AstroChemical Newsletter #20

June 2017

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Abstracts

Silicon-bearing molecules in the shock L1157-B1: first detection of SiS around a Sun-like protostar

L. Podio, C. Codella, B. Lefloch, N. Balucani, C. Ceccarelli, R. Bachiller, M. Benedettini, J. Cernicharo, N. Faginas-Lago, F. Fontani, A. Gusdorf, and M. Rosi

The shock L1157-B1 driven by the low-mass protostar L1157-mm is an unique environment to investigate the chemical enrichment due to molecules released from dust grains. IRAM-30m and Plateau de Bure Interferometer observations allow a census of Si-bearing molecules in L1157-B1. We detect SiO and its isotopologues and, for the first time in a shock, SiS. The strong gradient of the [SiO/SiS] abundance ratio across the shock (from >=180 to ~25) points to a different chemical origin of the two species. SiO peaks where the jet impacts the cavity walls ([SiO/H2] ~ 1e-6), indicating that SiO is directly released from grains or rapidly formed from released Si in the strong shock occurring at this location. In contrast, SiS is only detected at the head of the cavity opened by previous ejection events ([SiS/H2] ~ 2e-8). This suggests that SiS is not directly released from the grain cores but instead should be formed through slow gas-phase processes using part of the released silicon. This finding shows that Si-bearing molecules can be useful to distinguish regions where grains or gas-phase chemistry dominates.

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Kinetic Monte Carlo Simulations of the Grain-surface Back-diffusion Effect

Eric R. Willis, Robin T. Garrod

Rate-equation models are a widely used and inexpensive tool for the simulation of interstellar chemistry under a range of physical conditions. However, their application to grain-surface chemical systems necessitates a number of simplifying assumptions, due to the requirement to treat only the total population of each species, using averaged rates, rather than treating each surface particle as an independent entity. While the outputs from rate-equation models are strictly limited to such population information, the inputs—in the form of the averaged rates that control the time-evolution of chemical populations—can be guided by the results from more exact simulation methods. Here, we examine the effects of back-diffusion, wherein particles diffusing on a surface revisit binding sites on the lattice, slowing the total reaction rate. While this effect has been studied for two-particle systems, its influence at greater surface coverage of reactants has not been explored. Results from two Monte Carlo kinetics models (one a 2D periodic lattice, the other the surface of a three-dimensionally realized grain) were used to develop a means to

incorporate the grain-surface back-diffusion effect into rate-equation methods. The effects of grain size, grain morphology, and surface coverage on the magnitude of the back-diffusion effect were studied for the simple H+H reaction system. The results were fit with expressions that can be easily incorporated into astrochemical rate-equation models to accurately reproduce the effects of back-diffusion on grain-surface reaction rates. Back-diffusion reduces reaction rates by a maximum factor of around 5 for the canonical grain of ~10^6 surface sites, but this falls to unity at close to full surface coverage.

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Full-text URL: https://arxiv.org/abs/1704.05799

How hydroxylation affects hydrogen adsorption and formation on nanosilicates

Boutheïna Kerkeni, Marie-Christine Bacchus-Montabonel, Stefan T. Bromley

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(SiO2)y(H2O)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 (Mg4Si4O12)(H2O)N (N = 1–4) towards hydrogen physisorption, chemisorption and H2 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 H2 reaction barrier for the recombination of two chemisorbed H atoms tends to follow a linear correlation with respect to the 2H chemical binding energy, suggestive of a general Brønsted–Evans–Polanyi relation for H2 formation on silicate grains, independent of dust grain size, composition and degree of hydroxylation.

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Full-text URL: http://www.sciencedirect.com/science/article/pii/S2405675816300434

Formation of Complex Molecules in Prestellar Cores: a Multilayer Approach

A.I. Vasyunin, P. Caselli, F. Dulieu, I. Jiménez-Serra

We present the results of chemical modeling of complex organic molecules (COMs) under conditions typical for prestellar cores. We utilize an advanced gas-grain astrochemical model with updated gas-phase chemistry, with a multilayer approach to ice-surface chemistry and an up-to-date treatment of reactive desorption based on recent experiments of Minissale et al. (2016). With the chemical model, radial profiles of molecules including COMs are calculated for the case of the prototypical prestellar core L1544 at the timescales when the modeled depletion factor of CO becomes equal to that observed. We find that COMs can be formed efficiently in L1544 up to the fractional abundances of 10(-10) wrt. total hydrogen nuclei. Abundances of many COMs such as CH3OCH3, HCOOCH3, and others peak at similar radial distances of ~2000-4000 AU. Gas-phase abundances of COMs depend on the efficiency of reactive desorption,

which in turn depends on the composition of the outer monolayers of icy mantles. In prestellar cores, the outer monolayers of mantles likely include large fractions of CO and its hydrogenation products, which may increase the efficiency of reactive desorption according to Minissale et al. (2016), and makes the formation of COMs efficient under conditions typical for prestellar cores, although this assumption is yet to be confirmed experimentally. The hydroxyl radical (OH) appears to play an important role in gas-phase chemistry of COMs, which makes it deserving further detailed studies.

