the extensive and ubiquitous role of polycyclic aromatic hydrocarbons in space

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 play in the physics and chemistry of the interstellar medium of galaxies.

Polycyclic aromatic hydrocarbons (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 Early-stage researcher (ESR) positions are available across the EUROPAH network. 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 years* of your research career, since, *e.g.*,, completion of your masters' degree,
- not already possess a doctorate degree,
- be willing to move to a country within the network† 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, listing your favoured projects in order of preference, to recruitment@europah.eu by the deadline: 15th September 2016. After this first round each institute will contact successful candidates. You will then have to provide references may be required to attend interview. Note that only applications submitted through recruitment@europah.eu will be considered.

* full-time equivalent research experience

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

ESR 2 Density Functional Theory calculations of the catalytic activity of PAHs and their interaction with grain surfaces

Host Institute: Institute for Physics and Astronomy, Aarhus University

Host Country: Denmark

Start date: May 1st 2017

The candidate will be employed at the Institute for Physics and Astronomy at Aarhus University and will be enrolled in the PhD programme at Aarhus University under the supervision of Prof B. Hammer.

Project description

The rates of formation of small molecules like H_2, OH, H_2O and NH_3 in the interstellar medium can be greatly enhanced through catalytic effects. PAHs are proposed to act as catalysts for the formation of such species and this theoretical surface science project aims to elucidate these reactions. Specifically the aim is to: i) Calculate binding energies and addition barriers for oxygen and nitrogen on PAHs. ii) Calculate preferential adsorbate/functionalisation structures, iii) Calculate structural models for interstellar carbonaceous or silicate type nano-particulate dust grains, iv) Calculate the physisorption, chemisorption, and grafting of PAHs onto the surfaces of such dust grains, v) Calculate potential energy surfaces (PES) for Eley-Rideal type reactions, vi) Calculate pathways for conversion of small PAHs into larger PAHs/graphene layers. The project will include secondments to University of Milan (Italy) and Universite Paul Sabatier, Toulouse (France) for dynamic calculations for PAHs functionalization and reactivity and Graphic Science Ltd., our outreach-focussed enterprise partner, in developing outreach activities. The candidate will be enrolled in the Graduate School of Science and Technology at Aarhus University and will be expected to complete a PhD program which includes completion of local academic training requirements.

Group description

The Theoretical Surface Science Group at Aarhus University carries out research in the field of density functional theory calculations in surface and nanoscience with a particular emphasis on automation of equilibrium structure and reaction pathway determinations. http://phys.au.dk/forskning/forskningsomraader/condensed-matter-physics/theoretical-surface-science-group/. The group has extensive experience in the development and application of density functional theory techniques and works closely with experimentalists.

Institute description

The Graduate School of Science and Technology (GSST) is the largest graduate school at Aarhus University with almost 800 PhD students enrolled. PhD programmes at GSST are well structured, and participation in PhD courses, visits to international research institutions or universities and dissemination of knowledge are parts of the PhD education. Aarhus is Denmark's second largest city, a true student town, compact and close to the sea.

Ideal candidate

The successful candidate will have a masters' degree (or equivalent) in physics, chemistry or astronomy. Programming experience is required and candidates with experience using UNIX/Linux operating systems and coding in python will be preferred.

Working conditions and benefits

The candidate will become an employee of the Dep. Phys and Astron. and receive a competitive monthly gross salary in accordance with the EC Marie Sklodowska-Curie. The contract period will last for 3 years.

ESR #3 Photocatalytic activity of PAHs

Host Institute: Institute for Physics and Astronomy, Aarhus University

Host Country: Denmark

Start date: 1st May 2017

The candidate will be employed at the Institute for Physics and Astronomy at Arhus University and will be enrolled in the PhD programme at Aarhus University under the supervision of Assoc Prof L. Hornekær.

