AstroChemical Newsletter #24

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You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Complex organic molecules in diffuse clouds along the line of sight to Sgr B2

V. Thiel, A. Belloche, K. M. Menten, R. T. Garrod, and H. S. P. Müller

Up to now, mostly relatively simple molecules have been detected in interstellar diffuse molecular clouds in our galaxy, but more complex species have been reported in the diffuse/translucent medium of a z = 0.89 spiral galaxy. We aim at searching for complex organic molecules (COMs) in diffuse molecular clouds along the line of sight to Sgr B2(N), taking advantage of the high sensitivity and angular resolution of the Atacama Large Millimeter/submillimeter Array (ALMA). We use data acquired as part of the EMoCA survey performed with ALMA. To analyse the absorption features of the molecules detected towards the ultracompact HII region K4 in Sgr B2(N), we calculate synthetic spectra for these molecules and fit their column densities, line widths, centroid velocities, and excitation temperatures. We report the detection of CH3OH, CH3CN, CH3CHO, HC3N, and NH2CHO in Galactic center (GC) diffuse clouds and CH3OH and CH3CN in a diffuse cloud in the Scutum arm. The chemical composition of one of the diffuse GC clouds is found to be similar to the one of the diffuse/translucent medium of the z=0.89 spiral galaxy. The chemical processes leading to chemical complexity in the diffuse molecular ISM appear to have remained similar since z=0.89. As proposed in previous studies, the presence of COMs in diffuse molecular clouds may result from a cyclical interstellar process of cloud contraction and expansion between diffuse and dense states.

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Influence of surface and bulk water ice on the reactivity of a water-forming reaction

Thanja Lamberts and Johannes Kästner

On the surface of icy dust grains in the dense regions of the interstellar medium a rich chemistry can take place. Due to the low temperature, reactions that proceed via a barrier can only take place through tunneling. The reaction H + H2O2 → H2O + OH is such a case with a gas-phase barrier of ~26.5 kJ/mol. Still the reaction is known to be involved in water formation on interstellar grains. Here, we investigate the influence of a water ice surface and of bulk ice on the reaction rate constant. Rate constants are calculated using instanton theory down to 74 K. The ice is taken into account via multiscale modeling, describing the reactants and the direct surrounding at the quantum mechanical level with density functional theory (DFT), while the rest of the ice

is modeled on the molecular mechanical level with a force field. We find that H2O2 binding energies cannot be captured by a single value, but rather depend on the number of hydrogen bonds with surface molecules. In highly amorphous surroundings the binding site can block the routes of attack and impede the reaction. Furthermore, the activation energies do not correlate with the binding energies of the same sites. The unimolecular rate constants related to the Langmuir-Hinshelwood mechanism increase as the activation energy decreases. Thus, we provide a lower limit for the rate constant and argue that rate constants can have values up to two order of magnitude larger than this limit.

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Atom Tunneling in the Water Formation Reaction H2 + OH → H2O + H on an Ice Surface

Jan Meisner, Thanja Lamberts, and Johannes Kästner

OH radicals play a key role as an intermediate in the water formation chemistry of the interstellar medium. For example the reaction of OH radicals with H2 molecules is among the final steps in the astrochemical reaction network starting from O, O2, and O3. Experimentally it was shown that even at 10 K this reaction occurs on ice surfaces. As the reaction has a high activation energy only atom tunneling can explain such experimental findings. In this study we calculated reaction rate constants for the title reaction on a water-ice Ih surface. To our knowledge, low-temperature rate constants on a surface are not available in the literature. All surface calculations were done using a QM/MM framework (BHLYP/TIP3P) after a thorough benchmark of different density functionals and basis sets to highly accurate correlation methods. Reaction rate constants are obtained using instanton theory which takes atom tunneling into account inherently, with constants down to 110 K for the Eley-Rideal mechanism and down to 60 K for the Langmuir-Hinshelwood mechanism. We found that the reaction is nearly temperature independent below 80 K. We give kinetic isotope effects for all possible deuteration patterns for both reaction mechanisms. For the implementation in astrochemical networks, we also give fit parameters to a modified Arrhenius equation. Finally, several different binding sites and binding energies of OH radicals on the Ih surface are discussed and the corresponding rate constants are compared to the gas-phase case.

