AstroPAH

A Newsletter on Astronomical PAHs

Issue 107 • April 2024

Solar eclipse

Editorial

Dear Colleagues,

Welcome to our new AstroPAH volume no. 107! We hope all of you are healthy and doing well!

Those in North America this past month were able to experience a total solar eclipse on April 8^{th}. This moment was captured and features on our cover picture of the month. Until the next total solar eclipse on August 12, 2026, which will be mostly visible across Europe and Greenland!

The sudden passing of Prof. Harold Linnartz last December left a void in our community, and in honor of his legacy, the Laboratory for Astrophysics at the Leiden Observatory held a memorial symposium on April 13, 2024. A series of talks and short presentations throughout the day paid tribute to Prof. Linnartz's vast and expansive career and scientific contributions. A few of these moments taken from the symposium are part of this month's In Focus. In addition, to continue this tribute, a special issue in honor of Prof. Linnartz in the ACS journal Earth and Space Chemistry has been created. Articles on all aspects of molecular astrophysics are welcome, with a submission deadline on January 1, 2025 (see Announcements for more details).

We are also pleased to share with you more announcements, such as from the NanoSpace Astrochemistry Training School in Groningen, The Netherlands, along with a PhD position advertized by Otto Dopfer at the Berlin Institute of Technology, Germany. Note also the announcement of a special symposium organized by the American Association for Aerosol Research called *Planetary Aerosols: From Earth to Exoplanet*, with the aim to bring Earth and Planetary Science communities to improve our understanding of aerosols and cloud microphysics and chemistry. Abstract deadline will be on May 8, 2024.

We thank you all for your numerous contributions this month ranging from ion radiolysis of α-pinene to the IR absorption of phenylacetylene and a scientific biography of the late Dr. Timothy J. Lee and his legacy.

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: 23 May 2024.
Submission deadline: 10 May 2024.

Contact us:

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http://astropah-news.strw.leidenuniv.nl
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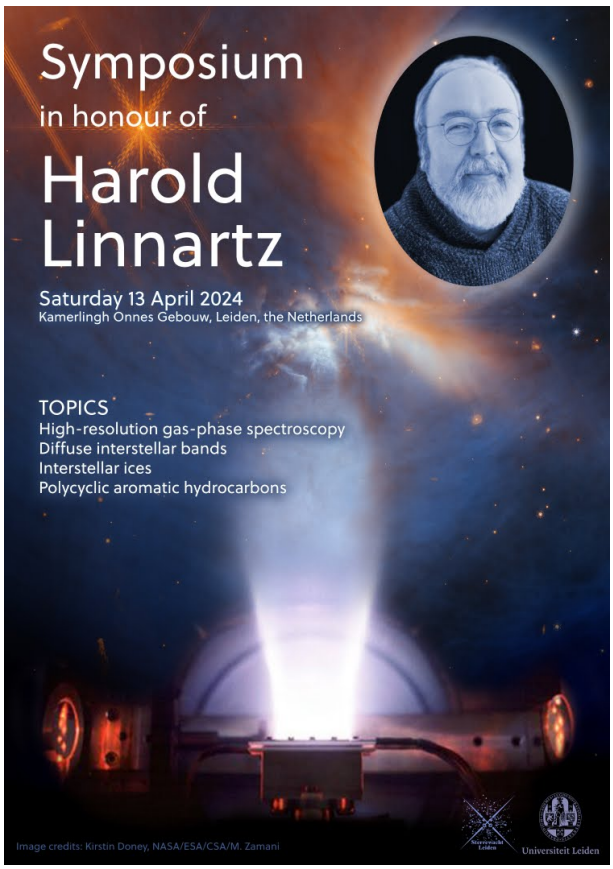
PAH Picture of the Month

The total solar eclipse of April 8, 2024, as observed from near Carbondale, Illinois.

Credits: Amlan Datta.

This newsletter is edited in LaTeX. Newsletter Design by: Isabel Aleman. Image Credits: Background image in this page: NASA, ESA, and the Hubble Heritage Team (STScI/AURA). Headers background: X-ray and optical image composition. X-ray by Chandra: NASA/CXC/Univ.Potsdam/L.Oskinova et al; Optical by Hubble: NASA/STScI; Infrared by Spitzer: NASA/JPL-Caltech.