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Single photon transient hot electron ionization of C60

K. Hansen

Recent experiments have demonstrated that C60 can ionize in a thermal process after absorption of a photon with energy far above the ionization energy. This indirect ionization mechanism is investigated here by calculating the total and singly charged ion yields, electron energy distributions, and effective electronic temperatures as a function of photon energy.

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Full-text URL: http://pubs.rsc.org/en/content/articlelanding/2017/cp/c7cp01705g#!divAbstract

Complex Organic Molecules Towards Embedded Low-Mass Protostars

Jennifer B. Bergner, Karin I. Oberg, Robin T. Garrod, Dawn M. Graninger

Complex organic molecules (COMs) have been observed towards several low-mass young stellar objects (LYSOs). Small and heterogeneous samples have so far precluded conclusions on typical COM abundances, as well as the origin(s) of abundance variations between sources. We present observations towards 16 deeply embedded (Class 0/I) low-mass protostars using the IRAM 30m telescope. We detect CH2CO, CH3CHO, CH3OCH3, CH3OCHO, CH3CN, HNCO, and HC3N towards 67%, 37%, 13%, 13%, 44%, 81%, and 75% of sources respectively. Median column densities derived using survival analysis range between 6.0x1e10 cm-2 (CH3CN) and 2.4x1e12 cm-2 (CH3OCH3) and median abundances range between 0.48% (CH3CN) and 16% (HNCO) with respect to CH3OH. Column densities for each molecule vary by about one order of magnitude across the sample. Abundances with respect to CH3OH are more narrowly distributed, especially for oxygen-bearing species. We compare observed median abundances with a chemical model for low-mass protostars and find fair agreement, although some modeling work remains to bring abundances higher with respect to CH3OH. Median abundances with respect to CH3OH in LYSOs are also found to be generally comparable to observed abundances in hot cores, hot corinos, and massive young stellar objects. Compared with comets, our sample is comparable for all molecules except HC3N and CH2CO, which likely become depleted at later evolutionary stages.

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Experimental investigation of the reaction of helium ions with dimethyl ether: stereodynamics of the dissociative charge exchange process

Andrea Cernuto, Paolo Tosi, Luca M. Martini, Fernando Pirani, Daniela Ascenzi

The fate of dimethyl ether (DME, CH3OCH3) in collisions with He+ ions is of high relevance for astrochemical models aimed at reproducing the abundances of complex organic molecules in the interstellar medium. Here we report an investigation on the reaction of He+ ions with DME carried out using a Guided Ion Beam Mass Spectrometer (GIB-MS), which allows measurements of reactive cross sections and branching ratio (BR) as a function of the collision energy. We obtain insights on the dissociative charge (electron) exchange mechanism by investigating the nature of the non-adiabatic transitions between the relevant potential energy surfaces (PESs) in an improved Landau-Zener approach. We find that the large interaction anisotropy could induce a pronounced orientation of the polar DME molecule in the electric field generated by He+ so that at short distances the collision complex is confined within pendular states, a particular case of bending motion, which give rise to intriguing stereodynamic effects. The positions of the intermolecular potential energy curve crossings indicate that He+ captures an electron from an inner valence orbital of DME, thus causing its dissociation. In addition to the crossing positions, the symmetry of the electron density distribution of the involved DME orbitals turns out to be a further major point affecting the probability of electron transfer. Thus, the anisotropy of the intermolecular interaction and the electron densities of the orbitals involved in the reaction are the key “ingredients” for describing the dynamics of this dissociative charge transfer

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H- Photodetachment and Radiative Attachment for Astrophysical Applications

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We combine R-matrix calculations, asymptotic relations, and comparison to available experimental data to construct an H- photodetachment cross section reliable over a large range of photon energies and take into account the series of auto-detaching shape and Feshbach resonances between 10.92 and 14.35 eV. The accuracy of the cross section is controlled by ensuring that it satisfies all known oscillator strength sum rules including contributions from the resonances and single-photon double-electron photodetachment. From the resulting recommended cross section, spontaneous and stimulated radiative attachment rate coefficients are obtained. Photodetachment rates are also computed for the standard interstellar radiation field, in diffuse and dense interstellar clouds, for blackbody radiation, and for high redshift distortion photons in the recombination epoch. Implications are investigated for these astrophysical radiation fields and epochs.

