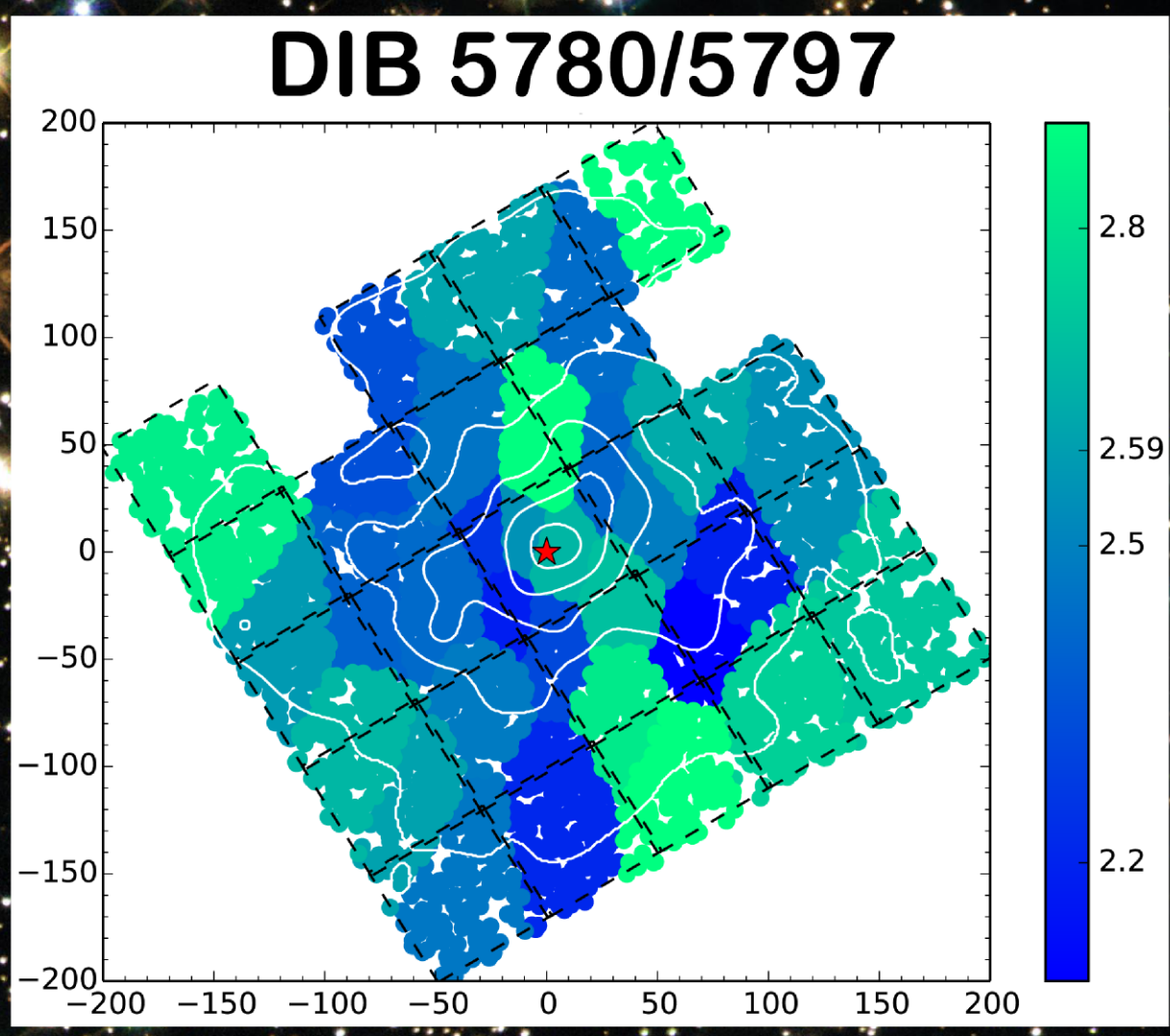


AstropAH

A Newsletter on Astronomical PAHs

Issue 42 | October 2017



Editorial

Dear Colleagues,

We are entering our 5th year of AstroPAH! It makes us very happy to keep you up to date about our community, and we hope to continue doing so for many years to come. Since our conception, the number of subscribers to AstroPAH has grown to more than 300 people, with roughly the same number of newsletter downloads each month.

For our 4-year anniversary, we are changing things up and introducing a new monthly release date. AstroPAH will now be released on the 3rd or 4th Thursday of the month. The release date for an upcoming issue will continue to be published on our website and in the previous issue as usual.

What better way to celebrate our anniversary than with a great Picture of the Month, sent by one of our subscribers - Martin Wendt. The picture shows the sub parsec variation of two Diffuse Interstellar Bands towards NGC 6397, as observed with the instrument MUSE installed on the VLT.

This month, our In Focus dives into a subject that has been on the rise since the launch of AstroPAH: Aude Simon and Mathias Rapacioli take us on a journey through the modeling of dissociation and isomerisation of PAHs.

Do not miss any of the interesting papers in our Abstract section, from calculations, to observational data analysis, to laboratory studies. We close this AstroPAH 4th anniversary issue with announcements of opportunities for Fellowships.

AstroPAH will continue to help you promote your science. Please visit our webpage or contact us. Send us your contributions anytime or for publication in November, see the deadlines below.

We thank you all for your contributions in these past 4 years and for the time to come.

