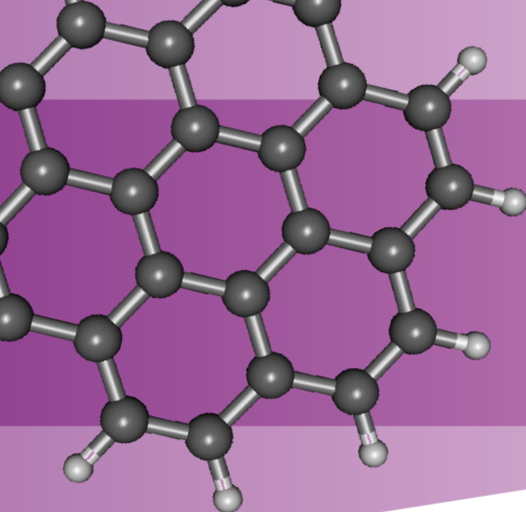
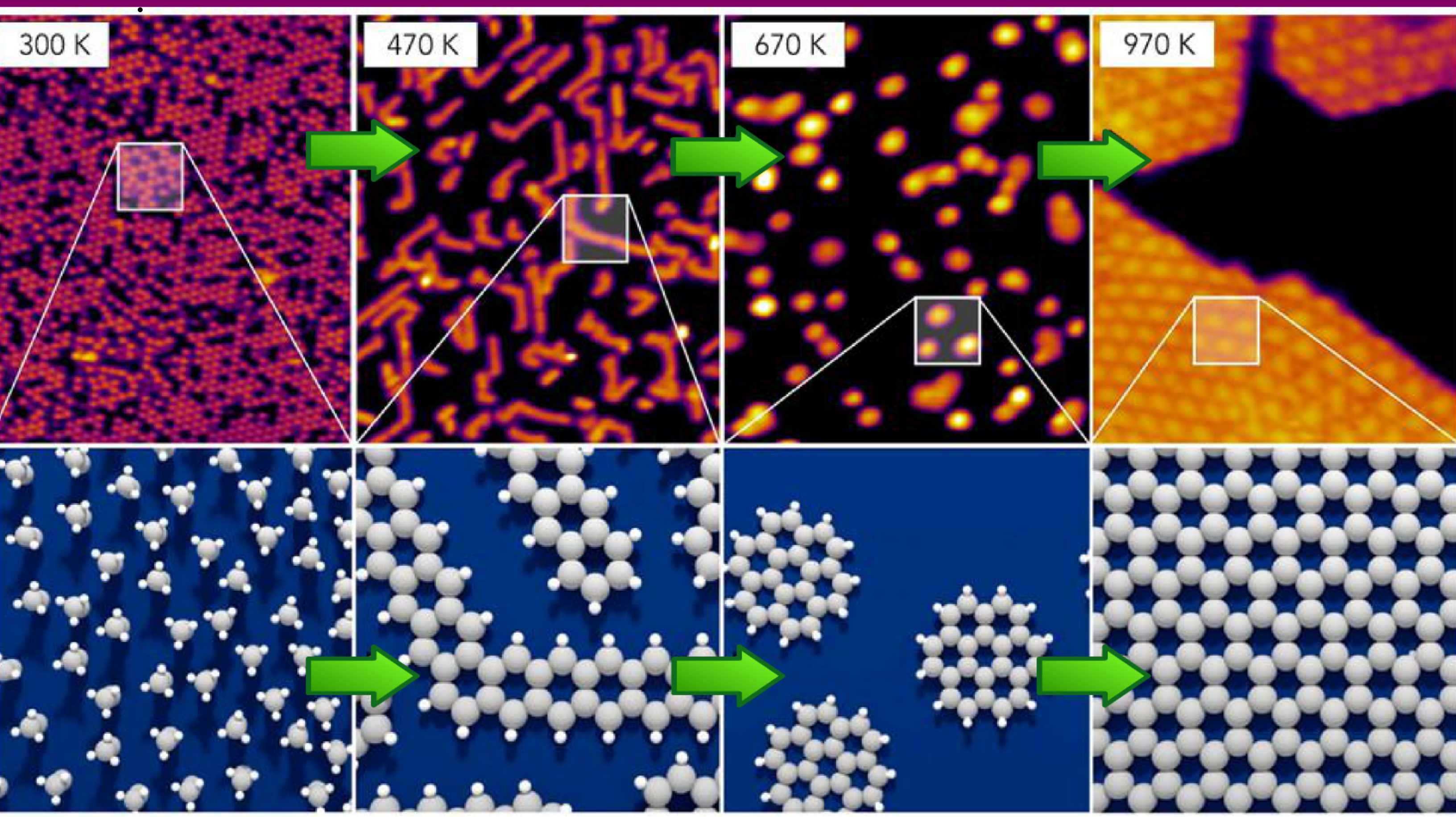


AstroPAH

A Newsletter on Astronomical PAHs

Issue 38 | May 2017



C_2H_4 → PAHs → Graphene

Editorial

Dear Colleagues,

This May we have another exciting newsletter issue for you on the story of PAHs!