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Different dust and gas radial extents in protoplanetary disks: consistent models of grain growth and CO emission

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ALMA observations of protoplanetary disks confirm earlier indications that there is a clear difference between the dust and gas radial extents. The origin of this difference is still debated, with both radial drift of the dust and optical depth effects suggested in the literature. In this work,

the feedback of realistic dust particle distributions onto the gas chemistry and molecular emissivity is investigated, with a particular focus on CO isotopologues. The radial dust grain size distribution is determined using dust evolution models that include growth, fragmentation and radial drift. A new version of the code DALI is used to take into account how dust surface area and density influence the disk thermal structure, molecular abundances and excitation. The difference of dust and gas radial sizes is largely due to differences in the optical depth of CO lines and millimeter continuum, without the need to invoke radial drift. The effect of radial drift is primarily visible in the sharp outer edge of the continuum intensity profile. The gas outer radius probed by 12CO emission can easily differ by a factor of ~2 between the models for a turbulent α ranging between typical values. Grain growth and settling concur in thermally decoupling the gas and dust components, due to the low collision rate with large grains. As a result, the gas can be much colder than the dust at intermediate heights, reducing the CO excitation and emission, especially for low turbulence values. Also, due to disk mid-plane shadowing, a second CO thermal desorption (rather than photodesorption) front can occur in the warmer outer mid-plane disk. The models are compared to ALMA observations of HD 163296 as a test case. In order to reproduce the observed CO snowline of the system, a binding energy for CO typical of ice mixtures needs to be used rather than the lower pure CO value.

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Detection of Interstellar Ortho-D2H+ with SOFIA

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We report on the detection of the ground-state rotational line of ortho-D2H+ at 1.477 THz (203 μm) using the German REceiver for Astronomy at Terahertz frequencies (GREAT) on board the Stratospheric Observatory For Infrared Astronomy (SOFIA). The line is seen in absorption against far-infrared continuum from the protostellar binary IRAS 16293-2422 in Ophiuchus. The para-D2H+ line at 691.7 GHz was not detected with the APEX telescope toward this position. These D2H+ observations complement our previous detections of para-H2D+ and ortho-H2D+ using SOFIA and APEX. By modeling chemistry and radiative transfer in the dense core surrounding the protostars, we find that the ortho-D2H+ and para-H2D+ absorption features mainly originate in the cool (T < 18 K) outer envelope of the core. In contrast, the ortho-H2D+ emission from the core is significantly absorbed by the ambient molecular cloud. Analyses of the combined D2H+ and H2D+ data result in an age estimate of ~5 × 10e5 yr for the core, with an uncertainty of ~2 × 10e5 yr. The core material has probably been pre-processed for another 5 × 10e5 years in conditions corresponding to those in the ambient molecular cloud. The inferred timescale is more than 10 times the age of the embedded protobinary. The D2H+ and H2D+ ions have large and nearly equal total (ortho+para) fractional abundances of ~10e−9 in the outer envelope. This confirms the central role of H3+ in the deuterium chemistry in cool, dense gas, and adds support to the prediction of chemistry models that also D3+ should be abundant in these conditions.

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The complexity of Orion : an ALMA point of view. I. Data and first results

