.M. Olivier, J.A. Rich, J.R. Rigby, C. Reuter, J.E. Rhoads, K. Sharon, J.D.T. Smith, M.I. Solimano, N. Sulzenauer, J.D. Vieira, D. Vizgan, A. Weiß, and K.E. Whitaker. *Spatial variations in aromatic hydrocarbon emission in a dust-rich galaxy.* *Nature*, Jun 2023. doi: 10.1038/s41586-023-05998-6.
- P. Woods. *Complex molecules in an early galaxy.* *Nature Astronomy*, 7(6):641–641, Jun 2023. doi: 10.1038/s41550-023-02021-w.
- J. Cami, J. Bernard-Salas, E. Peeters, and S. E. Malek. *Detection of C<sub>60</sub> and C<sub>70</sub> in a Young Planetary Nebula.* *sc*, 329:1180–, September 2010. doi: 10.1126/science.1192035.
- K. Sellgren, M. W. Werner, J. G. Ingalls, J. D. T. Smith, T. M. Carleton, and C. Joblin. *C<sub>60</sub> in Reflection Nebulae.* *apjl*, 722:L54–L57, October 2010. doi: 10.1088/2041-8205/722/1/L54.
- B. A. McGuire, A. M. Burkhardt, S. Kalenskii, C. N. Shingledecker, A. J. Remijan, E. Herbst, and M. C. McCarthy. *Detection of the Aromatic Molecule Benzonitrile (c-C<sub>6</sub>H<sub>5</sub>CN) in the Interstellar Medium.* *sc*, 359:202, January 2018. doi: 10.1126/science.aao4890.
- Brett A. McGuire, Ryan A. Loomis, Andrew M. Burkhardt, Kin Long Kelvin Lee, Christopher N. Shingledecker, Steven B. Charnley, Ilsa R. Cooke, Martin A. Cordiner, Eric Herbst, Sergei Kalenskii, Mark A. Siebert, Eric R. Willis, Ci Xue, Anthony J. Remijan, and Michael C. McCarthy. *Detection of two interstellar polycyclic aromatic hydrocarbons via spectral matched filtering.* *sc*, 371(6535):1265–1269, March 2021. doi: 10.1126/science.abb7535.
- E. Maltseva, A. Petrignani, A. Candian, C. J. Mackie, X. Huang, T. J. Lee, A. G. G. M. Tielens, J. Oomens, and W. J. Buma. *High-resolution IR Absorption Spectroscopy of Polycyclic Aromatic Hydrocarbons: The Realm of Anharmonicity.* *apj*, 814:23, November 2015. doi: 10.1088/0004-637X/814/1/23.
- Ozan Lacinbala, Géraldine Féraud, Julien Vincent, and Thomas Pino. *Aromatic and Acetylenic C–H or C–D Stretching Bands Anharmonicity Detection of Phenylacetylene by UV Laser-Induced Vibrational Emission.* *Journal of Physical Chemistry A*, 126(30):4891–4901, August 2022. doi: 10.1021/acs.jpca.2c01436.
- C. J. Mackie, A. Candian, X. Huang, E. Maltseva, A. Petrignani, J. Oomens, W. J. Buma, T. J. Lee, and A. G. G. M. Tielens. *The anharmonic quartic force field infrared spectra of three polycyclic aromatic hydrocarbons: Naphthalene, anthracene, and tetracene.* *jcp*, 143:224314, December 2015. doi: 10.1063/1.4936779.
- C. J. Mackie, A. Candian, X. Huang, E. Maltseva, A. Petrignani, J. Oomens, A. L. Mattioda, W. J. Buma, T. J. Lee, and A. G. G. M. Tielens. *The anharmonic quartic force field infrared spectra of five non-linear polycyclic aromatic hydrocarbons: Benz[a]anthracene, chrysene, phenanthrene, pyrene, and triphenylene.* *jcp*, 145:084313, August 2016. doi: 10.1063/1.4961438.
- C. J. Mackie, T. Chen, A. Candian, T. J. Lee, and A. G. G. M. Tielens. *Fully anharmonic infrared cascade spectra of polycyclic aromatic hydrocarbons.* *jcp*, 149(13):134302, October 2018. doi: 10.1063/1.5038725.
- C. J. Mackie, A. Candian, T. J. Lee, and A. G. G. M. Tielens. *Anharmonicity and the IR Emission Spectrum of Neutral Interstellar PAH Molecules.* *J. Phys. Chem. A*, 126(20):3198–3209, May 2022. doi: 10.1021/acs.jpca.2c01849.
- C. W. Bauschlicher, C. Boersma, A. Ricca, A. L. Mattioda, J. Cami, E. Peeters, F. Sánchez de Armas, G. Puerta Saborido, D. M. Hudgins, and L. J. Allamandola. *The NASA Ames Polycyclic Aromatic Hydrocarbon Infrared Spectroscopic Database: The Computed Spectra.* *apjss*, 189:341–351, August 2010. doi: 10.1088/0067-0049/189/2/341.