The Editorial Team

**Next issue: 23 November 2017.
Submission deadline: 10 November 2017.**

AstroPAH Newsletter

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Contents

PAH Picture of the Month	1
Editorial	2
In Focus	4
Recent Papers	11
Announcements	16

PAH Picture of the Month

Ratio of the equivalent widths of the Diffuse Interstellar Bands (DIB) at 5780 and 5797 Å toward the globular cluster NGC6397. This is depicted as a 2D color map (scale in arc-sec) based on 31 Voronoi-bins of about 10000 stellar spectra obtained with the instrument MUSE at VLT. The center of the globular cluster is at coordinate origin (0,0) and is marked with a red star. Superimposed with the image, brightness contours of the globular cluster are shown as white lines. More information can be found in <https://arxiv.org/abs/1709.03982>. In the Background: a Hubble image of NGC 6397.

Credits: M. Wendt. Background image: NASA/ESA and the Hubble Heritage Team (AURA/STScI).



Modeling Dissociation and Isomerisation of PAHs

by Aude Simon and Mathias Rapacioli

Since they were proposed as the AIBs carriers, Polycyclic Aromatic Hydrocarbons (PAHs) have been the object of many theoretical investigations. A large majority of which being dedicated to the determination of properties for their most stable structures. The stability of PAHs results from the presence of a π resonant system over a large number of hexagonal units, which is favored for planar geometries. Far fewer studies address the design of non equilibrium structures and of the energetic processing of PAHs leading them to escape from their most stable isomeric form. Indeed, although remaining most of the time at very low energy in their ground electronic state, astrophysical PAHs can sometime absorb significant amount of energy from photon absorption (for instance in photodissociation regions) or from collisions with energetic ions (for instance in shock waves). In this "In Focus" article, we present our recent theoretical studies concerning PAH dissociation and isomerisation. These channels for energy relaxation are important to investigate in the context of understanding PAH evolution, as well as PAHs' chemical role in the formation of small molecules such as H_2 and their possible link with fullerenes formation.

Let us first mention that in many cases, PAH evaporation is not highly dependent on the excitation condition but mainly on the amount of received energy. This is, for instance, the case when the excitation of the electronic system (by UV photon absorption, very fast collision) is followed by internal conversion and intramolecular vibrational redistribution (IVR) of the energy, leaving the molecule in its electronic ground state with an excess of energy distributed over vibrational modes. Such a final situation can also be reached from sequential absorption of IR photons. The subsequent dissociation will be qualified as 'statistical' dissociation as opposed to 'non-statistical' fragmentation such as dissociation in the excited states or knockout processes, i.e., direct ejection of an atom by a colliding particle before IVR can occur.

Focusing now on the modeling of statistical dissociation, two main approaches can be followed. The first one relies on the use of statistical theories, like for instance RRKM (Rice-Ramsperger-Kassel-Marcus) unimolecular dissociation theory, which requires the computation

of properties for some selected geometries. The advantage of such an approach is that these input quantities can be computed at the *ab initio* level, and it addresses very long timescales. One drawback is that all possible isomerisation and dissociation channels should in principle be included, which becomes hardly feasible even for medium-sized PAHs. In addition, it usually does not include anharmonic effects. An alternative approach consists in performing dynamical simulations of the evolution of PAHs with a large amount of energy (Simon *et al.* 2017, Gatchell *et al.* 2015). Within such an approach, if convergence is reached, all possible isomerisation and dissociation channels are in principle naturally included. One drawback is that the simulations have to be performed at relatively high energies to observe evaporation in a reasonable computational timescale. Such high energy simulations are, however, also interesting to interpret lower energy events as, in statistical dissociation, the relative ratios of the different products are mostly driven by their relative stabilities. Molecular dynamics simulations can therefore be seen as an efficient tool to explore all of these possible dissociation channels, including naturally entropic effects.

Approaching convergence from molecular dynamics (MD) simulations usually requires millions of single point energy and gradient calculations. This is, of course, out of reach for *ab initio* methods, even for Density Functional Theory (DFT) approaches. An attractive alternative is the Density Functional based Tight Binding (DFTB) scheme (Elstner & Seifert 2014), an approximated DFT scheme, whose computational efficiency relies on the use of tabulated values for integrals pre-computed at the DFT level. This approach could be qualified of semi-*ab initio*, and it presents the advantage of being parameterized in a general case and not for a specific system. It allows transferability and, in particular, the treatment of chemical reactivity and dissociation processes.

Dissociation dynamics of PAHs

PAHs undergoing statistical evaporation are known to lose H, H₂ and C₂H₂, as first shown by Jochims *et al.* (1994). In the experiments by these authors, loss of H is always the lowest energetic channel, followed by C₂H₂ and H₂ losses. The H vs C₂H₂ ratio increases with PAH size. For small systems like C₁₀H₈⁺, a DFT/RRKM mapping of dissociation/isomerisation channels remains feasible (Solenio & Mayer 2015). In order to address larger systems, we have recently achieved MD/DFTB simulations for PAH radical cations from naphthalene C₁₀H₈⁺ to coronene C₂₄H₁₂⁺ (Simon *et al.* 2017). In this study, the initial internal energy was taken in the 14-40 eV range so as to observe significant dissociation rates with a reasonable simulation time (100-500 ps). For each PAH and each energy, about 1000 simulations were successfully run with the initial energy randomly distributed over all the vibrational modes in order to approach statistics. Branching ratios and dissociation rates were obtained. The evolution of dissociation pathways and kinetics as a function of energy was studied (Fig. 1). We found that, overall, C₂H₂ and H are the most abundant ejected fragments, and that the H/C₂H₂ ratio increases when the PAH size is increased in the simulation, as well as, for a given PAH, when the energy is decreased. This is in agreement with experimental trends.