On our cover, beautiful images highlight the role of PAHs as intermediates in the formation of graphene from ethene.

This month's *In Focus* presents the new Dutch ORIGINS Center dedicated to research on life on Earth and in the Universe.

Do not miss any of the interesting papers we show in our Abstracts section and, if you are looking for a job on the physics and chemistry of interstellar and/or circumstellar clouds, check our Announcements as well!

AstroPAH can help you promote your science. Visit our webpage or contact us for more information. You can send us your contributions anytime. For publication in June, see the deadlines below.

We thank you all for your contributions so far!

The Editorial Team

Next issue: 20 June 2017.
Submission deadline: 9 June 2017.

Contact us:

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

PAH Picture of the Month

Top: Scanning tunneling microscopy (STM) images of different stages in the dehydrogenation process during annealing experiments from ethene (C_2H_4, T=300 K), through 1D linear PAHs of various lengths (T=470 K), 2D PAHs with 24 carbon atoms (coronene, T=670 K) and finally graphene (T=970 K). **Bottom:** simulated STM images. The full study is available here: Wang et al.,J. Phys. Chem. C, 2017, 121, DOI: 10.1021/acs.jpcc.7b01999

Credits: U. Landman and B. Yoon.

Newsletter Design: Isabel Aleman
Background image: NASA, ESA, and the Hubble Heritage Team (STScI/AURA)

The Dutch Origins Center

http://www.origins-center.nl

Presented by Frank Helmich, Jacintha Ellers, Matthias Heinemann, Inge Loes ten Kate, Jan-Willem Mantel, Roeland Merks, Sijbren Otto, Gijs Wuite on behalf of the Origins Center working group

http://www.origins-center.nl/partners/

The Dutch Science Agenda (Nationale WetenschapsAgenda - NWA)

In 2015, in response to a question from the Dutch ministers for Education, Arts and Science, and of Economic Affairs, multiple groups came together (from academia, medical centers, other higher education, funding agencies, research institutes, employer associations, etc.) to join in the so-called "Knowledge coalition". The aim of this coalition was to increase the influence of society on research, to stimulate cooperation between all the involved parties and to provide the basis of an extra investment in science and research 1 billion Euro per year extra.

The "Knowledge coalition" asked the general public to come up with questions that they felt were the important ones warranting further investigation. The response in May 2015 was overwhelming. Almost twelve thousand questions were received. These questions were grouped in 140 clusters, which were divided again in several Routes, and many were connected to the societal challenges of our time. One of these Routes was, however, dedicated to more fundamental questions and was appropriately named: The origin of life on Earth and in the Universe. It deals with curiosity driven questions such as: "Where do we come from?", "What is our future?", and "Is there life elsewhere in the Universe?"

The whole set of questions and Routes is available from the NWA website https://www.wetenschapsagenda.nl but this website is only available in the Dutch language.