- C. Boersma, C. W. Bauschlicher, A. Ricca, A. L. Mattioda, J. Cami, E. Peeters, F. Sánchez de Armas, G. Puerta Saborido, D. M. Hudgins, and L. J. Allamandola. *The NASA Ames PAH IR Spectroscopic Database Version 2.00: Updated Content, Web Site, and On(Off)line Tools*. *apjss*, 211:8, 2014. doi: 10.1088/0067-0049/211/1/8.
- C. W. Bauschlicher, Jr., A. Ricca, C. Boersma, and L. J. Allamandola. *The NASA Ames PAH IR Spectroscopic Database: Computational Version 3.00 with Updated Content and the Introduction of Multiple Scaling Factors*. *apjss*, 234:32, February 2018. doi: 10.3847/1538-4365/aaa019.
- A. L. Mattioda, D. M. Hudgins, C. Boersma, C. W. Bauschlicher, A. Ricca, J. Cami, E. Peeters, F. Sánchez de Armas, G. Puerta Saborido, and L. J. Allamandola. *The NASA Ames PAH IR Spectroscopic Database: The Laboratory Spectra*. *apjss*, 251(2):22, December 2020. doi: 10.3847/1538-4365/abc2c8.
- A. Ricca, J. E. Roser, E. Peeters, and C. Boersma. *Polycyclic Aromatic Hydrocarbons with Armchair Edges: Potential Emitters in Class B Sources*. *apj*, 882(1):56, September 2019. doi: 10.3847/1538-4357/ab3124.
- J. E. Roser and L. J. Allamandola. *Infrared Spectroscopy of Naphthalene Aggregation and Cluster Formation in Argon Matrices*. *apj*, 722(2):1932–1938, October 2010. doi: 10.1088/0004-637X/722/2/1932.
- J. E. Roser, A. Ricca, and L. J. Allamandola. *Anthracene Clusters and the Interstellar Infrared Emission Features*. *apj*, 783:97, March 2014. doi: 10.1088/0004-637X/783/2/97.
- J. E. Roser and A. Ricca. *PAH Clusters as Sources of Interstellar Infrared Emission*. *apj*, 801:108, March 2015. doi: 10.1088/0004-637X/801/2/108.
- A. Ricca, C. W. Bauschlicher, Jr., and L. J. Allamandola. *The Infrared Spectroscopy of Neutral Polycyclic Aromatic Hydrocarbon Clusters*. *apj*, 776:31, October 2013. doi: 10.1088/0004-637X/776/1/31.
- E. L. O. Bakes, A. G. G. M. Tielens, and C. W. Bauschlicher, Jr. *Theoretical Modeling of Infrared Emission from Neutral and Charged Polycyclic Aromatic Hydrocarbons. I*. *apj*, 556:501–514, July 2001. doi: 10.1086/321501.
- O. Berné, É. Habart, E. Peeters, A. Abergel, E. A. Bergin, J. Bernard-Salas, E. Bron, J. Cami, S. Cazaux, E. Dartois, A. Fuente, J. R. Goicoechea, K. D. Gordon, Y. Okada, T. Onaka, M. Robberto, M. Röllig, A. G. G. M. Tielens, S. Vicente, M. G. Wolfire, F. Alarcon, C. Boersma, A. Canin, R. Chown, D. Dicken, D. Languignon, R. Le Gal, M. W. Pound, B. Trahin, T. Simmer, A. Sidhu, D. Van De Putte, S. Cuadrado, C. Guilloteau, A. Maragkoudakis, B. R. Scheffer, T. Schirmer, I. Aleman, L. J. Allamandola, R. Auchettl, G. A. Baratta, S. Bejaoui, P. P. Bera, G. Bilalbegovic, J. H. Black, F. Boulanger, J. Bouwman, B. Brandl, P. Brechignac, S. Brunken, A. Burkhardt, A. Candian, J. Cernicharo, M. Chabot, S. Chakraborty, J. Champion, S. W. J. Colgan, I. R. Cooke, A. Coutens, N. L. J. Cox, K. Demyk, J. Donovan Meyer, C. Engrand, S. Foschino, P. Garcia-Lario, L. Gavilan, M. Gerin, M. Godard, C. A. Gottlieb, P. Guillard, A. Gusdorf, P. Hartigan, J. He, E. Herbst, L. Hornekaer, C. Jaeger, E. Janot-Pacheco, C. Joblin, M. Kaufman, F. Kemper, S. Kendrew, M. S. Kirsanova, P. Klaassen, C. Knight, S. Kwok, A. Labiano, T. S. Y. Lai, T. J. Lee, B. Lefloch, F. Le Petit, A. Li, H. Linz, C. J. Mackie, S. C. Madden, J. Mascetti, B. A. McGuire, P. Merino, E. R. Micelotta, K. Misselt, J. A. Morse, G. Mulas, N. Neelamkodan, R. Ohsawa, A. Omont, R. Paladini, M. E. Palumbo, A. Pathak, Y. J. Pendleton, A. Petrignani, t. Pino, E. Puga, N. Rangwala, M. Rapacioli, A. Ricca, J. Roman-Duval, J. E. Roser, E. Roueff, G. Rouille, F. Salama, D. A. Sales, K. Sandstrom, P. Sarre, E. M. Sciamma-O'Brien, K. Sellgren, M. J. Shannon, S. S. Shenoy, D. Teyssier, R. D. Thomas, A. Togi, L. Verstraete, A. N. Witt, A. Wootten, N. Ysard, H. Zettergren, Y. Zhang, Z. E. Zhang, and J. Zhen. *PDRs4All: A JWST Early Release Science Program on radiative feedback from massive stars*. *pasp*, 134(1035):054301, May 2022. doi: 10.1088/1538-3873/ac604c.
- M. J. Shannon and C. Boersma. *Organic Molecules in Space: Insights from the NASA Ames Molecular Database in the era of the James Webb Space Telescope*. page 99. *SciPy*, 2018. doi: 10.25080/majora-4af1f417-00f.