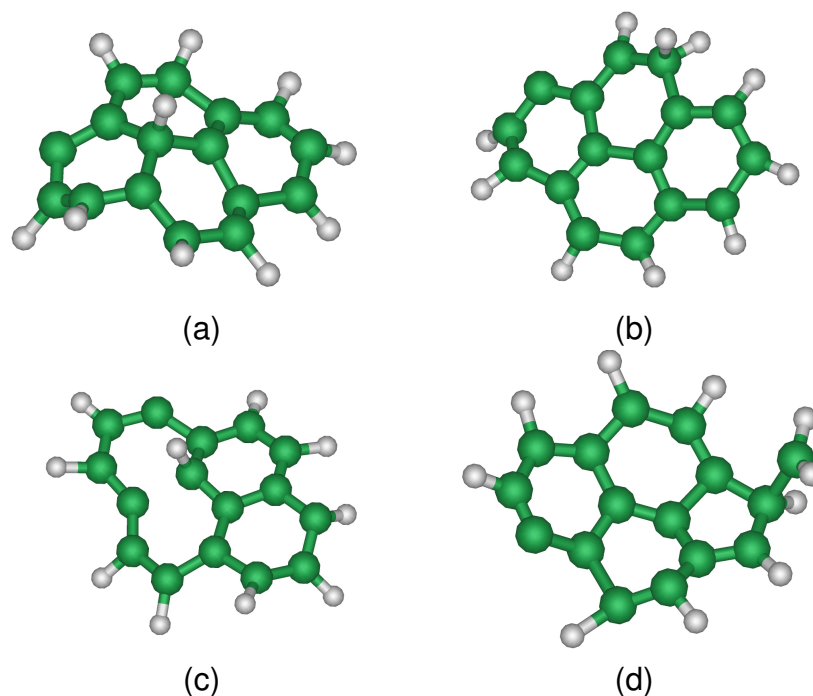


Figure 1: Snapshots extracted from MD/DFTB simulations for cationic pyrene: geometries preceding dissociation and presenting a hydrogen transfer on a central (a) or edge carbon atom (b), a ring opening (c) and a pentagonal cycle formation (d).

Isomerisation vs dissociation

In our MD studies, we observed that dissociation was frequently preceded by isomerisation (Fig. 1). From these qualitative results, we derived some classes of isomerisation reactions that we investigated at the DFT level and that are (i) the migration of a hydrogen atom over the carbonaceous skeleton, possibly leading to the evaporation of molecular hydrogen, (ii) the formation of pentagonal cycles and (iii) the formation of ethynyl derivatives, preliminary steps toward the loss of C_2H_2 fragments. Here, we focus on the first and second isomerisation types.

H-migration: We investigated, for different PAHs (Trinquier *et al.*, 2017a), the displacement of a hydrogen atom over the carbonaceous skeleton of a PAH, which leads to multiple isomers called H-shifted isomers (Fig. 2). A large majority of these isomers are stable and located between 3 and 6 eV above the corresponding optimised geometry. The most stable isomers correspond to the transfer of a hydrogen to the closest hydrogenated carbon atom (Fig. 2-b), presenting barriers as low as 3.5-4 eV. Interestingly, once this first hydrogen transfer has been initiated, the other barriers usually lie at about 1 eV above the minima they connect. The most stable isomers correspond to doubly hydrogenated carbon atoms on the edges. Such isomers can be seen as a preliminary step to a concerted mechanism leading to the loss of these two hydrogen atoms forming molecular hydrogen. This is particularly relevant in the astrophysical context, as PAHs are suspected to play a role in H_2 formation. Hydrogen-shifted isomers can also further lead to different isomers, presenting interesting patterns like ring opening or formation of pentagonal structures.

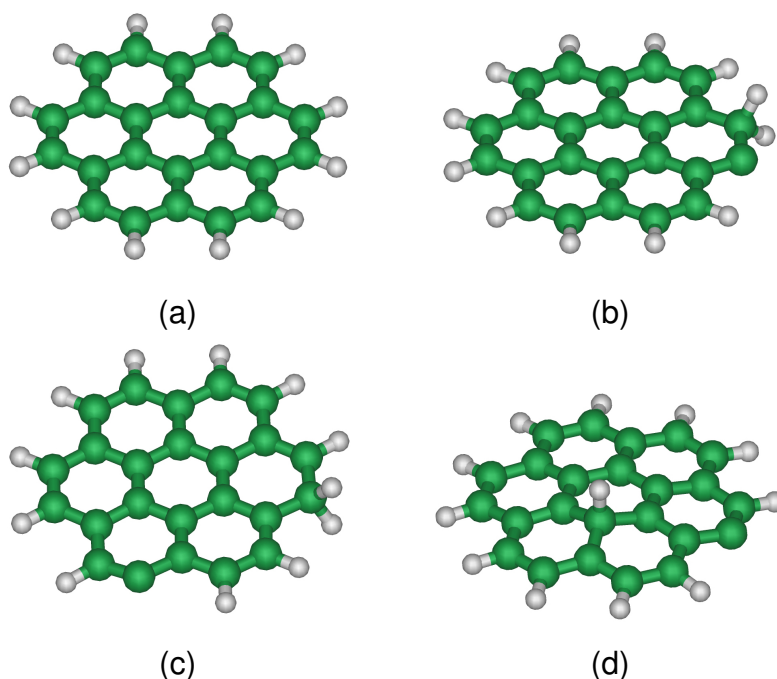


Figure 2: A selection of optimised H-shifted isomers for the coronene cation.