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The onset of energetic particle irradiation in Class 0 protostars

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The early stages of low-mass star formation are likely to be subject to intense ionization by protostellar energetic MeV particles. As a result, the surrounding gas is enriched in molecular ions, such as HCO+ and N2H+. Nonetheless, this phenomenon remains poorly understood for Class 0 objects. Recently, based on Herschel observations taken as part of the key program Chemical HErschel Surveys of Star forming regions

(CHESS), a very low HCO+/N2H+ abundance ratio of about 3-4, has been reported toward the protocluster OMC-2 FIR4. This finding suggests a cosmic-ray ionization rate in excess of 10^−14 s−1, much higher than the canonical value of 3×10−17 s−1 (value expected in quiescent dense clouds). To assess the specificity of OMC-2 FIR4, we have extended this study to a sample of sources in low- and intermediate mass. More specifically, we seek to measure the HCO+/N2H+ abundance ratio from high energy lines (J>6) toward this source sample in order to infer the flux of energetic particles in the warm and dense gas surrounding the protostars. We use observations performed with the Heterodyne Instrument for the FarInfrared spectrometer on board the Herschel Space Observatory toward a sample of 9 protostars. We report HCO+/N2H+ abundance ratios in the range of 5 up to 73 toward our source sample. The large error bars do not allow us to conclude whether OMC-2 FIR4 is a peculiar source. Nonetheless, an important result is that the measured HCO+/N2H+ ratio does not vary with the source luminosity. At the present time, OMC-2 FIR4 remains the only source where a high flux of energetic particles is clearly evident. More sensitive and higher angular resolution observations are required to further investigate this process.

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Chemical content of the circumstellar envelope of the oxygen-rich AGB star R Dor: Non-LTE abundance analysis of CO, SiO, and HCN

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(abridged) Our aim is to determine the radial abundance profile of SiO and HCN throughout the stellar outflow of R Dor, an oxygen-rich AGB star with a low mass-loss rate. We have analysed molecular transitions of CO, SiO, and HCN measured with the APEX telescope and all three instruments on the Herschel Space Observatory, together with literature data. Photometric data and the infrared spectrum measured by ISO-SWS were used to constrain the dust component of the outflow. Using both continuum and line radiative transfer methods, a physical envelope model of both gas and dust was established. We have performed an analysis of the SiO and HCN molecular transitions in order to calculate their abundances. We have obtained an envelope model that describes the dust and the gas in the outflow, and determined the abundance of SiO and HCN throughout the region of the outflow probed by our molecular data. For SiO, we find that the initial abundance lies between 5.5e-5 and 6.0e−5 w.r.t. H2. The abundance profile is constant up to 60 ±10 R∗, after which it declines following a Gaussian profile with an e-folding radius of (3.5±0.5)×1e13 cm. For HCN, we find an initial abundance of 5.0e−7 w.r.t. H2. The Gaussian profile that describes the decline starts at the stellar surface and has an e-folding radius re of (1.85±0.05)×1e15 cm. We cannot to unambiguously identify the mechanism by which SiO is destroyed at 60 ±10 R∗. The initial abundances found are larger than previously determined (except for one previous study on SiO), which might be due to the inclusion of higher-J transitions. The difference in abundance for SiO and HCN compared to high mass-loss rate Mira star IK Tau might be due to different pulsation characteristics of the central star and/or a difference in dust condensation physics.

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CN rings in full protoplanetary disks around young stars as probe of disk structure