*L. J. Allamandola, C. Boersma, T. J. Lee, J. D. Bregman, and P. Temi. PAH Spectroscopy from 1 to 5  $\mu\text{m}$ . *apjl*, 917(2):L35, aug 2021. doi: 10.3847/2041-8213/ac17f0.*





# Abstracts

## Catalytic role of HI in the interstellar synthesis of complex organic molecule

Shuming Yang<sup>1</sup>, Peng Xie<sup>2</sup>, Enwei Liang<sup>1</sup>, and Zhao Wang<sup>1</sup>

<sup>1</sup>Laboratory for Relativistic Astrophysics, Department of Physics, Guangxi University, Nanning 530004, China

<sup>2</sup>School of Chemistry and Chemical Engineering, Guangxi University, Nanning 530004, China

It has long been believed that the formation of biomolecules from closed-shell species in the gas phase of interstellar space is challenging due to the high temperature needed to activate the process. As a result, previous studies have predominantly focused on ion-molecule reactions or neutral-neutral reactions involving highly reactive radicals. This viewpoint does not entirely align with the astronomical observation that the majority of interstellar molecules detected so far are neutral species with closed shells. Consequently, researchers have explored catalyzed reactions as an alternative approach to synthesize complex interstellar molecules. However, the limited abundance of suggested catalysts often renders catalyzed reactions seemingly impossible in the ISM, since they require the simultaneous collision of three bodies.