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Aims. We wish to improve our understanding of the Orion central star formation region (Orion-KL) and disentangle its complexity. Methods. We collected data with ALMA during cycle 2 in 16 GHz of total bandwidth spread between 215.1 and 252.0 GHz with a typical sensitivity of 5 mJy/beam (2.3 mJy/beam from 233.4 to 234.4 GHz) and a typical beam size of 1.7"×1.0" (average pos. angle of 89◦). We produced a continuum map and studied the emission lines in 9 remarkable infrared spots in the region including the Hot Core and the Compact Ridge, plus the recently discovered Ethylene Glycol peak. Results. We present the data, and report the detection of several species not previously seen in Orion, including n- and i-propyl cyanide (C3H7CN), and tentative detection of a number of other species including glycolaldehyde (CH2(OH)CHO). The first detections of gGg′ ethylene glycol (gGg′ (CH2OH)2) and of acetic acid (CH3COOH) in Orion are presented in a companion paper. We also report for the first time in Orion the detection of several vibrationally excited states of cyanoacetylene (HC3N), and of its 13C isotopologues. We could not detect the 16O18O line predicted based on our detection of O2 with Herschel due to blending with a nearby line of vibrationally excited ethyl cyanide. We do not confirm the tentative detection of hexatriynyl (C6H) and cyanohexatriyne (HC7N) reported previously, nor of hydrogen peroxide (H2O2) emission. We report a complex velocity structure only partially revealed before. Components as extreme as -7 and +19 km s−1 are detected inside the hot region. Thanks to different opacities of various velocity components, we can order in some cases the position of these components along the line of sight. We propose that systematic redshifted and blueshifted wings of several species observed in the northern part of the region are linked to the explosion that occurred ∼500 years ago. The compact ridge, noticeably further south displays extremely narrow lines (∼1 km s−1) revealing a quiescent region that has not been affected by this explosion. This probably indicates that the compact ridge is either over 10,000 au in front or behind the rest of the region. Conclusions. Many lines remain unidentified, and only a detailed modeling of all known species, including vibrational states of isotopologues combined with the detailed spatial analysis offered by ALMA enriched with zero-spacing data, will allow new species to be detected.

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Ion irradiation of pure and amorphous CH4 ice relevant for astrophysical environments

F. A. Vasconcelos, S. Pilling, W. R. M. Rocha, H. Rothard, P. Boduch and J. J. Ding

This work presents a physicochemical study of frozen amorphous methane (at 16 K) under bombardment by medium-mass ions (15.7 MeV 16O5+) with implications for icy bodies in the outer Solar System exposed to the action of cosmic rays and energetic particles. The experiment was performed at the Grand Accélérateur National d'Ions Lourds (GANIL) located in Caen, France. The results demonstrate that irradiation of CH4-containing ices by swift medium mass ions with delivered energy covering both stopping power regimes until its implantation on ice (i.e. electronic and nuclear) leads to the production of many hydrocarbons, such as C2H2, C2H4, C2H6, and C3H8 (the most abundant daughter species produced). Values for the effective dissociation cross section of CH4 and the average value for the effective formation cross-sections of its daughter species were about 1e-14 cm2 and 1e-15 cm2, respectively. The half-life of methane ice in the presence of swift medium mass ions extrapolated to some outer Solar System environments is estimated to be around 10^6 years. The measured sputtering yield of methane due to incoming swift ions was about 7.30x10^5 molecules per impact. Such

parameters can be used as models to estimate the amount of CH4 and other molecular species desorbed from the icy surfaces that are constantly being incorporated to the gaseous atmosphere in the vicinity of these outer Solar System bodies due to the presence of energetic particles and cosmic rays.

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Announcements

3 yr PhD position at Leeds University, UK, in collaboration with the Leuven University, Belgium, in the field of astrochemistry

Interdisciplinary project on the stellar winds around evolved stars at Leuven University (Belgium) and the Leeds University (UK) funded by the ERC-CoG_2014 grant AEROSOL (PI. L. Decin, University of Leuven). Application deadline 30th June 2017. The project and the position We seek an excellent candidate for a PhD research position ready to play a key role in the interdisciplinary ERC Consolidator Grant AEROSOL (2016-2020, PI. Prof. Leen Decin). The aim of the project is to boost our understanding of the physics and chemistry characterizing the stellar winds around evolved stars. The project builds upon novel observations, detailed theoretical wind models, and targeted laboratory experiments (see http://fys.kuleuven.be/ster/Projects/aerosol/aerosol). The candidate will interact closely with a team consisting of astrophysicists, chemists, and computational mathematicians. Specifically, we seek a candidate with interest both in laboratory chemistry and in chemical modelling. In a first part of the project, the candidate will perform laboratory experiments aiming to understand the reactivity of Ni and Al in environments mimicking the winds of evolved stars. In a second phase, the student will study silicate dust formation using ab-initio quantum theory to establish likely reaction pathways occurring in stellar outflows. The candidate will perform his/her study at the University of Leeds supervised by Prof. John Plane (University of Leeds) and Prof. Leen Decin (University of Leuven, University of Leeds), working in collaboration with Dr David Gobrecht (University of Leuven). Candidates should have an interest in astrophysics, astrochemistry and/or physical chemistry. The ex-perimental work will be carried out in the modern and fully-equipped research laboratories at the Universities of Leeds. The (quantum) chemical computations will use the HPC facilities of the University of Leuven. The PhD student will interact closely with other team members at the Universities of Leuven and Leeds. Institute of Astronomy - University of Leuven The Institute of Astronomy (IoA) of the Leuven University in Belgium is a young and vibrant research group of some 50 scientists, engineers and administrative staff (fys.kuleuven.be/ster), including 6 full-time and 3 part-time professors. The institute is an expertise centre in stellar physics and is active in several international consortia and collaborations, involving telescopes at observatories worldwide and in space. Members of IoA have access to parallel computing facilities at Leuven University. The IoA is responsible for the organisation of the 2-year Master in Astronomy & Astrophysics of the Faculty of Science and owns the 1.2m Mercator telescope at Roque de los Muchachos, La Palma Observatory, Canary Islands. The institute has a long tradition in instrumental, observational, and theoretical studies of the late stages of evolution of low and intermediate mass stars. School of Chemistry - University of Leeds The Atmospheric and Planetary Chemistry (APC) Research Group within the School of Chemistry http://www.chem.leeds.ac.uk/research/groups/atmospheric-and-planetary-chemistry.html consists of ~40 scientists (3 Professors, academic staff, postdoctoral fellows and PhD students). Research into the Earth's at-mosphere focuses on field measurements of key