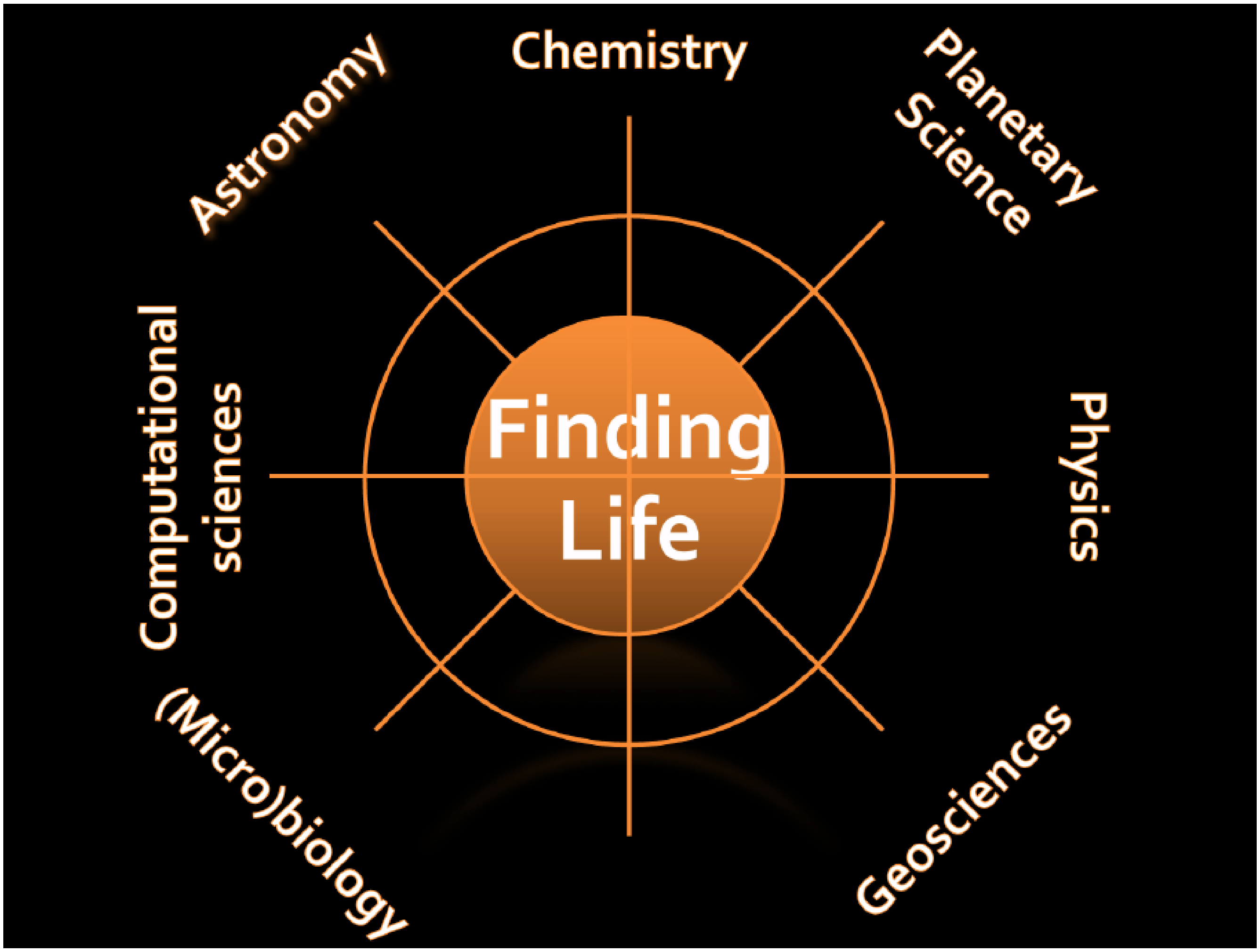

Figure 1: *The topic of "Finding Life" is shared among many disciplines. The other game-changing topics also include biophysics, ecology and evolution.*

The Origin of Life: on Earth and in the Universe

The question about the origin of life and its subsequent evolution is extremely broad and encompasses many disciplines. To study the cradle(s) of life and subsequent development and evolution, astrophysics, exo- and planetary science, geosciences, chemistry, molecular biosciences, biology, biophysics, ecology, mathematics, and computer science all have to work together. In order to achieve a coherent approach several workshops were organized in which over 100 Dutch scientists participated. The result is a list of 5 "game-changing" topics to tackle:

1. **Understanding the Origin and co-evolution of Earth-like planets and Life**
2. **Predicting evolution**
3. **Building and directing life from molecule to biosphere**
4. **Finding extraterrestrial life**
5. **Bridging long temporal and spatial scales**

These five topics should be seen as dots on the horizon that we want to reach in 10-20 years from now or possibly even later. This science has its basis in the disciplines involved, but it also has a strong interdisciplinary character.

It is worthwhile mentioning that most of our research topics are not easily usable for valorization. We stressed in our documents to the Cabinet and "Knowledge coalition" that the research would provide an empirical base for many applications in the future, e.g. in detection and treatment of diseases or estimating risks for the constant changing of our environment. However, we acknowledge that the inherent complexity of the game-changing topics requires to first overcome gaps in our fundamental knowledge that lay the basis for future applications.

In the workshops, we learned that bringing researchers from very different fields together brings out completely new ideas worthy of pursuing now or in the near future. It also showed that the languages and approaches used in different disciplines could be very different. Learning to speak each others language is therefore an indispensable ingredient in the approach.