Formation of five-member rings: We distinguish two classes of PAH isomers with 5-member rings:

(i) those with fused 5 and 7-member rings (Fig. 3 e-f) that can be regarded as azulene-type isomers, along with the particular class of Stone-Wales isomers. Their formation involves intramolecular C-C bonds, which can cost up to about 8 eV (Öttl *et al.* 2014).

(ii) those with one 5-member ring and a vinylidene group (fulvene-type isomers, Fig. 3-d and Fig. 4), that we frequently observed in our simulations for PAHs ranging from naphthalene to coronene cations.

We showed at the DFT level that, in all cases, the lowest energy path proceeds through a 1,2 H-migration, followed by a concerted mechanism involving C-C bond formation and cleavage (Trinquier *et al.* 2017b). The total energy barrier was estimated between 3.7 and 4.3 eV for neutral and cationic pyrene and coronene, while the final fulvene-type structures lied between 1.1 and 1.6 eV above normal form. In the case of phenanthrene, which has less geometrical constraints, this energy decreased to 0.65-0.69 eV. Overall, given the energies involved, the formation of fulvene-type isomers is clearly in competition with the lowest energy dissociation channels for neutral and cationic PAHs. Besides, given the important return barrier, such isomers are kinetically stable. Another point is that, starting with the inclusion of two fulvene motifs, PAHs become non planar (Fig. 4), which might be interesting in terms of fullerene precursor formation.

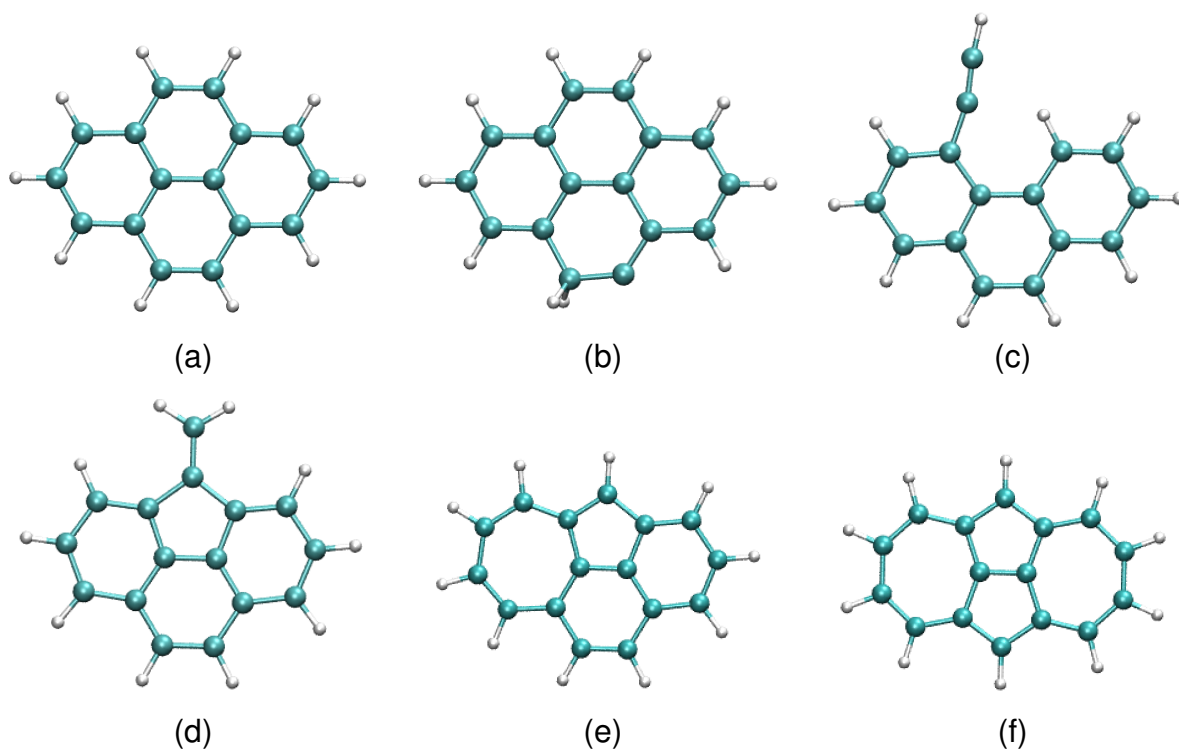


Figure 3: Optimised geometries of characteristic isomers of the pyrene cations (a) with the following patterns : H-shift (b), ethynyl (c) fulvene- (d), azulene- (e) and Stone-Wales- (f) type defects.

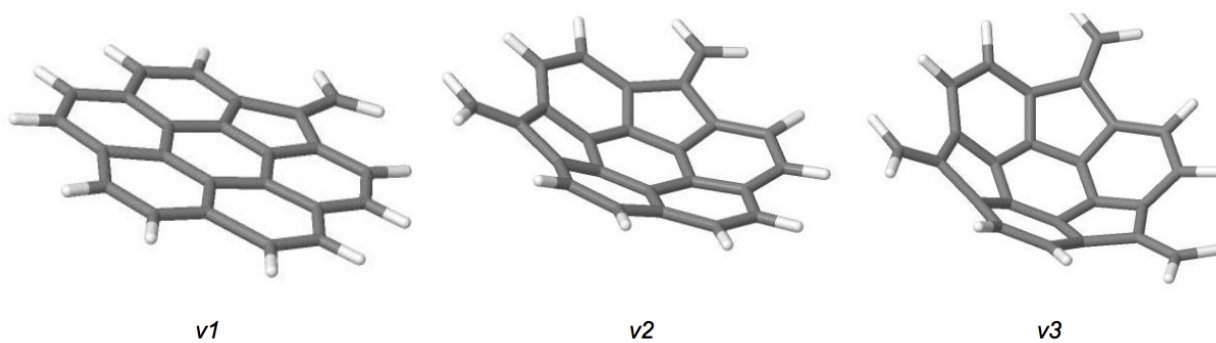


Figure 4: Optimized geometries of fulvene-type forms for coronene cation (from Trinquier *et al.* 2017b).