Project description

The ability of PAHs to act as catalysts and contribute to the chemical complexity of the ISM depends on the photo-stability of functionalised PAH molecules. In this experimental project you will study the photocatalytic activity of PAHs by measuring the photo-fragmentation and photo-catalytic reaction pathways of chemically functionalized PAHs using a range of surface science techniques, including mass spectrometry and scanning tunnelling microscopy under ultra-high vacuum conditions. The results will be compared to DFT calculations. The project will include a secondment to the FELIX Laboratory, Radboud University (Netherlands) for gas phase photo fragmentation experiments and Graphic Science Ltd., our outreach-focussed enterprise partner, in developing outreach activities. You will play an active role in the research group contributing to other experiments when required and supervising bachelor students' projects. The candidate will be enrolled in the Graduate School of Science and Technology at Aarhus University and will be expected to complete a PhD program which includes completion of local academic training requirements.

Group description The Surface Dynamics Group at Aarhus University carries out research in the fields of surface astrophysics and nanoscience with a particular emphasis on the role of carbon based materials. http://phys.au.dk/forskning/forskningsomraader/condensed-matter-physics/surface-dynamics-group/. The group has extensive experience in the use of surface science techniques, in particular STM and thermal desorption methods.

Institute description The Graduate School of Science and Technology (GSST) is the largest graduate school at Aarhus University with almost 800 PhD students enrolled. PhD programmes at GSST are well structured, and participation in PhD courses, visits to international research institutions or universities and dissemination of knowledge are parts of the PhD education. Aarhus is Denmark's secondest largest city, a true student town, compact and close to the sea.

Ideal candidate The successful candidate will have a masters' degree (or equivalent) in physics, chemistry or astronomy. Experimental laboratory experience is required and candidates with experience of ultra-high vacuum techniques will be preferred.

Working conditions and benefits The candidate will become an employee of the Dep. Phys and Astron. and receive a competitive monthly gross salary in accordance with the EC Marie Sklodowska-Curie. The contract period will last for 2 years under the EUROPAH network + 1 additional year under a Danish PhD student contract (3 years in total).

ESR #4 PAHs and the organic inventory of meteorites and comets
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 prof. Xander Tielens.

Project description

Carbonaceous meteorites and comets show a varied organic composition which is thought to reflect, at least partly, a heritage that dates back to interstellar clouds. However, a variety of processes on the parent asteroidal body and the comet will have modified any inherited material, including thermal processing in an aqueous or icy environment as well as processing by energetic ions and photons in the presence of nanograins. PAHs are one key component in the interstellar medium. The graduate student will develop models for the chemical evolution of PAHs in an aqueous environment and apply this to asteroids in the early solar system as well as for the photochemical evolution of ices and apply this to comets in the early solar system. He/she will identify chemical markers for these processes, make predictions for ALMA and JWST observations, and assess the astronomical implications by comparison to meteoritic and cometary composition.

As part of the study, secondments are foreseen to Heriot Watt University to study the characteristics of functionalized PAHs in ices, to Aarhus University to study the stability and catalytic activity of functionalized PAHs and to Graphic Science for the outreach project and travelling exposition development.

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 combins 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 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 world wide, with approximately 17000 students and 4000 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 astronomy, physics, physical chemistry, or Earth sciences. The successful student should have experience in experimental physics or computational chemistry preferably in one or more of the following areas: Raman and IR spectroscopy, density functional theory. A sound background in molecular astrochemistry is required, as is a good working knowledge in English. Certain restrictions on nationality apply related to mobility requirements from the Marie Curie Program.

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

ESR #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 Leiden Observatory and will aim 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 a large set of structurally different PAHs upon excitation by VUV and UV/VIS radiation from dye lasers, synchrotrons (DESIRS/SOLEIL) and free electron lasers (FELIX/FELICE/FLARE) using a mobile ion trap time-of-flight mass spectrometer. 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 chemical steps are backed-up by theoretical simulations and 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. The scheduled experiments take place in the Sackler Laboratory for Astrophysics (www.laboratory-astrophysics.eu). Leiden Observatory is actively involved in a large number of astronomical observing facilities, both ground and space based. The astrochemistry groups have 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 world wide, with approximately 17000 students and 4000 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. See also www.strw.leidenuniv.nl.