Symposium in honor of Harold Linnartz



On December 31, 2023 the AstroPAH community unexpectedly and mournfully lost one of its own, Prof. Harold Linnartz, director of the Laboratory for Astrophysics at the Leiden Observatory. In honor of his memory and legacy, a memorial symposium was held in Leiden on April 13, 2024. The symposium was a mixture of 20 min talks and shorter 5 minute pitches where former students, postdocs, and collaborators, shared their fond memories of Harold and his contribution to their scientific and personal endeavors. The mood of the symposium was far from sombre. It was positive and uplifting, where the community Prof. Harold Linnartz worked so hard on building came together to pay its respects and cherish his memory as a scientist who was a pillar of the community.

The recordings of the symposium are now available at:

Morning session: https://video.leidenuniv.nl/media/t/1_0hb71jau

Afternoon session: https://video.leidenuniv.nl/media/t/1_5qwb7u6x

Here we have selected a few snapshots taken during the symposium.

Figure 1 *– Prof. Stephan Schlemmer, University of Cologne, Germany, spoke about Harold's contribution to the spectroscopy of ions and the complexities of charge transfer in, e.g., Ar-N_2^+ complexes.*

Figure 2 *– Prof. Jan Cami, University of Western Ontario, USA, spoke about his and Harold's shared healthy obsession with the Diffuse Interstellar Bands (DIBs) and how insistant Harold was for thoroughness in the confirmation of C_{60}^+ as the first identified molecular carrier.*

Figure 3 *– Prof. Britta Redlich, Radboud University, The Netherlands, spoke about Harold's time during his PhD in Nijmegen, his work at the FELIX laboratory, and his talent for building successful teams.*

Figure 4 *– Assistant Professor Ko-Ju Chuang, Leiden University, The Netherlands, spoke about the future of the Laboratory for Astrophysics, its new location and future directions of the laboratory.*

Figure 5 *– Dr. Pavithraa Sundararajan, Leiden University, The Netherlands, presented Assistant Professor Ko-Ju Chuang with her hand-drawn potrait of Prof. Harold Linnartz to be displayed in the new Laboratory for Astrophysics.*

Heavy ion radiolysis of the chiral terpene α-pinene

A. L. F. de Barros[1,4], A. Ricca[2,3], A. Bychkova[4], C. A. P. da Costa[4], J. W. Costa[1], P. Boduch[4], H. Rothard[4], E. F. da Silveira[5] and A. Domaracka[4]

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Radiolysis of α-pinene by 61.3 MeV $^{-84}Kr^{15}$ ions was analyzed with the scope to simulate the effects of heavy ion cosmic ray bombardment on chiral molecules in typical interstellar medium. The α-pinene ice samples were irradiated at 10 K and their chemical evolution was monitored by mid-infrared Fourier transform (FTIR) spectroscopy to characterize the reaction products and to determine the extent of racemization. The integrated band strengths have been obtained for all the neutral α-pinene vibrational bands using the experimental band integrated absorbances and the theoretical absolute intensities calculated along the column densities. In the current heavy ion bombardment experiments, small molecules were formed and the precursor, α-pinene, was destroyed instead of being racemized. Twelve hydrocarbons were produced (final fluence of 2.0 $\times$ 10^{12} ions.cm^{-2}): methane (CH_4), acetylene (C_2H_2), ethylene (C_2H_4), propylene (C_3H_6), propane (C_3H_8), n-butane (C_4H_{10}), butene (C_4H_8), propyne (C_3H_4), benzene (C_6H_6), ethane (C_2H_6), vinylacetylene (C_4H_4) and 2-methyl-1,3-butadiene or isoprene (C_5H_8). The highest formation cross section ($\sim$ 40 $\times$ 10^{-15} cm^2) was observed for the C_3H_4 and the lowest was for C_3H_8 ($\sim$ 3 $\times$ 10^{-15} cm^2). The radiochemical yields for these molecules follow the same trends as those of their cross sections. The atom budget calculation confirms that all the expected products have been generated during the radiolysis and supports the conclusion that the proposed A-values are accurate. The α-pinene sputtering yield for this ion beam was found to be Y_0 = 1.84 $\times$ 10^6 molecules per impact.