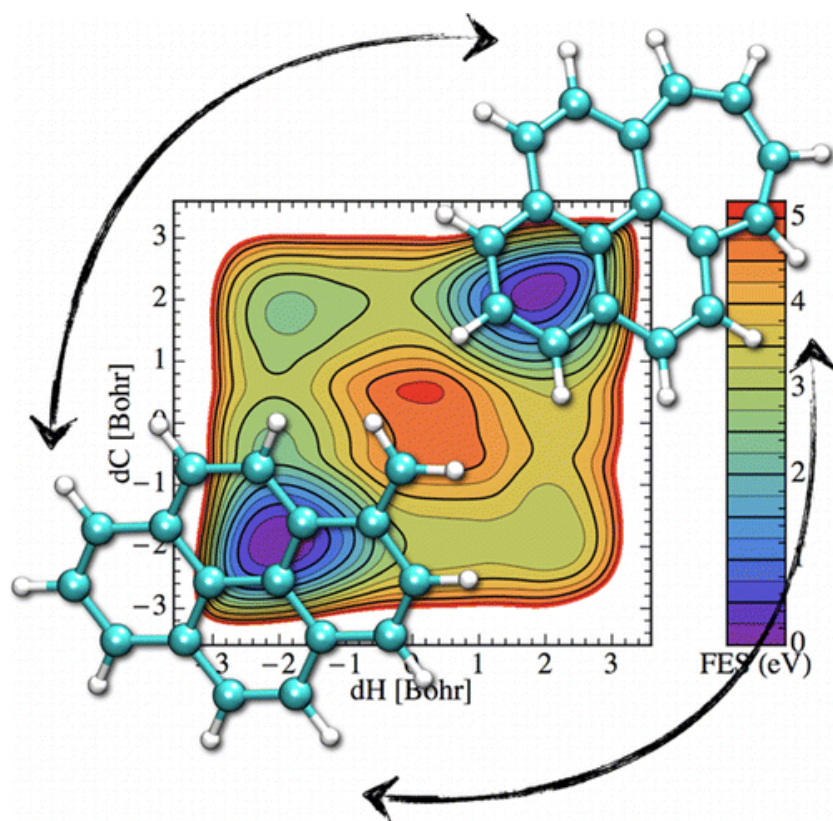


Figure 5: Free energy surface corresponding to the isomerisation between cationic methylene-pyrene and its tropylium like equivalent (from Rapacioli *et al.* 2015).

Let us finally mention that the mapping of free energy surfaces allows us to characterise the competition between several isomerisation/dissociation channels. Some theoretical tools have been developed in the recent years enabling such calculations. For instance, Parneix *et al.* (2017) recently showed that local dehydrogenation next to an aromatic ring favors ring opening, and thus the formation of one (5,7) member ring defect that could become competitive with the loss of a hydrogen atom. To do so, they determined entire free-energy profiles using the AIREBO reactive force field and advanced Monte Carlo techniques based on a biased exploration of the potential energy surface. Similarly, we have used a biased scheme, in which the exploration is achieved with MD simulations (metadynamics), to determine the free energy surface for cationic methylene-pyrene to tropylium-like pyrene isomerisation. (Fig. 5, Rapacioli *et al.* 2015)

Acknowledgments

The author would like to thank Georges Trinquier, Florent Xavier Gadéa, Arthur Huguenot, Jérôme Cuny and Fernand Spiegelman for collaborating on the topic presented here.



Aude Simon has been a CNRS research scientist since 2005, and she works at the University of Toulouse. She received her PhD in physical chemistry from the University of Paris XI. It was followed by a post-doc fellowship in the Chemistry Department of the University of Waterloo. She has experience in gas phase ion chemistry, quantum modeling and *ab initio* molecular dynamics. Her main current research interest is astrochemistry of large carbonaceous systems.

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Mathias Rapacioli has been a CNRS research scientist since 2007 at the Laboratory of Quantum Physics and Chemistry of Toulouse. He received his PhD in astrophysics from the University of Toulouse and was a post-doctoral fellow in the quantum chemistry group at Dresden Technical University. He is mostly doing methodological developments to investigate the properties of large molecules as well as atomic/molecular clusters, often of astrophysical interest.

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Abstracts

Mapping diffuse interstellar bands in the local ISM on small scales via MUSE 3D spectroscopy

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We map the interstellar medium (ISM) including the diffuse interstellar bands (DIBs) in absorption toward the globular cluster NGC 6397 using VLT/MUSE. This pilot study demonstrates the power of MUSE for mapping the local ISM on very small scales which provides a new window for ISM observations. Assuming the absorbers are located at the rim of the Local Bubble we trace small-scale variations in NaI and KI as well as in several DIBs structures on the order of mpc (milliparsec, a few thousand AU). The sightlines defined by binned stellar spectra are separated by only a few arcseconds and we probe the absorption within a physically connected region. This analysis utilized the fitting residuals of individual stellar spectra of NGC 6397 member stars and analyzed lines from neutral species and several DIBs in Voronoi-binned composite spectra with high signal-to-noise ratio (S/N). We verify the suitability of the MUSE 3D spectrograph for such measurements and gain new insights by probing a single physical absorber with multiple sight lines.