species in the atmosphere, laboratory studies of chemical oxidation of volatile organic compounds and the chemistry of meteor-ablated metals in the upper atmosphere, and detailed modelling using the Master Chemical Mechanism and the Whole Atmosphere Community Climate Model. The Planetary Chemistry research uses a combination of laboratory work, observations and modelling with an enhanced focus on chemistry at low temperatures using a pulsed Laval expansion, specialised flow tubes and theoretical models. The experience in combustion and high temperature pyrolysis chemistry is relevant for the conditions of 'super Earth' and 'hot Jupiter' exoplanets. The Group has extensive collaborations within Leeds (Physics and Astronomy, Institute for Climate and Atmospheric Science), nationally (National Centre for Atmospheric Science) and internationally (NASA, JPL and many university departments worldwide). Conditions The successful applicant will perform research in the context of AEROSOL. The PhD student will be able to take up personal training in science and people management, science communication, and grant application writing with the aim to develop a personal independent career track. The selected candidate will be offered a 3-year studentship, with a starting date between 1 July 2017 and 1 January 2018. In their application, candidates are requested to indicate their preferred starting date. Requirements and instructions to apply Applicants must possess a Master's degree in (astro)physics, chemistry or mathematics, or an equivalent diploma. High proficiency in English is assumed. Applications must include: • a Curriculum Vitae; • a statement of research interests (maximum 2 pages); • a letter detailing your specific qualifications for the position and your career/educational goals (maximum 1 page); • two letters of recommendation from people well acquainted with your academic achievements. The letters are to be submitted separately to the address mentioned below. Applications should be made using the University On-line Application System, where you can upload your supporting documents directly onto the system:
http://www.leeds.ac.uk/info/130206/applying/91/applying_for_research_degrees Please note: this opportunity is only available to those eligible for the UK/Non-UK EU fees rate.
http://www.leeds.ac.uk/info/102040/fees_and_costs/104/research_degrees_fees The short-listed applicants will be invited for an interview (live or via skype). More information can be obtained by contacting: Prof. L. Decin Institute for Astronomy Department of Physics and Astronomy, KU Leuven Celestijnenlaan 200D, 3001 Heverlee, Belgium Leen.Decin@kuleuven.be ++32-16-32 70 41 Prof. J. Plane Professor of Atmospheric Chemistry School of Chemistry University of Leeds, Leeds LS2 9JT, UK J.M.C.Plane@leeds.ac.uk ++44-113-343-8044

1 Postdoc and 2 PhD positions at KU Leuven, Belgium Observational and theoretical stellar astrophysics The winds of hot and cool massive stars

1 Postdoc and 2 PhD positions at KU Leuven, Belgium Observational and theoretical stellar astrophysics The winds of hot and cool massive stars ---------- The MAESTRO Project Throughout the Universe, the dynamics and chemical evolution of spiral galaxies like our Milky Way are largely controlled by the lives and deaths of stars with masses many times that of the Sun. But the evolution of these massive stars, in turn, is highly regulated by the huge amounts of mass expelled from their surfaces, by means of powerful starlight-driven wind outflows. These stellar winds critically determine how such massive stars evolve through their lives, how they finally die in giant supernova explosions, and how they after their violent deaths leave behind exotic remnants such as neutron stars and black holes. However, large uncertainties concerning such mass loss remain, affecting present-day predictions for massive-star evolution, including even massive-star progenitor models of gravitational wave sources. In this context, the MAESTRO project aims to fundamentally improve our understanding of the driving mechanism of massive-star winds. We will use novel theoretical and observational methods to probe the winds of hot and cool massive stars, throughout their entire evolution and across a large range of metallicity environments. Financed by the KU Leuven University in