Origins Center

The Netherlands has strong groups in all the mentioned disciplines and distances within the Netherlands are very small. This led to the concept of a Center that would concentrate on interdisciplinary research around the Origin of Life. This Origins Center would be a virtual Center with nodes all around the country. The Origins Center should support contact and foster collaboration, e.g. through shared PhD students and postdocs working in different institutes with senior staff. It also should be a platform in which we start dedicated workshops, invite experts from abroad and start thinking about lecture series for PhD and master students, as well as for the general public. By incorporating these activities and bringing in experts from around the world, we can begin an internationally based collaboration in which we can begin to tackle the five topics that were laid out above. Because these are such broad questions, experts from every sub-discipline within the aforementioned disciplines will play an important role in helping the Center move forward.

Below we give a description of two of our five long term goals that apply most to PAH research. All five goals can be found on the website http://www.origins-center.nl.

Our Game-Changing Goals

Understanding the Origin and Co-evolution of Earth-like Planets and Life

The Earth is currently the only place where life is known to exist and prevailing opinion suggests that it emerged rapidly within the first billion years following planetary accretion. Complex and intelligent life is the result of a long history of biological evolution that has developed in tandem with coupled atmosphere-ocean-deep Earth processes throughout the geological record. These billion-year timescales, culminating in the modern advanced society that we have today may or may not be typical for the development of comparable and potentially habitable planets elsewhere in the Universe. Delivering a full picture of the co-evolution of Earth and life and their interdependence requires integration of data and research from diverse disciplines including astronomy, astrobiology, (micro)biology and the earth- and planetary sciences. Here we identify three important steps, all based on a deep understanding of both planetary and biological evolution, necessary to provide new breakthroughs in constraining the conditions necessary for the development of habitable Earth-like planets.

1. Which are the boundary conditions under which life could begin?

   To answer this question, we must determine the starting point for life on Earth; to constrain the processes under which Earth-like planets accreted and evolved and to investigate the role of their composition. Detection and identification of abiotic sources of organic molecules that can serve as building blocks of life is needed. Another aspect to be investigated is demonstrating how life can begin from a mixture of organic molecules and mineralogical templates, as well as establishing the environments in which this was possible.

2. How can we trace the composition and extent of the biosphere and the geological record over time?

   For that purpose, it is necessary to identify the earliest life forms and their metabolisms. Ways to do this are: to determine reliable biosignatures to find traces of life in ancient rocks, to track the evolution of life from primitive single celled organisms to communities of more advanced multicellular life through time, and to resolve the persistence and development of life in interplay with planetary evolution and across global catastrophic events such as impacts, climate change, magnetic field excursions, large-scale volcanism, or global climatic changes.

3. What are the dependencies between physical-chemical planetary and biological evolution across a range of timescales?

   The goal here is to determine large-scale links between the biosphere, atmosphere, hydrosphere and geosphere throughout the geological record to the present day and to resolve the role of geological and deep geophysical processes versus shallow environmental processes in controlling near-surface environmental conditions and the evolution of life.

Finding Extraterrestrial Life

Being able to say that life exists in other places, within or outside our Solar system, will fundamentally change our view on the role of humanity in the Universe. Is the Earth unique as a cradle of life? We are in a position where we will find the answer in the next decades.

The enormous technological progress of the past decades has put us in a position to start examining the climate and the *habitability* of other worlds in detail. Within our own Solar System Mars, and the icy moons of Jupiter and Saturn are particularly interesting through the (former) presence of liquid water. Studies of the physical and chemical boundaries, and hallmarks of habitability based upon studies of Earth and in the wider Solar System will enable extrapolation to exoplanets.

An important challenge will be to recognize and understand the chemical *biomarkers* on other worlds, where both climatological and geological circumstances and the biological processes may be significantly different. Future efforts will focus on *in situ* detection of biomarkers on planetary surfaces, as well as through remote sensing. The *in situ* search for biosignatures focuses primarily on biomolecules, organic compounds that life uses, and biominerals on and embedded in the surface, whereas remote sensing focuses on the detection of atmospheric markers that betray the presence of biological activity, such as oxygen and methane on Earth.

The current progress in research into *exoplanets*, i.e., planets around stars other than the Sun, has been particularly remarkable. Thanks to technological advances in the last 2 decades, scientists are getting ever better at not only finding new exoplanets, but also at characterizing their atmospheric properties (as well as the chemistry of planetary systems in formation).