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: UHV vacuum technology, (Nd:YAG-dye) lasers, mass spectrometry, specifically TOF and ion trap, experimental control and data-acquisition schemes. A sound background in molecular physics is required, as is a good working knowledge in English. Certain restrictions on nationality apply related to mobility requirements from the Marie Curie Program.

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

ESR #6 Photophysics and photochemistry of PAH interactions in icy solids

Host Institute: Leiden Observatory, Leiden University

Host Country: The Netherlands

Start date: No later than summer of 2017.

The candidate will be employed in the Sackler Laboratory for Astrophysics at Leiden Observatory and will aim for a doctorate degree under the supervision of prof. Harold Linnartz.

Project description
PAHs are volatiles that are expected to freeze out onto cold dust grains, typically embedded in a matrix of amorphous water. This is fully in line with the observation that the typical PAH IR emission features vanish in regions where ices are known to govern interstellar chemistry. In an ice matrix, chemical processes are different and largely dominated by surface diffusion reactions. Such reactions can be triggered by energetic photons from the interstellar radiation field, ionizing PAHs (and charging ices), or fragmenting, offering pathways to recombine with other ice fragments.
The graduate student will investigate the spectroscopy and dynamics of PAHs and vacuum UV induced photoproducts of a series of model systems, varying in size and geometry, embedded in low temperature (10-15 K) amorphous water ices as PAH models in the bulk of model interstellar grain mantles. Both optical (electronic) and infrared (vibrational) spectra will be recorded in a unique and fully operational setup to study in situ and in real time chemical processes in interstellar ice analogues. We expect to gain insights in the solid state chemistry of PAHs and to realize a new tool to search for PAHs in space, namely through their electronic solid state features; observations with optical telescopes (VLT and from 2024 onwards with the E-ELT) make it possible to search for frozen PAH features. The data are included in the Leiden Database for Ice.
Secondments of in total 5 months are planned to Heriot Watt University in Edinburgh to work on electron induced ice chemistry. Special attention will be given to a 2 months outreach project in collaboration with Graphics Science, one of the industrial partners.
Group description The Sackler Laboratory for Astrophysics (www.laboratory-astrophysics.eu) at Leiden Observatory is a large experimental research facility fully dedicated to the physical and chemical characterization of molecular processes taking place in the interstellar medium. Both gas phase and solid state experiments are performed to interpret and guide astronomical observations and to derive the parameters needed as input in astrochemical models. With five ice setups, the laboratory is one of the largest interstellar ice research facilities worldwide. The laboratory is fully embedded within the infrastructural settings of Leiden Observatory that is actively involved in a large number of astronomical observing facilities, both ground and space based.

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. See also www.strw.leidenuniv.nl.

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: vacuum technology, optical and infrared optics, cryogenics, experimental control and data-acquisition schemes (labview). A sound background in molecular physics is required, as is a good working knowledge in. 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 the Leiden University. The initial appointment is for one year and the performance will be evaluated after 6 months. After a positive evaluation, the appointment will be extended for the full period. The monthly gross salary of the first three years will be in accordance with the EC Marie Sklodowska-Curie rates and will be paid by the host organization. The fourth year follows the Dutch regulations for PhD students. The salary may be subjected to tax according to applicable national regulations.

ESR #10 Non-thermal plasma decomposition of PAHs: Understanding the reaction pathways and mechanisms

Host Institute: Department of Electrical Engineering and Electronics, University of Liverpool

Host Country: UK

Start date: 1st May 2017

The candidate will be employed at the University of Liverpool and will read for a doctorate degree under the supervision of Dr. Xin Tu.