Belgium, the MAESTRO project will bridge the theoretical, computational, and observational expertise of 4 academic members of the Institute of Astronomy at KU Leuven, to build an interdisciplinary team tackling the above critical stellar physics questions, and to enhance the predictive power of contemporary stellar evolution models of massive stars. The Vacancies The Institute of Astronomy of the KU Leuven (Belgium) seeks highly motivated and excellent applicants to take on important roles in the MAESTRO project. Applications are invited for 1 postdoc and at least one2 PhD positions financed through a prestigious research grant (C1) from the KU Leuven university. The selected candidates will join the MAESTRO team, closely under the supervision of with Profs. Leen Decin, Hugues Sana, Jon Sunqvist and Alex de Koter, and as part of an international network of collaborators, to obtain crucial observational constraints and to develop new theoretical methods needed to advance our understanding of hot and cool massive-star winds. The MAESTRO project will open 6 positions in the next 3 years. Here, we sSpecifically advertise de following 1 postdoc and 2 PhD positions (with preferred starting date around 1 October 2017): - PhD position: Theory of Wolf-Rayet winds – The PhD student will aim to develop a theoretical framework for the radiative acceleration driving the winds of Wolf-Rayet (WR) stars; using this framework then, full dynamical wind models will be constructed to obtain theoretical predictions for global wind properties (e.g. mass-loss rate) and their scaling with fundamental stellar parameters. - PhD position: Observations and Diagnostics of Red Supergiant winds – The PhD student will aim to derive the geometrical and dynamical wind structure of Red Supergiants (RSGs) using existing retrieval methods and will study the current morphology and mass-loss evolution during the RSG life time, as well as the mass-loss signatures at low metallicities. - Postdoc position: Observations of hot and cool massive stars – The postdoc will be responsible for the observational aspects of the MAESTRO project. Tasks involve, e.g.: collect, reduce and/or organize a multi-wavelength data-set covering hot (OB, WR) and cool (RSGs) massive stars across a wide metallicity range, develop and/or adapt the necessary techniques to analyse crowded regions and unresolved small clusters. Lead the analysis of these data, including part of the daily supervision of students in the MAESTRO project. - Time resolved photometry and spectroscopy of young clusters The Host Institute The Institute of Astronomy (IoA) of Leuven University in Belgium consists of a young and vibrant research group of some 50 scientists, engineers, and administrative staff (fys.kuleuven.be/ster), including 6 full-time and 3 part-time professors. The institute is an expertise centre in stellar physics and is active in several international consortia and collaborations, involving telescopes at observatories worldwide and in space. Members of IoA have access to parallel computing facilities at Leuven University. The IoA is responsible for the organisation of the 2-year Master in Astronomy & Astrophysics of the Faculty of Science and owns the 1.2m Mercator telescope at Roque de los Muchachos, La Palma Observatory, Canary Islands. The institute has a long tradition in instrumental, observational, and theoretical studies of stellar evolution. The PhD Contract The selected PhD students will be offered a 4-year contract, including a mid-term evaluation after 2 years. The salary will be commensurate to the standard scale for PhD students in Belgium; it includes social and medical insurance as well as pension rights. The preferred starting date is 1 August October 1st 2017 but can be negotiated. The successful PhD applicants(will) have to register at and comply with the regulations of the Arenberg Doctoral School of the Leuven University. Good command of the English language is a requirement to be approved by the doctoral school. The successful PhD applicants will follow a doctoral programme including personal training in management, science communication, and teaching. As part of the doctoral program, the students will have to take up a teaching task of at maximumally 4 hours per week in one of the Bachelor (in Dutch) or Master (in English) programmes. PhD students at IoA are also required to perform at least one Mercator observing run of 10 nights per year for the pooled IoA long-term monitoring programmes. The Postdoc Contract The selected post-doc will be offered a 2-year contract with a possible extension of maximum 1 year. The salary will be commensurate to the standard scale for post-doc researcher