Conclusion

With the Origins Center we aim to stimulate interdisciplinary projects, including research on the compounds of the Interstellar Medium that play an important role in the formation and evolution of stars, planets, comets and asteroids. Also, the relation between molecules present in the ISM and those present in the early atmosphere and rocks of the Earth/exoplanets will be a topic that deserves a place within the Origins Center and which is closely connected to PAH research.

Although we feel strongly encouraged by the response of the scientific community within the Netherlands, funding is not yet guaranteed. However, if the Origins Center is funded we will have some very busy years ahead. **Connecting the disciplines and all Dutch institutes is a major undertaking in itself; however, since science is an international collaborative effort it is also necessary to connect the Origins Center to scientists and research institutes abroad. We hope this article will inspire international interest about our virtual center, and we invite you to contact us if you have any comments, questions or ideas about collaborations or specific research to be done in support of the Origins Center's goals.**

Our opening symposium will be held in Groningen August 31 and September 1 of this year http://www.origins-symposium.nl under the supervision of the Royal Society of Arts and Sciences. You are invited to register.

Effect of Alignment on Polarized Infrared Emission from Polycyclic Aromatic Hydrocarbons

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Polarized emission from polycyclic aromatic hydrocarbons (PAHs) potentially provides a new way to test the basic physics of the alignment of ultrasmall grains. In this paper, we present a new model of polarized PAH emission that takes into account the effect of PAH alignment with the magnetic field. We first generate a large sample of the grain angular momentum **J** by simulating the alignment of PAHs due to resonance paramagnetic relaxation that accounts for various interaction processes. We then calculate the polarization level of the PAH emission features for the different phases of the interstellar medium, including the cold neutral medium (CNM), reflection nebulae (RNe), and photodissociation regions. We find that a moderate degree of PAH alignment can significantly enhance the polarization degree of the PAH emission compared to the previous results obtained with randomly oriented angular momentum. In particular, we find that the smallest negatively charged PAHs in RNe can be excited to slightly suprathermal rotation due to enhanced ion collisional excitation, resulting in an increase of the polarization with the ionization fraction. Our results suggest that an RN is the most favorable environment in which to observe polarized PAH emission and to test the alignment physics of nanoparticles. Finally, we present an explicit relationship between the polarization level of PAH emission and the degree of external alignment for the CNM and RNe. The obtained relationship will be particularly useful for testing the alignment physics of PAHs in future observations.

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ApJ, 2017, 838, id. 112

http://iopscience.iop.org/article/10.3847/1538-4357/aa65cf/meta

Dust dynamics and evolution in HII regions - II. Effects of dynamical coupling between dust and gas

V. V. Akimkin, M. S. Kirsanova, Ya. N. Pavlyuchenkov, D. S. Wiebe

Institute of Astronomy of the Russian Academy of Sciences

In this paper, we extend the study initiated in Paper I by modelling grain ensemble evolution in a dynamical model of an expanding HII region and checking the effects of momentum transfer from dust to gas. The radiation pressure on the dust, the dust drift, and the lug on the gas by the dust are all important process that should be considered simultaneously to describe the dynamics of HII regions. With accounting for the momentum transfer from the dust to the gas, the expansion time of the HII region is notably reduced (for our model of RCW120, the time to reach the observed radius of the HII region is reduced by a factor of 1.5). Under the common approximation of frozen dust, where there is no relative drift between the dust and gas, the radiation pressure from the ionizing star drives the formation of the very deep gas cavity near the star. Such a cavity is much less pronounced when the dust drift is taken into account. The dust drift leads to the two-peak morphology of the dust density distribution and significantly reduces the dust-to-gas ratio in the ionized region (by a factor of 2 to 10). The dust-to-gas ratio is larger for higher temperatures of the ionizing star since the dust grains have a larger electric charge and are more strongly coupled to the gas.

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Search for Hydrogenated C_{60} (fulleranes) in Circumstellar Envelopes

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The recent detection of fullerene (C_{60}) in space and the positive assignment of five diffuse interstellar bands to C_{60}^+ reinforce the notion that fullerene-related compounds can be efficiently formed in circumstellar envelopes and be present in significant quantities in the interstellar medium. Experimental studies have shown that C_{60} can be readily hydrogenated, raising the possibility that hydrogenated fullerenes (or fulleranes, $C_{60}H_m$, $m = 1 - 60$) may be abundant in space. In this paper, we present theoretical studies of the vibrational modes of isomers of $C_{60}H_m$. Our results show that the four mid-infrared bands from the C_{60} skeletal vibrations remain

prominent in slightly hydrogenated C_{60}, but their strengths diminish in different degrees with increasing hydrogenation. It is therefore possible that the observed infrared bands assigned to C_{60} could be due to a mixture of fullerenes and fulleranes. This provides a potential explanation for the observed scatter of the C_{60} band ratios. Our calculations suggest that a feature around 15 µm due to the breathing mode of heavily hydrogenated C_{60} may be detectable astronomically. A preliminary search for this feature in 35 C_{60} sources is reported.