Project description The objective of this project is to investigate the energetic processing of PAHs and related species driven by non-thermal plasma and to gain in-depth insight into the reaction mechanisms and pathways of the plasma process. A fundamental understanding of the roles of different energetic or reactive species for the decomposition of PAHs and formation of fragments and by-products (*e.g.* light hydrocarbons, carbon, etc) in the plasma will be available by combined means of gas analysis (FTIR/GC/GCMS), and advanced plasma diagnostics. The ESR will be trained in the use of equipment for gas analysis and plasma diagnostics at the University of Liverpool. The project will involve collaborations (secondments) with both academic and industrial partners.

Group description Our group has been working for many years on interdisciplinary research at the interface of plasma physics and plasma chemistry directed towards environmental and energy applications. Our research has been largely focused on the development and deployment of novel plasma processes for environmental clean-up, energy conversion and fuel synthesis, waste-to-energy and synthesis of carbon nanomaterials. The group has a wide range of plasma systems with state-of-art electrical, optical diagnostic tools (Emission spectrometers, ICCD cameras, Langmuir probes and laser systems), gas analytic facilities (e.g. GC, FTIR, GC-MS and ozone monitor). The students will be trained to use all the analytical equipment they are not already familiar with and will be expected to become competent in the use of the plasma systems.
https://www.liverpool.ac.uk/electrical-engineering-and-electronics/staff/xin-tu/

Institute description The University of Liverpool (http://www.liv.ac.uk) is a member of the prestigious Russell Group, comprising the leading research universities in the UK. The research quality of the Department of Electrical Engineering and Electronics in RAF (2014) has been judged as 90 % world leading or international excellence. The Technological Plasma Group at the University of Liverpool is one of the leading plasma groups in the world, working on low temperature plasmas and their applications in pollution control, energy conversion, bio-engineering, sterilization/ decontamination, surface modification and material processing.

Ideal candidate The ideal candidate should have a strong background and interest in one of the following research areas: plasma chemistry, plasma physics, hydrocarbon chemistry or catalysis. The candidate should have a first class MEng or MSc degree (or equivalent) in Chemical Engineering, Chemistry, Physics or a related subject. Good written and oral communication skills are essential (for candidates who are not from a majority English-speaking country, please check postgraduate English language entry requirements of the University of Liverpool).

Working conditions and benefits The candidate will be employed at the University of Liverpool and enrolled for a PhD program. The contract will be for 3 years. The monthly gross salary will be in accordance with the EC Marie Sklodowska-Curie rates and will be paid by the University of Liverpool. Salary may be subjected to tax according to applicable national regulations.

ESR #11 Spectroscopy of charged PAHs in ion traps

Host Institute: Institute of Physics I, University of Cologne

Host Country: Germany

Start date: 1st April 2017 (A later start up to 1st September 2017 at the latest can be considered)

The candidate will be employed at the Institute of Physics I (University of Cologne) and will read for a doctorate degree under the supervision of Prof. S. Schlemmer and Dr. S. Brünken.

Project description Spectroscopic signatures of PAHs from the mid-infrared to UV spectral region are needed to compare to astronomical observations. The aim of this project is to develop, implement and investigate sensitive action spectroscopic schemes, like multiple-photon dissociation (MPD) or rare-gas messenger techniques, to measure vibrational and ultimately electronic spectra of different classes of PAH ions under conditions resembling those in space. Experiments will be performed on mass-selected, cold and isolated gas-phase PAH ions in cryogenic 22-pole ion trap instruments, one located in Cologne, and one at the infrared Free Electron Laser Facility (FELIX) at the Radboud University (Nijmegen, Netherlands). Complementary measurements of electronic PAH spectra will be conducted during a six month secondment to the Université Paul Sabatier (Toulouse, France) using the PIRENEA cold FTICR setup.

Group description The Cologne Laboratory Astrophysics group offers a longstanding expertise in gas-phase laser spectroscopy and in the development and operation of sophisticated experimental instrumentation, like the ion-trap instruments to be used in this research project. Being embedded in the astrophysical institute and through many international collaborations in diverse fields of astrophysics/-chemistry, the group provides a stimulating and multi-disciplinary environment.