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Accepted for publication in A&A

<http://arxiv.org/abs/1709.03982>

Spectroscopy of prospective interstellar ions and radicals isolated in para-hydrogen matrices

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para-Hydrogen (*p*-H₂) serves as a new host in matrix-isolation experiments for an investigation of species of astrochemical interest. Protonated and mono-hydrogenated species are produced upon electron bombardment during deposition of *p*-H₂ containing a precursor in a small proportion. The applications of this novel technique to generate protonated polycyclic aromatic hydrocarbons (H+PAH), protonated polycyclic nitrogen heterocycles (H+PANH), and their neutral counterparts, which are important in the identification of interstellar unidentified infrared emission bands, demonstrate its superiority over other methods. The clean production with little fragmentation, ease of distinction between protonated and neutral species, narrow lines and reliable relative infrared intensities of the lines, and broad coverage of the spectral range associated with this method enable us to assign the isomers unambiguously. The application of this method to the protonation of small molecules is more complicated partly because of the feasible fragmentation and reactions, and partly because of the possible proton sharing between the species of interest and H₂, but, with isotopic experiments and secondary photolysis, definitive assignments are practicable. Furthermore, the true relative infrared intensities are critical to a comparison of experimental results with data from theoretical calculations. The spectra of a proton-shared species in solid *p*-H₂ might provide insight into a search for spectra of proton-bound species in interstellar media. Investigations of hydrogenated species involving the photolysis of Cl₂ or precursors of OH complement those using electron bombardment and provide an improved ratio of signal to noise. With careful grouping of observed lines after secondary photolysis and a comparison with theoretical predictions, various isomers of these species have been determined. This photolytic technique has been applied in an investigation of hydrogenated PAH and PANH, and the hydrogenation reactions of small molecules, which are important in interstellar ice and the evolution of life. The electronic transitions of molecules in solid *p*-H₂ have been little investigated. The matrix shift of the origins of transitions and the spectral width seem to be much smaller than those of noble-gas matrices; these features might facilitate a direct comparison of matrix spectra with diffuse interstellar bands, but further data are required to assess this possibility. The advantages and disadvantages of applying these techniques of *p*-H₂ matrix isolation to astrochemical research and their future perspectives are discussed.

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Phys. Chem. Chem. Phys., 2017, Advance Article

<http://pubs.rsc.org/en/Content/ArticleLanding/2017/CP/C7CP05680J#ldivAbstract>

Adsorption of molecular hydrogen on coronene with a new potential energy surface

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Benchmark interaction energies between coronene, C₂₄H₁₂, and molecular hydrogen, H₂, have been computed by means of high level electronic structure calculations. Binding energies, equilibrium distances and strengths of the long range attraction, evaluated for the basic configurations of the H₂-C₂₄H₁₂ complex, indicate that the system is not too affected by the relative orientations of the diatom, suggesting that its behavior can be approximated to that of a pseudoatom. The obtained energy profiles have confirmed the noncovalent nature of the bonding and served to tune-up the parameters of a new force field based on the atom-bond approach which correctly describes the main features of the H₂-coronene interaction. The structure and binding energies of (para-H₂)_N- coronene clusters have been investigated within an additive model for the above mentioned interactions and exploiting basin-hopping and path integral Monte Carlo calculations for $N = 1-16$ at $T = 2$ K. Differences with respect to the prototypical (Rare Gas)_N-coronene aggregates have been discussed.

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Phys. Chem. Chem. Phys. 19, 26358 (2017)

<https://doi.org/10.1039/C7CP03819D>

Origin of spectral band patterns in the cosmic unidentified infrared emission

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The cosmic unidentified infrared emission (UIE) band phenomenon is generally considered as indicative of free-flying polycyclic aromatic hydrocarbon molecules in space. However, a coherent explanation of emission spectral band patterns depending on astrophysical source is yet to be resolved under this attribution. Meanwhile astronomers have restored the alternative origin as due to amorphous carbon particles, but assigning spectral patterns to specific structural elements of particles is equally challenging. Here we report a physical principle in which inclusion of nonplanar structural defects in aromatic core molecular structures (π -domains) in-

duces spectral patterns typical of the phenomenon. We show that defects in model π -domains modulate the electronic-vibration coupling that activates the delocalized π -electron contribution to aromatic vibrational modes. The modulation naturally disperses C=C stretch modes in band patterns that readily resemble the UIE bands in the elusive 6-9 μm range. The electron-vibration interaction mechanics governing the defect-induced band patterns underscores the importance of π -delocalization in the emergence of UIE bands. We discuss the global UIE band regularity of this range as compatible with an emission from the delocalized sp^2 -phase, as π -domains, confined in disordered carbon mixed-phase aggregates.

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Accepted for publication in Physical Review Letters

<https://journals.aps.org/prl/accepted/d207bYe2Pb51f768586e7022d0813dda2785e7b66>

On Graphene in the Interstellar Medium

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The possible detection of C_{24} , a planar graphene, recently reported in several planetary nebulae by García-Hernández et al. (2011, 2012) inspires us to explore whether and how much graphene could exist in the interstellar medium (ISM) and how it would reveal its presence through its ultraviolet (UV) extinction and infrared (IR) emission. In principle, interstellar graphene could arise from the photochemical processing of polycyclic aromatic hydrocarbon (PAH) molecules which are abundant in the ISM through a complete loss of their hydrogen atoms, and/or from graphite which is thought to be a major dust species in the ISM through fragmentation caused by grain-grain collisional shattering. Both quantum-chemical computations and laboratory experiments have shown that the exciton-dominated electronic transitions in graphene cause a strong absorption band near 2755 Å. We calculate the UV absorption of graphene and place an upper limit of ~ 5 ppm of C/H (i.e., $\sim 1.9\%$ of the total interstellar C) on the interstellar graphene abundance. We also model the stochastic heating of graphene C_{24} in the ISM, excited by single starlight photons of the interstellar radiation field and calculate its IR emission spectra. We also derive the abundance of graphene in the ISM to be < 5 ppm of C/H by comparing the model emission spectra with that observed in the ISM.