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http://adsabs.harvard.edu/abs/2017arXiv170501807Z

How hydroxylation affects hydrogen adsorption and formation on nanosilicates

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Silicate dust constitutes one of the primary solid components of the Universe and is thought to be an essential enabler for complex chemistry in a number of astronomical environments. Hydroxylated silicate nanoclusters $(MgO)_x(SiO_2)_y(H_2O)_z$, where strongly absorbed water molecules are dissociated on the silicate surface, are likely to be persistent in diffuse clouds. Such precursor species are thus also primary candidates as seeds for the formation and growth of icy dust grains in dense molecular clouds. Using density functional calculations we investigate the reactivity of hydroxylated pyroxene nanoclusters $(Mg_4Si_4O_{12})(H_2O)_N$ (N=1-4) towards hydrogen physisorption, chemisorption and H_2 formation. Our results show that increased hydroxylation leads to a significant reduction in the energy range for the physisorption and chemisorption of single H atoms, when compared to bare silicate grains and bare bulk silicate surfaces. Subsequent chemisorption of a second H atom is, however, little affected by hydroxylation. The H_2 reaction barrier for the recombination of two chemisorbed H atoms tends to follow a linear correlation with respect to the $2H_{\rm chem}$ binding energy, suggestive of a general Brønsted-Evans-Polanyi relation for H_2 formation on silicate grains, independent of dust grain size, composition and degree of hydroxylation.

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Molecular Astrophysics, 2017, 7, 1

http://www.sciencedirect.com/science/article/pii/S2405675816300434

Corannulene and its complex with water: A tiny cup of water

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We report the results of a broadband rotational spectroscopic study of corannulene, $C_{20}H_{10}$, all of its singly substituted ^{13}C isotopologues, and a complex of corannulene with one molecule of water. Corannulene is a polycyclic aromatic hydrocarbon (PAH) with a curved structure that results in a large dipole moment. Observation of ^{13}C isotopic species in natural abundance allowed us to precisely determine the molecular structure of corannulene. The differences between the experimental CC bond lengths correlate to the double-bond characters predicted using Kekules resonance structures. In the case of $C_{20}H_{10}$–H_2O, the water molecule is found to reside inside the bowl-like structure of corannulene. Our experimental and theoretical results indicate that the water molecule rotates freely around its C_2 axis and that dispersion interactions are the dominant contribution to the binding.

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http://pubs.rsc.org/en/content/articlelanding/2017/cp/c7cp01506b#!divAbstract

Announcements

Post-doctoral position on the physics and chemistry of interstellar and circumstellar clouds at the CSIC

Advertised by Marcelino Agundez

We seek a candidate with a PhD, preferentially in Astrophysics, for a postdoctoral research position on the study of the physics and chemistry of interstellar and/or circumstellar clouds. The goal of the project is to develop models that include basic physical and chemical processes to confront with astronomical observations obtained with millimeter-to-optical observatories (ALMA, IRAM, SOFIA, JWST, GTC). The ideal candidate should have experience in the development of numerical models studying aspects such as the energy balance, hydrodynamics, shocks, chemical processes on the gas phase and on grain surfaces, radiative transfer, etc. We will also consider candidates with a background in the analysis of data gathered with (sub-)millimeter, infrared, and optical telescopes. The postdoc will take part of the Molecular Astrophysics group of CSIC, based in Madrid (Spain). The selected candidate will be employed for a period of 2 to 3 years (depending of funding and status of the project) with a salary that will depend on research experience. The preferred starting date is September 2017, although it may be adapted to the selected candidate.

If you are interested, please send a Curriculum Vitae and a short letter of motivation to the following e-mail address: marcelino.agundez@icmm.csic.es. Applications received before June 2017 will receive full consideration.

Application deadline: 31 May 2017.

Contact: marcelino.agundez@icmm.csic.es

AstroPAH Newsletter

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

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