Institute description The University of Cologne, located in a vibrant, international and multi-cultural city, is one of the oldest and largest universities in Germany, recognized for its high standards of graduate education and international reputation of academic accomplishment. It is one of eleven German Universities of Excellence, offering exceptional institutional support for international students.

Ideal candidate We are looking for a highly motivated candidate holding (or expecting to receive) a Master's degree or equivalent in (Astro-/) Physics, Chemistry or a related field. Experience with experimental work, in particular in the fields of gas phase laser spectroscopy and mass spectroscopy under ultra-high vacuum conditions is highly desirable. The ability to work both independently and within a team is a key asset. The working language is English.

Working conditions and benefits The successful candidate will be employed by the University of Cologne as a research assistant for the duration of 3 years, and be enrolled as a doctoral student to obtain the degree Dr. rer. nat. (equivalent to PhD). The monthly gross salary will be in accordance with the EC Marie Sklodowska-Curie rates and will be paid by the host organization, including a generous mobility and family allowance. The salary may be subjected to tax and deductions for health insurance and other social benefits according to applicable national regulations. The University of Cologne is an equal opportunities employer. Preference will be given to suitably qualified women, all other qualifications and requirements being equal.

ESR #12 Non-adiabatic dynamics and dissipation in the reactivity of PAH-related complexes

Host Institute: Laboratoire Collisions Agrégats Réactivité (LCAR), Université Toulouse III Paul Sabatier (UPS)

Host Country: France

Start date: 1st July 2017 - 1st October 2017

The candidate will be employed at LCAR and enrolled in the UPS doctorate school of matter sciences (EDSDM, www.edsdm.ups-tlse.fr), under the supervision of CNRS researcher Didier Lemoine.

Project description *Objectives*: Depending on the background and experience of the candidate the objectives are to be chosen from:
i) Model and simulate energy relaxation in PAH complexes, following either UV irradiation or reactive H atom collisions; ii) Investigate dynamically the various relaxation channels and energy transfer mechanisms: electronic-to-vibrational relaxation, phonon excitations, nonadiabatic transitions and electronic excitations in large PAHs; iii) Apply a multiangle-like approach (e.g. Time-Dependent Density Functional-based Tight Binding "TD-DFTB" approach with classical molecular dynamics, quantum wave packet dynamics coupled with a quantum bath of phonon modes or electron-hole pair states to treat the reaction dynamics of small molecules with a surface or large PAH, Multi-Configuration Time-Dependent Hartree algorithm for low-dimensionality systems with fully quantum and fully explicit description of all considered degrees of freedom) to study the photoreactivity of water cluster/ice or H atoms interacting with PAHs, the photofragmentation of PAH clusters and the Eley-Rideal reaction dynamics of H_2 formation on PAHs.
Expected results: i) Theoretical/computational tools for the simulation of coupled electronic and vibrational dynamics, considering all degrees of freedom either explicitly or via bath representations; ii) Assess the role of electronic excitations in the fragmentation/reactivity of PAH-related complexes; iii) Quantify electronic/vibrational dissipation in the reaction dynamics of small molecules.
Planned secondments: Graphic Science, 2 months: outreach project and website development; Aarhus University, 2 x 3 months: apply Density Functional Theory to generate potential energy surfaces or to benchmark the DFTB approach (collaboration with Bjørk Hammer, supervisor ESR 2).
PhD additional training: at www.edsdm.ups-tlse.fr select English and click "Doctoral program"

Group description The PhD research will be co-supervised by Didier Lemoine, Bruno Lepetit and Fernand Spiegelman, between the LCAR-Theory and LCPQ-MAD teams (www.lcar.ups-tlse.fr/spip.php?rubrique35&lang=en and www.lcpq.ups-tlse.fr/spip.php?rubrique35&lang=en) gathering a number of complementary skills, thus backing up the broad and rich PhD project. The two teams have access to local HPC (high performance computing) resources in both LCAR and LCPQ institutes. In addition, there is strong theory-experiment interplay with the team of Christine Joblin (IRAP, UPS), supervisor ESR 13, which will also benefit the PhD project.