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Monthly Notices of the Royal Astronomical Society, stae757, accepted (2024)

https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stae757/7630226
https://doi.org/10.1093/mnras/stae757

Attosecond metrology of the two-dimensional charge distribution in molecules

V. Loriot[1], A. Boyer[1], S. Nandi[1], C. M. González-Collado[2], É. Plésiat[3], A. Marciniak[1], C. L. Garcia[1], Y. Hu[1], M. Lara-Astiaso[2], A. Palacios[2,4,5], P. Decleva[6], F. Martín[2,3,5] and F. Lépine[1]

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Photoionization as a half-scattering process is not instantaneous. Usually, time delays in photoionization are on the order of tens of attoseconds. In going from a single atom to a nano-object, one can expect the delay to increase, since the photoelectron scatters over a larger distance. Here we show that this intuition is not correct when comparing three-dimensional and planar molecules. Using attosecond interferometry, we find that the time delays in two-dimensional (2D) carbon-based molecules can be significantly shorter than those of three-dimensional counterparts. The measured time delay carries the signature of the spatial distribution of the 2D hole created in the residual molecular cation, allowing us to obtain its dimensions with angstrom accuracy. Our results demonstrate that the photoionization delay depends on the symmetry and shape of the created hole, as we show by identifying a quadrupole contribution in the measured delay of 2D molecules.

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Nature Physics (2024)

https://www.nature.com/articles/s41567-024-02406-2
https://doi.org/10.1038/s41567-024-02406-2
https://arxiv.org/abs/2209.02445

A scientific biography of Dr. Timothy J. Lee

P. P. Bera[1,2], X. Huang[1,3], R. C. Fortenberry[4], H. F. Schaefer III[5], and M. Head-Gordon[6]

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[2]Bay Area Environmental Research Institute, Mountain View, CA, USA
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[4]Department of Chemistry Biochemistry, University of Mississippi, University, MS, USA
[5]Center for Computational Quantum Chemistry, University of Georgia, Athens, GA, USA
[6]Department of Chemistry, University of California, Berkeley, CA, USA;g Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

A scientific biography is presented as an introduction to a collection of papers by his colleagues and co-workers honouring the scientific contributions and legacy of the late Dr. Timothy J. Lee (1959–2022). Tim Lee performed highly regarded research on the methods and applications of computational quantum chemistry, particularly coupled cluster theory, and computational spec- troscopy, with impacts in interstellar chemistry, aiding NASA missions, atmospheric chemistry, as well as fundamental science. His presence is deeply missed.

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Molecular Physics, e2313816 (2024)

https://doi.org/10.1080/00268976.2024.2313816

The Infrared Absorption Spectrum of Phenylacetylene and its Deuterated Isotopologue in the Mid- to Far-IR

V. J. Esposito[1], P. Ferarri[2], W. Jan Buma[2,3], R. C. Fortenberry[4], C. Boersma[1], A. Candian[5] and A. G. G. M. Tielens[6,7]

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[2]Radboud University, Institute for Molecules and Materials, HFML-FELIX, Nijmegen, The Netherlands
[3]Van't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands
[4]Department of Chemistry & Biochemistry, University of Mississippi, University, Mississippi, USA
[5]Anton Pannekoek Institute for Astronomy, University of Amsterdam, Amsterdam, The Netherlands
[6]Leiden Observatory, Leiden University, Leiden, The Netherlands
[7]Astronomy Department, University of Maryland, College Park, Maryland, USA

Anharmonicity strongly influences the absorption and emission spectra of polycyclic aromatic hydrocarbon (PAH) molecules. Here, IR-UV ion-dip spectroscopy experiments together with detailed anharmonic computations reveal the presence of fundamental, overtone, as well as 2- and 3-quanta combination band transitions in the far- and mid-infrared absorption spectrum of phenylacetylene and its singly deuterated isotopologue. Strong absorption features in the 400–900 cm^{-1} range originate from CH(D) in-plane and out-of-plane wags and bends, as well as bending motions including the C≡C and CH bonds of the acetylene substituent and the aromatic ring. For phenylacetylene, every absorption feature is assigned either directly or indirectly to a single or multiple vibrational mode(s). The measured spectrum is dense, broad, and structureless in many regions but well characterized by computations. Upon deuteration, large isotopic shifts are observed. At frequencies above 1500 cm^{-1} for d_1–phenylacetylene, a one-to-one match is seen when comparing computations and experiment with all features assigned to combination bands and overtones. The C≡C stretch observed in phenylacetylene is not observed in d_1–phenylacetylene due to a computed 40-fold drop in intensity. Overall, a careful treatment of anharmonicity that includes 2- and 3-quanta modes is found to be crucial to understand the rich details of the infrared spectrum of phenylacetylene. Based on these results, it can be expected that such an all-inclusive anharmonic treatment will also be key for unraveling the infrared spectra of PAHs in general.