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Accepted for publication in ApJ

<http://arxiv.org/abs/1710.05081>

Interstellar Silicon Depletion and the Ultraviolet Extinction

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Spinning small silicate grains were recently invoked to account for the Galactic foreground anomalous microwave emission. These grains, if present, will absorb starlight in the far ultraviolet (UV). There is also renewed interest in attributing the enigmatic 2175 Å interstellar extinction bump to small silicates. To probe the role of silicon in the UV extinction, we explore the relations between the amount of silicon required to be locked up in silicates $[\text{Si}/\text{H}]_{\text{dust}}$ and the 2175 Å bump or the far-UV extinction rise, based on an analysis of the extinction curves along 46 Galactic sightlines for which the gas-phase silicon abundance $[\text{Si}/\text{H}]_{\text{gas}}$ is known and both the 2175 Å bump and the far-UV rise exhibit considerable variations. We derive $[\text{Si}/\text{H}]_{\text{dust}}$ either from $[\text{Si}/\text{H}]_{\text{ISM}} - [\text{Si}/\text{H}]_{\text{gas}}$ or from the model-independent Kramers-Kronig relation which relates the wavelength-integrated extinction to the total dust volume, where $[\text{Si}/\text{H}]_{\text{ISM}}$ is the interstellar silicon reference abundance and taken to be that of proto-Sun or B stars. The approach is less model-dependent since it does not require the knowledge of the detailed optical properties and size distribution of the dust. We also derive $[\text{Si}/\text{H}]_{\text{dust}}$ from fitting the observed extinction curves with a mixture of amorphous silicates and graphitic grains. We find that in all three cases $[\text{Si}/\text{H}]_{\text{dust}}$ shows no correlation with the 2175 Å bump, while the carbon depletion $[\text{C}/\text{H}]_{\text{dust}}$ tends to correlate with the 2175 Å bump. This supports carbon grains instead of silicates as the possible carrier of the 2175 Å bump. We also find that neither $[\text{Si}/\text{H}]_{\text{dust}}$ nor $[\text{C}/\text{H}]_{\text{dust}}$ alone correlates with the far-UV extinction, suggesting that the far-UV extinction is a combined effect of small carbon grains and silicates.

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ApJ, in press (2017)

<http://arxiv.org/abs/1710.04905>

Announcements

PhD Positions European Training Network EUROPAH

EUROPAH is a European Training Network (ETN) funded by the European Commission under the Horizon 2020 Marie Skłodowska-Curie Action. 13 research groups, spread across 10 universities and 3 industrial partners in 6 different countries, have come together to train a new generation of astrophysicists through an EU-wide PhD training network.

The joint scientific research goal is to understand the role that Polycyclic Aromatic Hydrocarbons (PAHs) play in the physics and chemistry of the interstellar medium of galaxies.

PAHs are universally ubiquitous and lock-up close to 15% of the elemental carbon in space. They play a key role in maintaining the ionization balance and in the heating of interstellar gas; hence controlling the phase structure of the interstellar medium (ISM) of galaxies and regulate star formation. PAHs are also central to the chemical complexity of space and the organic inventory of regions of star and planet formation. On Earth, PAHs are pernicious pollutants affecting the atmosphere and aquatic environments. Understanding PAHs and their multitude of roles in the Universe is thus a key question in both astrophysics and terrestrial chemistry.

What is offered 16 early-stage researcher (ESR) positions were created across the EUROPAH network. Most of these have been filled, but there are still three open positions at Leiden & Aarhus. Each ESR will be enrolled in a PhD program and complete a specially designed training schedule in tandem with performing research and innovation projects at their host organisation. This will be a highly multidisciplinary network that combines astronomy, molecular physics, molecular spectroscopy, environmental science, quantum chemistry, surface sciences, plasma physics and scientific communication. The training program is aimed at developing a research-oriented, creative and innovative mindset and will place you well for a future career in academia or in industry.

Who can apply Details on the individual positions are provided below. To qualify as an ESR in the EUROPAH network you must:

- have the background and expertise required for the position as described below
- be in the first four years¹ of your research career, since, e.g., completion of your masters' degree,
- not already possess a doctorate degree,

¹full-time equivalent research experience

- be willing to move to a country within the network² in which you have not lived for more than 12 months over the last 3 years,
- be proficient in both written and spoken English.

This information is also available through the EUROPAH website at www.europah.eu.

What to do Please forward a 2-page CV and 1-page cover letter to tielens@strw.leidenuniv.nl and linnartz@strw.leidenuniv.nl. Please provide 3 references from former supervisors who are familiar with your background and experience. You may be required to attend an interview. We will consider applicants until the position is filled.

ESR position 5: Molecule formation through PAH fragmentation in the gas phase

Host Institute: Leiden Observatory, Leiden University

Host Country: The Netherlands

Start date: No later than summer of 2017.