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Bright ring-like structure emission of the CN molecule has been observed in protoplanetary disks. We investigate if such structures are due to the morphology of the disk itself or if they are instead an intrinsic feature of CN emission. We also address to which physical and chemical parameters CN is most sensitive, in order to use it as a diagnostic. Using the 2D thermochemical code DALI, a set of disk models are run for different stellar spectra, masses and physical structures. An updated chemical network that accounts for the most relevant CN reactions is adopted. Ring-shaped emission is found to be a common feature of all models: the highest abundance is found in the upper outer regions of the disk, and the column density peaks at 50-70 AU for T Tauri stars with standard accretion rates. The emission profile follows the column density suggesting that optical depth and non-LTE effects are minimal up to the N=3-2 transition. Higher mass disks generally show brighter CN. Higher UV fields, such as appropriate for T Tauri stars with high accretion rates or for Herbig Ae stars or for higher disk flaring, generally result in brighter and larger rings. These trends are due to the main formation paths of CN, which all start with vibrationally excited H2* molecules, produced through FUV pumping of H2. The model results compare well with observed disk-integrated CN fluxes and with the observed location of the CN ring in TW Hya. CN rings are produced naturally in protoplanetary disks and do not require a specific underlying disk structure (dust cavity or gap). The strong link between FUV flux and CN emission can provide information on the vertical structure of the disk and on the distribution of dust grains affecting UV penetration, and could help to break some degeneracies in the SED fitting. In contrast with C2H or c-C3H2, the CN flux is not very sensitive to carbon and oxygen depletion.

12 pages, 18 figures, accepted for publication in A&A
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The 12C/13C Ratio in Sgr B2(N): Constraints for Galactic Chemical Evolution and Isotopic Chemistry

D. T. Halfen , N. J. Woolf, and L. M. Ziurys

A study has been conducted of 12C/13C ratios in five complex molecules in the Galactic center. H2CS, CH3CCH, NH2CHO, CH2CHCN, and CH3CH2CN and their 13C-substituted species have been observed in numerous transitions at 1, 2, and 3 mm, acquired in a spectral-line survey of Sgr B2(N), conducted with the telescopes of the Arizona Radio Observatory (ARO). Between 22 and 54 individual, unblended lines for the 12C species and 2–54 for 13C-substituted analogs were modeled in a global radiative transfer analysis. All five molecules were found to consistently exhibit two velocity components near VLSR ~ 64 and 73 km s-1, with column densities ranging from Ntot ~ 3e14 – 4e17 cm-2 and ~2e13 – 1e17 cm-2 for the 12C and 13C species, respectively. Based on 14 different isotopic combinations, ratios were obtained in the range 12C/13C = 15 ± 5 to 33 ± 13, with an average value of 24 ± 7, based on comparison of column densities. These measurements better anchor the 12C/13C ratio at the Galactic center, and suggest a slightly revised isotope gradient of 12C/13C = 5.21(0.52) DGC + 22.6(3.3). As indicated by the column densities, no preferential 13C enrichment was found on the differing carbon sites of CH3CCH, CH2CHCN, and CH3CH2CN. Because of the elevated temperatures in Sgr B2(N), 13C isotopic substitution is effectively “scrambled,” diminishing chemical fractionation effects. The

resulting ratios thus reflect stellar nucleosynthesis and Galactic chemical evolution, as is likely the case for most warm clouds.

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Deuterated methanol on a solar system scale around the HH212 protostar

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Context: Methanol is thought to be mainly formed during the prestellar phase and its deuterated form keeps memory of the conditions at that epoch. Thanks to the unique combination of high angular resolution and sensitivity provided by ALMA, we wish to measure methanol deuteration in the planet formation region around a Class 0 protostar and to understand its origin. Aims: We mapped both the 13CH3OH and CH2DOH distribution in the inner regions (~100 au) of the HH212 system in Orion B. To this end, we used ALMA Cycle 1 and Cycle 4 observations in Band 7 with angular resolution down to ~0.15". Results: We detected 6 lines of 13CH3OH and 13 lines of CH2DOH with upper level energies up to 438 K in temperature units. We derived a rotational temperature of (171 ± 52) K and column densities of 7×10^16 cm−2 (13CH3OH) and 1×10^17 cm−2 (CH2DOH), respectively. Consequently, the D/H ratio is (2.4 ± 0.4)×10^−2, a value lower by an order of magnitude with respect to what was previously measured using single dish telescopes toward protostars located in Perseus. Our findings are consistent with the higher dust temperatures in Orion B with respect to that derived for the Perseus cloud. The emission is tracing a rotating structure extending up to 45 au from the jet axis and elongated by 90 au along the jet axis. So far, the origin of the observed emission appears to be related with the accretion disk. Only higher spatial resolution measurements however, will be able to disentangle between different possible scenarios: disk wind, disk atmosphere, or accretion shocks.