Fortunately, this is not always the case, particularly when the concentration of the catalyst significantly exceeds that of the reactants, as neutral atomic hydrogen (HI). By utilizing quantum chemical calculations, we modeled the pathways involved in generating adenine and guanine in the gas-phase interstellar environment encompassed by HI. We discovered that the presence of HI leads to alternative pathways that substantially decrease the energy barriers for reactions, resulting in a significant enhancement of the reaction rate. Consequently, these reactions become thermodynamically feasible in star-forming regions where reactants have been observed. Our findings indicate that HI can effectively serve as a catalyst for organic synthesis in interstellar space, suggesting that HI-catalyzed reactions could represent a significant mechanism for the interstellar formation of complex organic molecules from species with closed shells.

E-mail: [zw@gxu.edu.cn](mailto:zw@gxu.edu.cn)

Res. Astron. Astrophys., **23**:055019 (2023)

<https://doi.org/10.1088/1674-4527/accb25>

<http://arxiv.org/abs/2305.11409>

# The Astroduct+PAH Model: A Unified Description of the Extinction, Emission, and Polarization from Dust in the Diffuse Interstellar Medium

Brandon S. Hensley<sup>1</sup> and B. T. Draine<sup>1</sup>

<sup>1</sup>Department of Astrophysical Sciences, Princeton University, Princeton, NJ 08544, USA

We present a new model of interstellar dust in which large grains are a single composite material, “astroduct”, and nanoparticle-sized grains come in distinct varieties including polycyclic aromatic hydrocarbons (PAHs). We argue that a single-composition model for grains larger than  $\sim 0.02\ \mu\text{m}$  most naturally explains the lack of frequency dependence in the far-infrared (FIR) polarization fraction and the characteristic ratio of optical to FIR polarization. We derive a size distribution and alignment function for 1.4:1 oblate astroduct grains that, with PAHs, reproduce the mean wavelength dependence and polarization of Galactic extinction and emission from the diffuse interstellar medium while respecting constraints on solid phase abundances. All model data and Python-based interfaces are made publicly available.

E-mail: [bhensley@astro.princeton.edu](mailto:bhensley@astro.princeton.edu)

Astrophys. J., **948**:55 (2023)

<https://ui.adsabs.harvard.edu/abs/2023ApJ...948...55H/abstract>

<https://doi.org/10.3847/1538-4357/acc4c2>

# Gas phase hydrogenated and deuterated fullerene cations

Xiaoyi Hu<sup>1,2,3</sup>, Zhenru Dong<sup>1,2</sup>, Yanan Ge<sup>1,2</sup>, Jia Liu<sup>1,2</sup>, Yang Chen<sup>3</sup>, Junfeng Zhen<sup>1,2,4</sup>, and Liping Qin<sup>1,2</sup>

<sup>1</sup>Deep Space Exploration Laboratory / CAS Key Laboratory of Crust-Mantle Materials and Environment, University of Science and Technology of China, Hefei 230026, China

<sup>2</sup>CAS Center for Excellence in Comparative Planetology, University of Science and Technology of China, Hefei 230026, China

<sup>3</sup>CAS Center for Excellence in Quantum Information and Quantum Physics, Hefei National Laboratory for Physical Sciences at the Microscale, and Department of Chemical Physics, University of Science and Technology of China, Hefei 230026, China

<sup>4</sup>CAS Key Laboratory for Research in Galaxies and Cosmology, Department of Astronomy, University of Science and Technology of China, Hefei 230026, China

H/D accretion, especially onto ionized fullerenes, is expected to be very efficient in space. In this work, we study hydrogenated and deuterated fullerene cations and their photodissociation behavior in the gas phase. The experimental results show that hydrogenated fullerene cations (i.e.,  $[C_{60}H_n]^+$  and  $[C_{70}H_n]^+$ ,  $n$  up to 30) and deuterated fullerene cations (i.e.,  $[C_{60}D_n]^+$  and  $[C_{70}D_n]^+$ ,  $n$  up to 21) are formed efficiently through the ion-atom collision reaction pathway. Upon irradiation, the hydrogenated and deuterated fullerene cations dissociate into fullerene cations and H/H<sub>2</sub> or D/D<sub>2</sub> species. The structures of the newly formed hydrogenated and deuterated fullerene cations (C<sub>58</sub> and C<sub>60</sub>) and the bonding energies for these reaction pathways are investigated by means of quantum chemical calculations. The competition between hydrogenation and dehydrogenation is confirmed, and the hydrogenation-to-dehydrogenation ratio in the accretion processes in the gas phase is determined. We infer that the proportion of accreted hydrogen and deuterium atoms on the surface of fullerenes is similar as that of hydrogen and deuterium atoms in the interstellar environment where these fullerenes are located, especially when the interstellar environments are similar to our experimental conditions, i.e., the hot environment.