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The Journal of Chemical Physics, **160**, 114312 (2024)

https://doi.org/10.1063/5.0191404

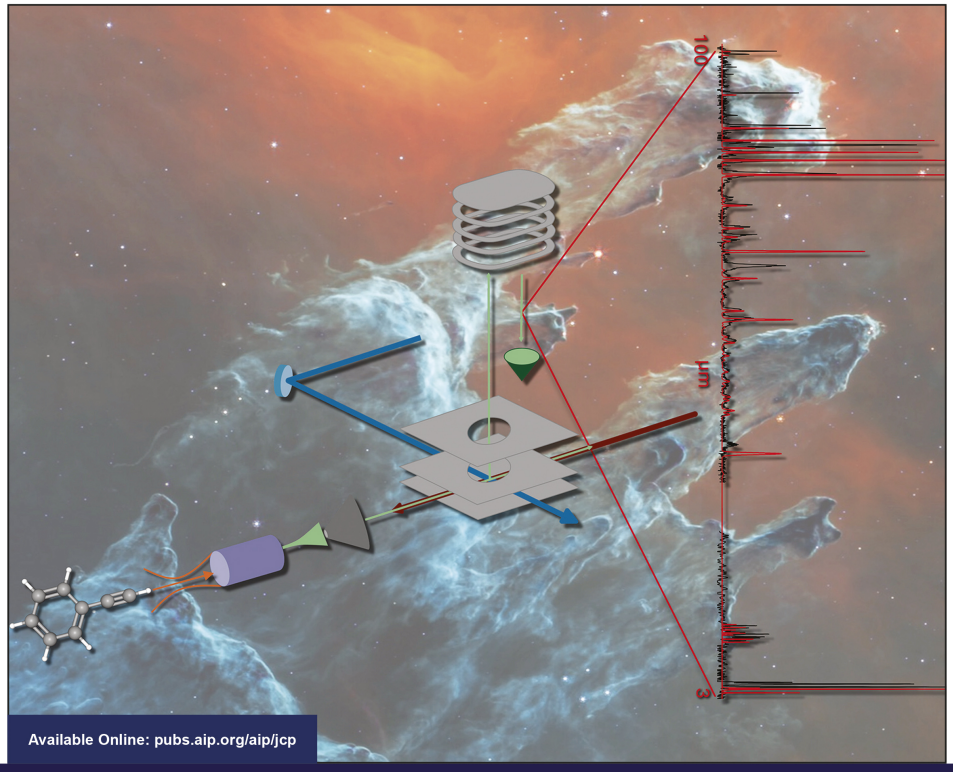
The Journal of Chemical Physics

AIP Publishing

Vol. 160, Iss. 11, 21 Mar. 2024

The infrared absorption spectrum of phenylacetylene and its deuterated isotopologue in the mid- to far-IR

Vincent J. Esposito, Piero Ferrari, Wybren Jan Buma, Ryan C. Fortenberry, Christiaan Boersma, Alessandra Candian, and Alexander G. G. M. Tielens



This paper was featured on the cover of the Journal of Chemical Physics. It was also selected for the 2024 JCP Emerging Investigators Special Collection. The image depicts the experimental setup at FELIX as well as the combined experimental (black) and computational (red) absorption spectrum. Background Image: ©ESA, Credit: NASA, ESA, CSA, STScI, J. DePasquale (STScI), A. Pagan (STScI)

Meetings

Special Symposium
"Planetary Aerosols: From Earth to Exoplanet"
American Association for Aerosol Research (AAAR)

Alburquerque, New Mexico, USA

21–25 October, 2024

https://web.cvent.com/event/a3a3aa41-527e-4e88-814a-45b56c7cdbde

We would like to invite members of the community to a special symposium **"Planetary Aerosols: From Earth to Exoplanet"** at the American Association for Aerosol Research (AAAR) 42nd Annual Conference October 21–25, 2024 in Alburquerque, New Mexico.