Astronomy & Astrophysics Letter, in press
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Testing the variability of the proton-to-electron mass ratio from observations of methanol in the dark cloud core L1498

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The dependence of the proton-to-electron mass ratio, mu, on the local matter density was investigated using methanol emission in the dense dark cloud core L1498. Towards two different positions in L1498, five methanol transitions were detected and an extra line was tentatively detected at a lower confidence level in one of the positions. The observed centroid frequencies were then compared with their rest frame frequencies derived from least-squares fitting to a large data set. Systematic effects, as the underlying methanol hyperfine structure and the Doppler tracking of the telescope, were investigated and their effects were included in the total error budget. The comparison between the observations and the rest frame frequencies constrains potential mu variation at the level of Dmu/mu < 6x10^(-8), at a 3 sigma confidence level. For the dark cloud we determine a total CH3OH (A+E) beam averaged column

density of 3-4x10^(12) cm^(-2) (within roughly a factor of two), an E- to A-type methanol column density ratio of N(A-CH3OH)/N(E-CH3OH) 1.00 +/- 0.15, a density of n(H2) = 3x10^5 cm^(-3) (again within a factor of two), and a kinetic temperature of Tkin = 6 +/- 1 K. In a kinetic model including the line intensities observed for the methanol lines, the n(H2) density is higher and the temperature is lower than that derived in previous studies based on different molecular species; the intensity of the 1_0 --> 1_-1 E line strength is not well reproduced.

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Evidences for disks an an early stage in class 0 protostars

M. Gerin, J. Pety, B. Commerçon, A. Fuente4 J. Cernicharo, N. Marcelino, A. Ciardi, D. C. Lis, E. Roueff, H.A. Wootten, and E. Chapillon

The formation epoch of protostellar disks is debated because of the competing roles of rotation, turbulence, and magnetic fields in the early stages of low-mass star formation. Magnetohydrodynamics simulations of collapsing cores predict that rotationally supported disks may form in strongly magnetized cores through ambipolar diffusion or misalignment between the rotation axis and the magnetic field orientation. Detailed studies of individual sources are needed to cross check the theoretical predictions. We present 0.06 – 0.1 ″ resolution images at 350 GHz toward B1b-N and B1b-S, which are young class 0 protostars, possibly first hydrostatic cores. The images have been obtained with ALMA, and we compare these data with magnetohydrodynamics simulations of a collapsing turbulent and magnetized core. The submillimeter continuum emission is spatially resolved by ALMA. Compact structures with optically thick 350 GHz emission are detected toward both B1b-N and B1b-S, with 0.2 and 0.35″ radii (46 and 80 au at the Perseus distance of 230 pc), within a more extended envelope. The flux ratio between the compact structure and the envelope is lower in B1b-N than in B1b-S, in agreement with its earlier evolutionary status. The size and orientation of the compact structure are consistent with 0.2″ resolution 32 GHz observations obtained with the Very Large Array as a part of the VANDAM survey, suggesting that grains have grown through coagulation. The morphology, temperature, and densities of the compact structures are consistent with those of disks formed in numerical simulations of collapsing cores. Moreover, the properties of B1b-N are consistent with those of a very young protostar, possibly a first hydrostatic core. These observations provide support for the early formation of disks around low-mass protostars.

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The profile of the bending mode band in solid CO2

Baratta, G. A. and Palumbo, M. E.

Solid carbon dioxide (CO2) is one of the most abundant species detected in icy grain mantles in dense molecular clouds. Its identification is based on the comparison between astronomical and laboratory spectra. In the past 30 years the profile of solid CO2 infrared absorption bands has been extensively studied experimentally, however the debate on the structure (amorphous versus crystalline) of CO2 samples obtained in laboratory by the thin-film technique is still open. The aim of this work is to investigate if the presence of the double peak feature in the profile of the CO2 bending mode band is