E-mail: jfzhen@ustc.edu.cn

Res. Astron. Astrophys., Forthcoming Article (2023)

<https://doi.org/10.1088/1674-4527/acd994>

# PAH Emission Features in Star Forming Regions and Late Type Stars

Rahul Kumar Anand<sup>1</sup>, Shantanu Rastogi<sup>1</sup>, and Brijesh Kumar<sup>2</sup>

<sup>1</sup>Department of Physics, DDU Gorakhpur University, Gorakhpur 273009, India

<sup>2</sup>Aryabhata Research Institute of Observational Sciences, Manora Peak, Nainital-263001, India

Mid infrared emission spectra, obtained from ISO archive, of thirteen astrophysical objects as well as computed spectra of 27 polycyclic aromatic hydrocarbon (PAH) molecules are studied. All the objects show strong aromatic infrared band (AIB) features with variations that correlate with object type. Based on AIB peak positions the features for IRC +10216, Monoceros R2, IC 5117 and PN-SwSt 1 are classified as type 'A', 'B' or 'C' for the first time. The AIBs at 6.2, 7.7 and 11.2  $\mu\text{m}$  are used to obtain band intensity ratios for 6.2/7.7 and 11.2/6.2, which respectively indicate PAH size as number of carbon atoms and the ionization conditions of the medium. The smaller value of 6.2/7.7 points towards the presence of large PAH molecules while higher value of 11.2/6.2 ratio relate to harsh conditions around the object. In general, for star forming regions the 6.2/7.7 band ratio obtained is  $>1$  and the 11.2/6.2 ratio is  $>2$ , while for late type carbon stars these values are  $<1$  and  $<2$ . This indicates that small/medium sized ionized PAHs are likely in star forming regions and large PAHs in evolved stars. For each of the 27 plain PAH molecules, the integrated intensity in these bands is obtained from the computed infrared spectra and the band ratios calculated. The ratio 6.2/7.7 in several computed medium and large sized PAH cations is in the range of observed ratio in most objects, but some molecules show large variations in band ratios, indicating that PAHs possible in ISM could be more complex and with irregular structures.

E-mail: shantanu.r@hotmail.com

J. Astrophys. Astron., **44**:47 (2023)

<https://www.ias.ac.in/article/fulltext/joaa/044/0047>

<https://doi.org/10.1007/s12036-023-09941-z>



# Processing of methane and acetylene ices by galactic cosmic rays and implications to the color diversity of Kuiper Belt objects

Chaojiang Zhang<sup>1,2</sup>, Cheng Zhu<sup>1,2</sup>, Andrew M. Turner<sup>1,2</sup>, Ivan O. Antonov<sup>1,2</sup>, Adrien D. Garcia<sup>3</sup>, Cornelia Meinert<sup>3</sup>, Leslie A. Young<sup>4</sup>, David C. Jewitt<sup>5</sup>, and Ralf I. Kaiser<sup>1,2</sup>

<sup>1</sup>Department of Chemistry, University of Hawaii at Mānoa, Honolulu, HI 96822, USA

<sup>2</sup>W.M. Keck Laboratory in Astrochemistry, University of Hawaii at Mānoa, Honolulu, HI 96822, USA

<sup>3</sup>Université Côte d'Azur, Institut de Chimie de Nice, UMR 7272 CNRS, Nice 06108, France

<sup>4</sup>Department of Space Studies, Southwest Research Institute, Boulder, CO 80302, USA

<sup>5</sup>Department of Earth and Space Sciences, University of California, Los Angeles, Los Angeles, CA 90095, USA

Kuiper Belt objects exhibit a wider color range than any other solar system population. The origin of this color diversity is unknown, but likely the result of the prolonged irradiation of organic materials by galactic cosmic rays (GCRs). Here, we combine ultrahigh-vacuum irradiation experiments with comprehensive spectroscopic analyses to examine the color evolution during GCR processing methane and acetylene under Kuiper Belt conditions. This study replicates the colors of a population of Kuiper Belt objects such as Makemake, Orcus, and Salacia. Aromatic structural units carrying up to three rings as in phenanthrene (C<sub>14</sub>H<sub>10</sub>), phenalene (C<sub>9</sub>H<sub>10</sub>), and acenaphthylene (C<sub>12</sub>H<sub>8</sub>), of which some carry structural motives of DNA and RNA connected via unsaturated linkers, were found to play a key role in producing the reddish colors. These studies demonstrate the level of molecular complexity synthesized of GCR processing hydrocarbon and hint at the role played by irradiated ice in the early production of biological precursor molecules.