From the H_2SO_4 haze of Venus to the thick organic haze of Titan and thin organic haze of Pluto, photochemically produced hazes are prevalent in our solar system and recent observations suggest that they are common components of exoplanet atmospheres as well. Additionally, haze is thought to have existed at several points during the evolution of Earth's atmosphere with implications for habitability and the emergence of early life. Just as on the modern Earth, aerosols in these diverse atmospheres play a central role in atmospheric chemistry, dynamics, and radiative balance. Through their interaction with light, aerosols affect observable planetary atmospheric spectra providing information on composition and structure while also potentially complicating interpretation. With new and forthcoming measurement capabilities such as from the James Webb telescope and NASA's Dragonfly mission, there exists an opportunity and a need to improve our understanding of aerosols much different from those prevalent in the modern Earth's atmosphere.

The aim of this session is to facilitate cross- and inter-disciplinary work in the Earth and planetary science communities to improve our understanding of aerosol and cloud microphysics and chemistry. We invite submissions from laboratory, observational, modeling, and instrument/method development work that focus on aerosols in atmospheres different from that of the modern Earth.

We welcome submissions on any aspect of planetary aerosols including laboratory experiments, modeling, and measurements/observations. A goal of the session is to facilitate multi-disciplinary connections between planetary and aerosol scientists. The symposium abstract is copied at the bottom of this announcement. Confirmed invited speakers include Dr. Ella Sciamma-O'Brien (NASA Ames Research Center).

Regular abstract deadline: May 8, 2024

Abstracts for late-breaking posters accepted until: July 22, 2024

Submission information: available here.

We hope you are able to join us in Albuquerque!

— Prof. Ellie Browne (CU Boulder) and Dr. Melissa Trainer (NASA Goddard)

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NanoSpace Astrochemistry Training School:

A COST/DAN summer school on the astrochemistry of star & planet formation

First Announcement

Groningen, The Netherlands
26-30 August, 2024

https://meetings.iac.es/nats2024/

We are very happy to announce the 'NanoSpace Astrochemistry Training School: A COST/DAN summer school on the astrochemistry of star & planet formation' to be held **26–30 August 2024 in Groningen, The Netherlands**.

The list of lecturers/trainers confirmed is the following:

Sergio Ioppolo, Aarhus University, Denmark
Thanja Lamberts, Leiden University, The Netherlands
Sandra Brunken, Radboud University, The Netherlands
Javier Goicoechea, Instituto de Fisica Fundamental (IFF-CSIC), Spain
Floris van der Tak, SRON, The Netherlands
Jacques le Bourlot, Observatoire de Paris, France
Maryvonne Gerin, French National Centre for Scientific Research (CNRS), France
Inga Kamp, University of Groningen, The Netherlands
Gerrit Groenenboom, Radboud University, The Netherlands
Alessandra Candian, University of Amsterdam, The Netherlands
Emma Postolec, University of Groningen, The Netherlands
Aditya Arabhavi, University of Groningen, The Netherlands

This Astrochemistry Training School is organized by the COST Action NanoSpace (CA21126) (https://research.iac.es/proyecto/nanospace/) in collaboration with the Dutch Astrochemistry Network (DAN). The main goal of the COST/DAN Astrochemistry Training School is to provide PhD students and young researchers specialised knowledge and training in the field of astrochemistry (e.g., theoretical and experimental tools). The program will include several sessions on astrophysical context, chemical processes in space, laboratory techniques, numerical models and theory, and the future of astrochemistry, as well as series of practical exercises and a participant poster session.

The school will be in person with attendance limited to 50-60 trainees and with priority given to PhD students and Young Researchers, who are strongly encouraged to participate. There is no registration fee and the NanoSpace COST Action will provide financial support (i.e. reimbursement after the event) for a significant number of participants (at least 20-30), with high priority to those with a primary affiliation in an institution located in an Inclusiveness Target Country (ITC) / Near Neighbour Country (NNC) participating in the Action. The information requested in the registration form (https://meetings.iac.es/nats2024/pages/registration.php) will be used to select the final list of registered participants as well as those eligible for financial support, which will be notified in advance of the Training School (i.e., in the last week of May). The attendees are expected to arrange their own travel and accommodation following the instructions given by the organizing committee at the due time.