related to the crystalline or amorphous structure of the sample. We performed new laboratory experiments depositing CO2 under ultra high vacuum (UHV) conditions at 17 K. We investigated, using infrared transmission spectroscopy, the influence of various experimental parameters on the profile of the CO2 bands, namely deposition rate, sample thickness, annealing, and presence of water, methanol or carbon monoxide co-deposited with CO2. We found that, within experimental uncertainties, under UHV conditions the profile of the CO2 bands in pure solid samples does not depend on the deposition rate or the sample thickness in the ranges investigated. In all cases the bending mode band profile shows a double peak (at 660 and 655 cm-1). The spectra also show the Fermi resonance features that cannot be active in crystalline samples. On the other hand, when a small fraction of water or methanol is co-deposited with CO2 the double peak is not observed while it is observed when a CO2:CO mixture is considered. Furthermore, we measured the density of solid CO2 and the refractive index (at 543.5 nm) at 17 K and at 70 K: rho(17K)=1.17 g cm-3, rho(70K)=1.49 g cm-3, n(17K)=1.285, and n(70K)=1.372. Our experimental results indicate that the presence of the double peak in the profile of the bending mode band is not an indication of a crystalline structure of the sample and they do not exclude the presence of amorphous solid CO2 in space.

A&A, in press
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Full-text URL: https://www.aanda.org/articles/aa/pdf/forth/aa30945-17.pdf

Announcements

Volatile elements in the Solar System

https://solarsystem2018.wordpress.com Winter school at the Ecole de Physique des Houches in the French Alps, March 11-16, 2018 The school will focus on the origin and evolution of water and associated volatile elements – carbon, nitrogen, noble gases – in the early Solar System. The elemental and isotopic compositions of these elements and species have been shaped by heritage from the interstellar medium and/or photon/ionizing particles – matter interactions in the disk. These elements/species have played a fundamental role in the condensation of solids, in the accretion of planets, and in the formation of their atmospheres. The analysis of extraterrestrial material (primitive meteorites, lunar and martian meteorites), as well as recent space missions, have permitted to document the compositions of the nebular gas, of asteroids, of comets and of differentiated bodies. This is an interdisciplinary school, at the frontier between planetary science, chemistry of interstellar medium and cosmochemistry. The school is open to Ph.D. students and researchers who wish to broaden their knowledge. The lectures will be accessible to non specialists, but a background in planetary sciences, geo/cosmochemistry or astrophysics is required. All lectures will be in English. Scientific Organizers: David Bekaert (CRPG-Université de Lorraine), Evelyn Füri (CRPG-CNRS), Yves Marrocchi (CRPG-CNRS), Bernard Marty (CRPG-CNRS), Alessandro Morbidelli (Observatoire de la Côte d'Azur), Laurette Piani (CRPG-CNRS), Lionel Vacher (CRPG-CNRS).

Paid Twinkle Space Mission Tutors

The education branch of the Twinkle space mission are looking for PhD students and post-docs in the London area to join their team of tutors, at a rate of £18/hour. Starting Autumn 2017, the tutors are paid to mentor small groups of sixth form students on a publishable research project. This is particularly suitable for those with expertise in atomic and molecular physics and/or astronomy and astrophysics. The program

consists of 2 contact hours + 1.5 hours preparation time/fortnight for 12 fortnightly session over the 2017/2018 school year. An experienced team is on hand for support throughout. To learn more, you are invited to come along to the Royal Astronomical Society on Monday 25th September, 3.30-5pm. Please see the flyer attached and visit http://bit.ly/ORBYTS-2017-18 You can contact orbyts@twinkle-spacemission.co.uk with any queries. www.orbyts.co.uk http://www.twinkle-spacemission.co.uk/edutwinkle/