E-mail: ralfk@hawaii.edu

Sci. Adv., **9**:eadg6936 (2023)

<https://www.science.org/doi/10.1126/sciadv.adg6936>

# Spatial variations in aromatic hydrocarbon emission in a dust-rich galaxy

Justin Spilker<sup>1</sup>, Kedar Phadke<sup>2</sup>, and the JWST TEMPLATES Early Release Science team<sup>3</sup>

<sup>1</sup>Department of Physics and Astronomy and George P. and Cynthia Woods Mitchell Institute for Fundamental Physics and Astronomy, Texas A&M University, USA

<sup>2</sup>Department of Astronomy, University of Illinois, USA

<sup>3</sup><https://sites.google.com/view/jwst-templates/>

Dust grains absorb half of the radiation emitted by stars throughout the history of the universe, re-emitting this energy at infrared wavelengths. Polycyclic aromatic hydrocarbons (PAHs) are large organic molecules that trace millimeter-size dust grains and regulate the cooling of the interstellar gas within galaxies. Observations of PAH features in very distant galaxies have been difficult due to the limited sensitivity and wavelength coverage of previous infrared telescopes. Here we present JWST observations that detect the 3.3 $\mu\text{m}$  PAH feature in a galaxy observed less than 1.5 billion years after the Big Bang. The high equivalent width of the PAH feature indicates that star formation, rather than black hole accretion, dominates the infrared emission throughout the galaxy. The light from PAH molecules, large dust grains, and stars and hot dust are spatially distinct from one another, leading to order-of-magnitude variations in the PAH equivalent width and the ratio of PAH to total infrared luminosity across the galaxy. The spatial variations we observe suggest either a physical offset between the PAHs and large dust grains or wide variations in the local ultraviolet radiation field. Our observations demonstrate that differences in the emission from PAH molecules and large dust grains are a complex result of localized processes within early galaxies.

We used the JWST MIRI instrument to detect the 3.3/ $\mu\text{m}$  PAH feature in the  $z=4.22$  galaxy SPT0418-47, now the most distant detection of any PAH feature and by far the highest-redshift detection of the 3.3/ $\mu\text{m}$  feature. PAH emission has been suggested as a useful indicator of the star formation rates of galaxies, and our JWST program aimed (in part) to determine whether the 3.3/ $\mu\text{m}$  features could be used as such for high-redshift galaxies. We found order-of-magnitude variations in the ratio of PAH to total infrared luminosity in different regions of the galaxy. Whether these variations are common in high-redshift galaxies, as well as their physical origin, will continue to be investigated in the future. These data were acquired as part of the TEMPLATES Early Release Science program and are publicly available, and a python notebook detailing the data processing is available from the collaboration github page.

E-mail: [jspilker@tamu.edu](mailto:jspilker@tamu.edu)

Nature, **123**:000 (2023)

<https://www.nature.com/articles/s41586-023-05998-6>

<https://github.com/JWST-Templates/Notebooks>



# Meetings

## Surveying the Milky Way The Universe in Our Own Backyard

**Pasadena, CA - USA  
23–27 October, 2023**

<https://conference.ipac.caltech.edu/milkywaysurveys/>

### **Overview:**

We are pleased to announce the conference “Surveying the Milky Way: The Universe in Our Own Backyard”, to be held October 23–27, 2023, on the Caltech campus in Pasadena, CA. This conference is organized by IPAC, which is part of Caltech.

The goal of the conference is to highlight the role of modern surveys of the Milky Way in bridging our knowledge of Galactic star formation and the interstellar medium, the structure of the Galaxy, stellar astrophysics and time domain astronomy with information on extragalactic systems. The conference will also be an occasion to celebrate IPAC’s historical involvement in surveys that greatly advanced our understanding of the Galaxy, with missions such as 2MASS, IRAS, WISE and Spitzer.