The candidate will be employed at the Leiden Observatory and will read for a doctorate degree under the supervision of Profs. Xander Tielens and Harold Linnartz.

Project description Interstellar PAHs are extensively processed by UV photons in the ISM, weeding out less stable species. Indeed, the IR spectral signatures of PAHs show variations from source to source and within sources. These variations are thought to reflect changes in the composition of the interstellar PAH family driven by the local physical conditions. In particular, photochemistry may dominate the composition of the interstellar PAH family and be an important source of small hydrocarbon radicals and chains and other carbon compounds in photon-dissociation regions and in the diffuse ISM. The graduate student will characterize photo-fragmentation reactions of PAHs upon excitation by VUV and UV/VIS radiation from dye lasers, synchrotrons (DESIRS/SOLEIL) and free electron lasers (FELIX/FELICE/FLARE) using the mobile ion trap time-of-flight mass spectrometer i-POP. The photo-fragmentation channels typically sequential H-atom, H₂, C₂, or C₂H₂ loss ultimately result in a bare carbon skeleton, which may isomerize to form e.g. fullerenes and fullerene cages, as well as fragment to smaller and smaller graphene-like structures. The astronomical implications will be assessed. In particular, identified complex molecule formation paths will be implemented in astrochemical models. Secondments are planned to Universität zu Köln (Germany) for 4 months to acquire experience in the use of ion traps and to Hiden Analytical (UK) for 2 months for mass spectrometry training.

Group description The interstellar medium group at Leiden observatory (<http://ism.strw.leidenuniv.nl/research.html#moluni>) studies the origin and evolution of the organic inventory of space, and combines that with studies on the structure and evolution of the interstellar medium of galaxies. In addition, we have an active program on the coagulation of dust particles, to aggregates, pebbles, and larger bodies in the general ISM and in protoplanetary disks. Leiden Observatory is actively involved in a large number of astronomical observing facilities, both ground- and space-based. Observations and modeling studies are supported by in house laboratory

²you must also be eligible for a working permit for this country

studies. It has a very active research program concerning polycyclic aromatic hydrocarbon molecules in Space, analysis and interpretation of space-based infrared data, simulations of inter- and circumstellar conditions, controlled growth of pure or mixed interstellar ice analogs and simulation of chemical processes that occur in and on top of the ice.

Institute description Leiden University is a prominent research university in Europe, situated for decades in the top 100 of best Universities worldwide, with approximately 17 000 students and 4 000 staff members. The university consists of 6 faculties, a School of education, and a campus in The Hague, and focuses on the independent practice of research-oriented work in an academic setting. Leiden Observatory is one of the largest academic observatories in the world and ranked in the top 5. It has a very active research programme with 25 scientific staff, 45 post-docs, 80 graduate students and 40 master students. Bachelor and master courses are ETCS courses.

Ideal candidate The position is open to students with the equivalent of a masters degree in physics or physical chemistry. The successful student should have hands-on experience in experimental physics preferably in one or more of the following areas: UV spectroscopy, mass spectrometry, (free electron) laser systems, and ion traps. A good working knowledge in English is required. Certain restrictions on nationality apply.

Working conditions and benefits The appointment is for 4 years and is anticipated to end with a Ph.D. degree at Leiden University. The initial appointment is for one year and your performance will be evaluated after 6 month. After a positive evaluation, the appointment will be extended for the full period. The monthly gross salary will be in accordance with the EC Marie Skłodowska-Curie rates and will be paid by the host organization. The salary may be subjected to tax according to applicable national regulations.

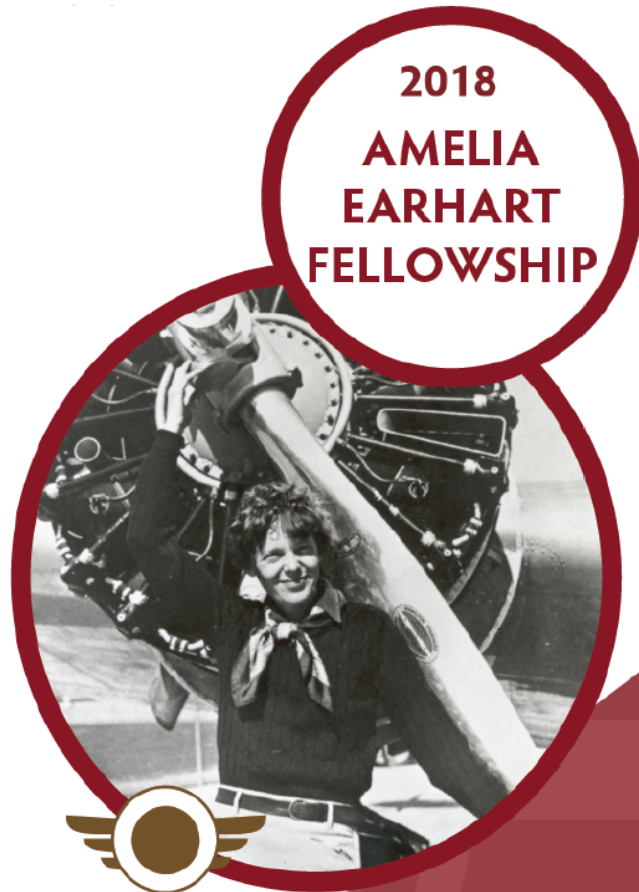
2018 Zonta International Amelia Earhart Fellowship

Application deadline: November 15th



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To download the 2018 AE Fellowship application, [click here](#).

AstroPAH Newsletter

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

Next issue: 23 November 2017
Submission deadline: 10 November 2017