Institute description www.lcar.ups-tlse.fr ; www.lcpq.ups-tlse.fr ; www.univ-tlse3.fr

Ideal candidate holding a Master's degree in physics (or physical chemistry) with most of the following expertise: quantum physics/chemistry, molecular reaction dynamics, surface science, computational skills, numerical analysis and interest for methodological developments

Working conditions and benefits The successful candidate will be employed by UPS under a three-year PhD contract and enrolled as a doctoral student to obtain a PhD. The gross salary will be in accordance with the EC Marie Sklodowska-Curie rates and will be paid by UPS, including a mobility

allowance to cover secondments and a family allowance if applicable. The salary will be subjected to tax and deductions for health insurance and other social benefits according to French regulations.

ESR #16 Innovating in Outreach in a European Network Environment

Host Institute: *Graphic Science Ltd.*

Host Country: *UK*

Start date: *To be agreed between 1st April 2017 - 1st October 2017*

The candidate will be employed at Graphic Science Ltd. and will read for a doctoral degree at University of Bristol under the supervision of Professor Justin Dillon.

Project description

The project's focus addresses the research question: "How can innovative communication practices enable communities with low science capital to engage more effectively in citizen participation on complex scientific issues?" In developing a thesis responding to this question, the appointee will: i) Develop a coherent programme of outreach activities with associated training and materials that will allow members of the EUROPAH network to engage EU citizens with the results, processes and wider scientific context of their research. (The activities will be targeted at a specific group defined early in the process, characterised as traditionally underserved, possessing low science capital and being present across a range of European States.) ii) Develop and test a set of robust, rigorous and appropriate evaluation tools to accurately assess the impact of that outreach on both the audiences engaged and upon the researchers themselves, with a view to identifying learning from each side. iii) Disseminate findings and propose a contextually-appropriate framework of best practice for raising science capital among the target audiences. iv) Develop mechanisms for embedding further Public Engagement activity into the member institutions of the network with a view to establishing an ongoing legacy of Public Engagement activity. v) Participate in the co-development on new activities including a bid to present at the Royal Society Summer Exhibition during the operational period of EUROPAH.

Host description

Graphic Science is a communications and education agency specialising in taking science, technology, engineering and maths (STEM) to a variety of audiences. We have substantial in-house expertise in the development and evaluation of new resources. Team members have many years' experience using iterative prototyping and substantial audience/user testing. We employ a range of quantitative and qualitative research methodologies including surveys, interviews and focus groups, content and discourse analysis. Analytic tools include excel and nvivo. Prof Graham Turner holds a professorship within the area of communication. He is a specialist in applied languages, translation and communication with particular reference to 'hard-to-reach' minority language communities including Deaf sign language users. https://www.hw.ac.uk/schools/management-languages/staff-directory/graham-turner.htm

Ideal candidate

The ideal candidate will have a Bsc. BA. degree (or equivalent) in a STEM subject area and be an effective and experienced STEM communicator. They should have worked across a range of media, and with varied and preferably under-served audiences. A good knowledge of science in general is essential and a knowledge of physical chemistry or chemical physics desirable. They should be able to demonstrate a good grasp of the cultural and political background to the Public Engagement with STEM movement across the continent of Europe. They must be sufficiently capable in their use of English (IELTS 6.5 minimum) to enable them to undertake effective postgraduate research.

Working conditions and benefits

The appointment will be for a fixed term of 36 months, based at Graphic Science in the South West of England with frequent travel to Heriot Watt University (Edinburgh, Scotland) where, subject to negotiations, the candidate will be registered at the Graduate School. There will be a number of

visits to other institutions within the network. The monthly gross salary will be in accordance with the EC Marie Sklodowska-Curie rates and will be paid by the host organization. The salary will be subject to tax according to applicable UK regulations.