### **Themes will include:**

- Star Formation and ISM
- Structure of the Galaxy
- Metallicity and Merging History
- The Galactic Center
- Time Domain Astronomy
- Surveys of the Milky Way

### **List of Invited Speakers:**

Rachel Akeson (Caltech-IPAC)  
Sean Carey (Caltech-IPAC)  
David Elia (INAF, Italy)  
Neal Evans (University of Texas at Austin)  
Claude-Andre Faucher Giguere (University of Northwestern)  
Adam Ginsburg (University of Florida)  
Mark Krumholz (Australian National University)  
Jorge Pineda (JPL)  
Mattia Sormani (Heidelberg University, Germany)

Jiayi Sun (MacMaster University, Canada)  
Gail Zasowski (University of Utah)  
Catherine Zucker (STScI)

### **Registration and Abstracts Submission:**

The registration for the conference opened on June 1. We welcome abstracts for proposed contributed talks and for posters.

#### *Important dates:*

<i>June 30</i>	abstract deadline for contributed talks
<i>August 21</i>	conference program published
<i>August 25</i>	deadline for regular in-person meeting registration
<i>September 15</i>	abstract deadline for posters
<i>September 22</i>	deadline for late in-person meeting registration
<i>October 16</i>	deadline for online meeting registration

To register and submit an abstract, please visit [our website](#).

### **Hybrid Format:**

We strongly encourage in-person participation; we can accommodate about 300 participants in the Caltech Ramo Auditorium. Caltech requires all in-person attendees to have received a WHO-recognized COVID-19 vaccine and booster. Currently, masks are not required indoors, but we will inform you if requirements change.

We will also enable online attendance. We do charge online participants a nominal registration fee to offset the costs of the virtual platforms. The registration deadline for remote participants is October 16. To register, please visit [our website](#).

### **Activities for Early Career Researchers:**

We are planning to organize lunches with the invited speakers in order to bring together more senior with early career scientists. We will provide more information closer to the conference date.

### **Social Dinner:**

We will have an optional social dinner on Wednesday, October 25, at the Mexican restaurant [Mijares](#). When registering for the conference, there will be an option for purchasing a ticket for the dinner. Please note that the dinner is limited to 100 attendees (first come, first served).

### **Accommodations:**

We have reserved a block of rooms at the [Hyatt Hotel in Pasadena](#). The deadline to book a room is 9/25/2023.

**E-mail for contact:** [mw2023@lists.ipac.caltech.edu](mailto:mw2023@lists.ipac.caltech.edu)





# Announcements

## PhD positions Molecular Physics / Physical Chemistry Laboratory Astrophysics

**Advertised by Otto Dopfer**

A fully funded PhD position (3 years) from DFG (German Science Foundation) is available in the laser molecular spectroscopy group of Otto Dopfer at the Berlin Institute of Technology (TU Berlin), Germany. The funded project involves the IR and electronic characterization of diamondoid cations and their derivatives and clusters using laser spectroscopic, mass spectrometric, and quantum chemical methods.

The laboratory astrochemistry work is strongly related to the problem of the diffuse interstellar bands (DIBs), the unidentified/aromatic IR emission bands (UIR/AIB) and hydrocarbon chemistry in water ices. Available equipment on our laboratory astrochemistry group includes a variety of pulsed and tuneable IR and UV lasers, several ion sources and cryogenic rf-traps, as well as several types of tandem mass spectrometers.

Previous papers of the group in this field include:

- Angew. Chem. Int. Ed. 51, 4925-4929 (2012) DOI: [10.1002/anie.201108937](https://doi.org/10.1002/anie.201108937)
- Astrophys. J. Lett. 900, L20 (2020), DOI: [10.3847/2041-8213/abafbd](https://doi.org/10.3847/2041-8213/abafbd)
- Astrophys. J. 940, 104 (2022), DOI: [10.3847/1538-4357/ac9733](https://doi.org/10.3847/1538-4357/ac9733)
- Phys. Chem. Chem. Phys. 25, 13593-13610 (2023), DOI: [10.1039/D3CP01514A](https://doi.org/10.1039/D3CP01514A)
- Phys. Chem. Chem. Phys. 25, 5529-5549 (2023), DOI: [10.1039/d2cp04556g](https://doi.org/10.1039/d2cp04556g)
- J. Phys. Chem. Lett. 13, 449-454 (2022), DOI: [10.1021/acs.jpcllett.1c03948](https://doi.org/10.1021/acs.jpcllett.1c03948)