in Belgium and will depend on the number of years of experience after PhD. It includes social and medical insurance as well as pension rights. The preferred starting date shall be between 1 August October 1st 2017 and January 1st 2018 but can be negotiated. The postdoc will also be encouraged to take up training in science and people management, science communication and grant application writing with the aim to develop a personal independent career track. Requirements and Instructions to Apply PhD applicants must hold a M.Sc. degree in physics, astrophysics or mathematics or else own an equivalent diploma. The degree must be dated at the latest one month before the position can be taken up. Expertise in astrophysics is an asset but not a requirement. Post-doc applicants must hold a PhD in astrophysics or an equivalent diploma. The ideal candidates will have a strong observational and data analysis background, including expertise relevant for the atmosphere analysis of hot and/or cool massive stars. Prior-experience with UV, optical, IR and/or sub-mm observations and facilities such as the HST, ESO/VLT (XShooter, UVES, SPHERE, MUSE, KMOS), ALMA and JWST, or similar facilities, will be viewed positively by the selection committee. Similarly, preference will be given to applicants who demonstrate expertise with low-metallicity environments, crowded regions, IFU spectroscopy and/or future JWST observations. PhD and postdoc applicants: Proficiency in English is assumedrequired. The application package should be sent as one single PDF containing (i) a curriculum vitae with a full publication list, (ii) a statement of interest (max. one page for PhD applicants and 2 pages for postdocs) and (iii) a summary of the research experience (e.g. master thesis; also max. one page for PhD applicants and 3 pages for postdocs). Exclusively for PhD applicants, (iv) a list of all master courses with their number of study points and the scores obtained. Applicants must also provide the names and contact details of two reference persons who would be prepared to send confidential recommendation letters should they be requested to do so. The selection committee will send out requests for such letters for those applicants on the short-list after an initial ranking. The short-listed applicants will be invited for an interview (live or via skypeSkype). The application material should be sent by e-mail to Leen.Decin@kuleuven.be with subject “MAESTRO-” at the latest by 1 July 15, 2017. Interviews will be held during the summer and selected candidates will be contacted at the latest by August 31, 2017. Only Ccomplete applications received by July 15th 2017 will be considered. Information on the positions and on the MAESTRO project may be obtained by contacting the co-promotors of the project: Prof. Leen Decin: email (Leen.Decin@kuleuven.be) or phone (+32-16-32.70.41) Prof. Hugues Sana: email (Hugues.Sana@kuleuven.be) or phone (+32-16-37.43.61) Prof. Jon Sundqvist: email (Jon.Sundqvist@kuleuven.be) or phone (+32-487-36.31.20) Prof. Alex de Koter: email (A.deKoter@uva.nl) or phone (+31-20-525.74.91) or at the website https://fys.kuleuven.be/ster/Projects/maestro

PhD at LOMC, Le Havre University, France

Dear Colleagues. A PhD on the electron/molecule reactive collisions will be funded at fall at LOMC-UMR-6294, Le Havre University, Normandy, France. The announcement follows. Thank you for spreading it around. Best regards, Ioan Schneider Electron-Molecule Collisions: Study of the Reactive Mechanisms and Applications. Doctoral School: Physics, Engineering, Materials, Energy (PSIME), Normandie Université. Research group: ‘Reactive Processes’, LOMC-UMR-6294, Université du Havre Normandie. Supervisor: Ioan F. SCHNEIDER, Université du Havre Normandie. Co-supervisor: Arnaud BULTEL, CORIA-UMR-6614, Université de Rouen Normandie. Sponsor: Normandy region (La Région Normandie). Key words: reactive collisions, dissociative recombination, rate coefficients, quantum methods, plasmas, kinetics, collisional-radiative model. Context and motivation: The electronic collisions are major processes in the plasmas of hypersonic entries of spacecrafts in the planetary atmospheres, in the edge of the fusion plasmas, in the interstellar molecular clouds, flames and ionic propulsion plasmas [1]. Sophisticated experiments measuring the rate coefficients of these processes are supported and