Cosmic Rays: the salt of the star formation recipe

Department of Physics and Astronomy, University of Florence, Arcetri - Italy Cosmic rays are a key ingredient in many fields of Astrophysics and in particular in star formation, but despite their great relevance our understanding is still relatively incomplete. Thanks to the data delivered by the new generation of radio and (sub)millimeter telescopes, we have now the opportunity of attaining a comprehensive knowledge about the role of cosmic rays in the physics and chemistry of the interstellar medium, hence about the processes leading to star and planet formation. Observations are needed to constrain the multiple aspects of the proposed theoretical models and models are required to properly interpret observations. Despite the importance of cosmic rays in star formation, the interplay between observers, chemical modellers, and theoreticians is still missing. Therefore, the proposed workshop has the goal of bringing together experts in theory and simulations of cosmic-ray propagation, astrochemists, and observers to share ideas, discuss about recent and present results, and identify the key challenges regarding the chemistry and the physics of cosmic rays for the near future. The discussion arising from this workshop will settle the ground for a more efficient exploitation of the current facilities (Radionet facilities as NOEMA, IRAM 30m, APEX, Effelsberg, LOFAR, VLBI; and other such as ALMA and VLA). We stress that bf we expect not only participants who already work on cosmic rays, but also experts on different aspects of star formation with the aim of make everyone aware about the relevance of cosmic rays in their respective research. Specific science topics: - Role of cosmic rays in star and planet formation - Cosmic-ray fingerprints in different environments - Impact of cosmic rays on the formation of interstellar molecules: observations, models, and laboratory experiments - Cosmic-ray factories: local acceleration in protostellar shocks - Cosmic rays and the origin of Life: ISM, comets, planets, and early Earth Invited speakers already confirmed: Elena Amato (INAF-OAA), Anabella Araudo (Astronomical Institute of Prague), Paola Caselli (MPE), Jan Forbrich (U. Hertfordshire), Stefano Gabici (APC), Daniele Galli (INAF-OAA), Philipp Girichidis (Leibniz-Institut), Guillaume Gronoff (NASA), Izaskun Jiménez-Serra (QMUL), Alexandre Marcowith (LUPM), Jesús Martín-Pintado (INTA-CSIC), Guillermo Muñoz-Caro (INTA-CSIC), David Neufeld (JHU), Elisabetta Palumbo (INAF-OACT) Scientific Organizing Committee: Marco Padovani (INAF-OAA, co-chair), Víctor M. Rivilla (INAF-OAA, co-chair), Patrick Hennebelle (CEA/IRFU/SAp), Ana López-Sepulcre (IRAM/IPAG), Leonardo Testi (ESO/INAF-OAA), Serena Viti (UCL) More detailed information and registration instructions are published on the conference website: https://www.arcetri.astro.it/cosmicrays/

Postdoctoral fellowship in theoretical astrochemistry at ITAMP

The Institute for Theoretical Atomic Molecular and Optical Physics (ITAMP) at the Harvard-Smithsonian Center for Astrophysics in Cambridge, MA invites applications for a postdoctoral fellowship in theoretical astrochemistry. Research areas include, but are not limited to, primordial chemistry, and atomic and molecular processes in interstellar space and exoplanet atmospheres. The awardee will be selected through a rigorous competition for an initial two years and can be extended to a third year. Applications process will be accepted in early September through November 17, 2017. Interested applicants are encouraged to visit itamp.harvard.edu for further information and

access the online application process. A statement of proposed research and a description of current research, in addition to a biographical sketch and letters of recommendation are to be included with all applications. Preference will be given to applicants who have recently been awarded their degrees. ITAMP is the premier institute of theoretical atomic molecular and optical (AMO) physics in the United States and is funded by the National Science Foundation. Application Deadline: Friday, November 17, 2017 Application link and more information at https://www.cfa.harvard.edu/itamp-postdoctoral-fellowship The Institute for Theoretical Atomic Molecular and Optical Physics (ITAMP) Harvard-Smithsonian Center for Astrophysics 60 Garden Street, Mailstop 14 Cambridge, MA 02138

2018 Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments

The Abdus Salam International Centre for Theoretical Physics (ICTP) and the International Atomic Energy Agency (IAEA) will jointly organize this School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments. The one-week event at ICTP in Trieste, from 16 to 20 April 2018, will provide training and information exchange for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research, industrial plasmas, laser-produced plasmas, astrophysical plasmas, and warm and hot dense matter. The training is aimed at advanced Ph.D. students, postdocs and other young researchers. The information exchange will span several disciplines: from molecules to materials and from method developments to data treatments. Topics related to energetic events and electronically excited states are emphasized throughout the programme. The schedule features lectures by international experts, invited and contributed research talks, posters and discussion sessions, with ample time available for interaction and discussions. Dates: 16 - 20 April 2018 Location: International Centre for Theoretical Physics (ICTP) - Miramare, Trieste, Italy Organized by: Atomic and Molecular Data Unit, International Atomic Energy Agency (IAEA) Web page: https://www-amdis.iaea.org/Workshops/ICTP2018/ Contact e-mail: smr3197@ictp.it Deadline for abstracts: 20 November 2017