Qualified candidates hold a MSc in Physics, Physical Chemistry, or related fields, with focus on experimental work. Experience in one or more of the following fields is not mandatory but highly advantageous:

1. laser spectroscopy, mass spectrometry, ion sources and traps, cluster science
2. vacuum, optics, data acquisition, construction of apparatus
3. writing of publications and reports
4. strong communication and presentation skills

Interested candidates are encouraged to send their application (in a single pdf file) to Prof. Otto Dopfer (dopfer@physik.tu-berlin.de), including a cover letter, a CV, previous certificates (BSc and MSc), a statement of qualifications relevant for the position (max. 1 page), a statement of research interests (max. 1 page) as well as names and complete addresses of two persons willing to provide reference letters.

Evaluation of the applications will begin at July 31 (2023) and will continue until the position is filled. The desired starting date is as soon as possible but this is negotiable to some extent.

Berlin is an international city and offers an exciting scientific and cultural environment.

**Deadline:** 31 July 2023

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

**Webpage:** <https://www.tu.berlin/en/lmsu>

# Postdoctoral Positions

## Reaction Dynamics & Materials in Extreme Environments

**Advertised by Ralf Kaiser**

The Reaction Dynamics & Materials in Extreme Environments Group, Department of Chemistry, University of Hawai'i at Manoa, invites applications for two Postdoc and/or Visiting Scientist positions in the areas of gas phase reaction dynamics and combustion chemistry. The prime directive of the experimental gas phase studies is to investigate the formation of (precursors to) polycyclic aromatic hydrocarbons (PAHs) (project I) and silicon carbides (project II) exploiting crossed molecular beams coupled with atom/radical sources along with universal, ion-imaging, and laser induced fluorescence detection. The experimental results are merged with electronic structure calculations, dynamics simulations, and astrochemical modeling to eventually untangle the roles of these bimolecular gas phase reactions in the formation of nanoparticles (soot, grains) in combustion flames and deep space (interstellar medium, circumstellar envelopes).

Recent works on our gas phase projects can be found at:

- Sci. Adv., 7, eabg7003 (2021)
- Sci. Adv., 7, eabf0360 (2021)
- Sci. Adv., 7, eabd4044 (2021)
- Sci. Adv., 7, eabd4044 (2021)
- Nat. Commun. 13, 786 (2022)
- JACS, 143, 14227-14234 (2021)
- JACS, 144, 22470-22478 (2022)
- JACS, 144, 8649-8657 (2022)
- JACS, 145, 3084-3091 (2023)
- Angew. Chem. Int. Ed. 62, e202216972 (2023)
- Chem. Sci., 14, 5369-5378 (2023)
- Nat. Commun., 14, 1527 (2023)

The appointment period is initially for one year, but can be renewed annually based on availability of funds and satisfactory progress as defined by first author publications. The salary is competitive and commensurate with experience. Successful applicants should have a strong background in experimental reaction dynamics and laser systems. Experience in LabView, programming, and/or Autocad/SolidWorks is desirable. Solid communication skills in English (written, oral), a publication record in internationally circulated, peer-reviewed journals, and independent working skills are mandatory.

Please send a letter of interest, three letters of recommendation, CV, and publication list to Prof. Ralf I. Kaiser, Department of Chemistry, University of Hawai'i at Manoa, Honolulu, HI 96822, USA [ralfk@hawaii.edu]. Applicants must demonstrate their capability to prepare manuscripts for publications independently. The review of applications will start July 1, 2023, and continues until the position is filled. A description of our research group can be found [here](#). Only complete applications will be reviewed.

**Deadline:** 1 July 2023

**E-mail for contact:** ralfk@hawaii.edu

**Webpage:** <https://www.uhmreactiondynamics.org/>

## AstroPAH Newsletter

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

[astropah@strw.leidenuniv.nl](mailto:astropah@strw.leidenuniv.nl)

Next issue: 20 July 2023

Submission deadline: 7 July 2023