extended by quantum state-to-state computations, in order to deeply understand the role of these collisions in the kinetics and hydrodynamics of the invoked environments, and in order to fill the data bases (NIST, ADAS, UMIST, KIDA, etc.) in view of detailed modelling. Objectives of the doctoral work: We will study the collisions between electrons and molecules – neutral and ionized - in particular the Hydrogen (molecular benchmark), the hydrides – containing Oxygen, Carbon, Argon, metalic elements, etc. – and species containing halogenes or Sulphur. Three activities will be simultaneously developped. The first one will be the production of molecular structure data – potential energy curves and inter-channel couplings – by using quantum chemistry and R-matrix methods. The second one will be the modelling of the reactional dynamics (recombination, attachement, dissociation,ionization, excitation) by collisional methods and theoretical spectroscopy methods. And finally the third will be that of the use of the rate coefficients in the kinetic models. Methodological details: Many of the reactions invoked occur simultaneously and, consequently, are in mutual competition. They are complex processes, where the super-excited states amplify resonantly the excitation, the ionization and the dissociation. Several fragmentation continua – electron/molecule, atom/atom, etc. – and several infinite series of bound states overlap. Our methods are the only capable to manage this complexity, and to link it to the kinetic models. They are based on the Multichannel Quantum Defect Theory (MQDT) [2-6], on the R-matrix theory [7] and on the Configuration Interaction theory [8]. The kinetics driven by these processes will be described by collisional-radiative models [9]. Collaborations : In France: Laboratories CORIA (Rouen), LSPM (Villetaneuse), Aimé Cotton (Orsay), LPP (Ecole Polytechnique), Ecole Centrale de Paris, IPAG (Grenoble), LUPM (Montpellier). Abroad: University College London, University of Central Florida - Orlando, University of California – Davis, Max-Planck-Institut für Kernphysik - Heidelberg, Stockholm University, Politecnico and Aldo Moro University - Bari, University of Calcutta, University of Douala, University of Burundi, Politehnica University and West University of Timisoara, Tunis El Manar University. References : [1] I. F. Schneider, O. Dulieu et J. Robert (Editeurs) Eur. Phys. J./Web of Conferences 84, 2015 (http://www.epj-conferences.org/articles/epjconf/abs/2015/03/contents/contents.html). [2] Ch. Jungen, “Elements of Quantum Defect Theory”, in M. Quack and F. Merkt (editors), Handbook of High Resolution Spectroscopy, Wiley, Chichester, New York 2010. [3] J. Zs. Mezei et al, Plasma Sources Science and Technology 24, 035005, 2015. [4] M. D. Epée Epée et al, Monthy Notices of the Royal Astronomical Society 455, 276–281, 2016. [5] D. A. Little et al, Phys. Rev. A 90, 052705, 2014. [6] S. Niyonzima et al, Phys. Rev. A 87, 022702, 2013. [7] J. Tennyson, Physics Reports 491, 29-76, 2010. [8] V. Laporta et al, Plasma Physics and Controlled Fusion 59, 045008, 2017. [9] A. Bultel et al, Physics of Plasmas 13, 043502, 2006.

Quantemol is hiring

Quantemol Ltd. (www.quantemol.com) is a scientific software and consultancy company developing state of the art simulation software for industrial applications in the integrated circuit (IC) fabrication industry, and providing simulation and plasma chemistry consultancy to industrial clients. We are based in University College London, located in the heart of the city, with clients which include large international blue-chip corporations. Quantemol is looking to fill two positions: Chemical Reactions Modeller We are looking for a Chemical Reactions Modeller who will be able to construct and validate plasma chemistry reaction sets by comparison with laboratory measurements. This is a fantastic opportunity for someone looking to utilise their technical background in a commercial environment. You will be collaborating with a wide range of researchers from around the globe, and have the opportunity to travel and present at events where the latest innovations in plasma science are showcased. You will be a technical expert for our customer base, and work with our unique database of validated plasma chemistries (QDB) validating data for plasma modelling. You will have or be about to obtain a PhD in an appropriate

field. For more information on the Chemical Reactions Modeller role, and how to apply, please see: http://www.quantemol.com/2017/05/12/chemical-reactions-modeller-vacancy/ Data Scientist We are looking for a Data Scientist (PhD) to manage and develop QDB, a database of plasma process data. This is a fantastic opportunity for someone looking to utilise their technical background in a commercial environment. You will be collaborating with a wide range of researchers from around the globe, and have the opportunity to travel and present at events where the latest innovations in plasma science are showcased. We are looking for candidates with knowledge of research techniques and information systems. You will have good knowledge of and experience with Python (essential), MySQL, and Unix/Linux administration. Familiarity with the Django web framework, Mezzanine, and version control with Git would be an advantage, as would experience at front-end development with HTML/CSS and JavaScript/JQuery. Applicants must have a PhD in an appropriate field. For more information on the Data Scientist role, and how to apply, please see: http://www.quantemol.com/2017/05/12/data-scientist-vacancy/ Informal enquiries should be addressed to: Prof Jonathan Tennyson, Department of Physics and Astronomy, University College London, London WC1E 6BT, UK Email: j.tennyson@ucl.ac.uk