*****Deadline for registration: 15th May 2024*****

Anibal Garcia-Hernandez,
NanoSpace Action Chair on behalf of the Organizing Committee

E-mail for contact: nats2024@iac.es

Announcements

Call for Papers

Special Issue in honor of Harold Linnartz in the journal ACS Earth and Space Chemistry

Advertised by Xander Tielens

This Special Issue honoring the legacy of Harold Linnartz will feature a broad range of contributions on all aspects of molecular astrophysics, including but not limited to gas-phase spectroscopy, spectroscopy and dynamics of ices, photo physics of Polycyclic Aromatic Hydrocarbons and related compounds, astronomical observations involving molecules, modeling of astrophysical conditions, planets to galaxies, all from a broad perspective. **Details on the submission process can be found on the ACS/Earth and Space Chemistry website:** https://axial.acs.org/earth-space-and-environmental-chemistry/call-for-papers-special-issue-in-honor-of-harold-linnartz.

On New Year's eve, our friend and colleague, Harold Linnartz suddenly passed away at the age of 58. Harold was the head of the Astrophysics Laboratory of Leiden Observatory. Harold was a highly respected leader in the field of molecular astrophysics, specifically in the areas of molecular spectroscopy and its application to the carriers of the Diffuse Interstellar Bands, in the spectroscopy and reactions of low temperature solids as relevant to interstellar ices, and in the photochemistry of PAHs as they speak to the challenges of the AIBs.

With this Special Issue in the journal *ACS Earth and Space Chemistry*, we want to honor Harold's scientific legacy. In this special issue, we will welcome articles on all aspects of molecular astrophysics; in particular those that touch closely on Harold's scientific interests, which were very broad as, in his scientific career, he focused on unlocking the chemistry of the heavens in the broadest sense.

As a spectroscopist pur sang, shining light on molecules in space was one of his guiding principles. Fathom the behavior of molecules under the extreme conditions of space was another. Topics that may be covered in the Special Issue include: gas-phase spectroscopy, spectroscopy and dynamics of ices, photo physics of Polycyclic Aromatic Hydrocarbons and related compounds, astronomical observations involving molecules, modeling of astrophysical conditions, planets to galaxies, all from a broad perspective. In the submission process, please select Harold Linnartz Special Issue from the drop-down menu. Submitted manuscripts will follow the normal refereeing process of the journal and peer review decisions will be made by the journal Editors.
Submission deadline is 01 January 2025.

Guest Editors

Wim Ubachs, Department of Physics and Astronomy, Vrije Universiteit, Amsterdam, The Netherlands (w.m.g.ubachs@vu.nl)

Xander Tielens, Astronomy Department, University of Maryland, College Park, USA & Leiden Observatory, Leiden University, The Netherlands (tielens@umd.edu).

Deadline: 1 January 2025

E-mail for contact: tielens@umd.edu

Webpage: https://axial.acs.org/earth-space-and-environmental-chemistry/call-for-papers-special-issue-in-honor-of-harold-linnartz

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 in the gas phase 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 and a photoelectron spectrometer.

Previous publications of the group in this field include:

- Angew. Chem. Int. Ed. 51, 4925-4929 (2012) DOI: 10.1002/anie.201108937
- Astrophys. J. Lett. 900, L20 (2020), DOI: 10.3847/2041-8213/abafbd
- Astrophys. J. 940, 104 (2022), DOI: 10.3847/1538-4357/ac9733
- J. Phys. Chem. Lett. 13, 449-454 (2022), DOI: 10.1021/acs.jpclett.1c03948
- Chem. Eur. J. 28, e202200577 (2022), DOI: 10.1002/chem.202200577
- Phys. Chem. Chem. Phys. 24, 16101-16111 (2022), DOI: 10.1039/D2CP01947G
- Phys. Chem. Chem. Phys. 25, 13593-13610 (2023), DOI: 10.1039/D3CP01514A
- Phys. Chem. Chem. Phys. 25, 22734-22743 (2023), DOI: 10.1039/D3CP03417H
- Phys. Chem. Chem. Phys. 25, 5529-5549 (2023), DOI: 10.1039/d2cp04556g
- Mol. Phys. 122, e2231566 (2024), DOI: 10.1080/00268976.2023.2231566

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 (as 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 April 26 (2024) 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: April 26, 2024

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

Webpage: https://www.tu.berlin/en/lmsu

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl Next issue: 23 May 2024

astropah@strw.leidenuniv.nl Submission deadline: 10 May 2024