Current and Future Perspectives of Chemical Modelling in Astrophysics

Abstract booklet

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Contents

Talks: Day 1 – Monday 17 July

Dust grains processes: experiments

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The dust component of interstellar matter comprises nearly 1% of its mass. Bare dust grains are made of silicate or carbonaceous materials. In cold regions, the dust is covered by ice mantles composed of H2O and other species such as CO, CO2, CH3OH, and NH3. The increasing interest of the astrophysical community on dust is motivated by its important role in the physics and chemistry of inter- and circumstellar regions. In particular, models aiming to reproduce molecular abundances in the gas invoke the dust when gas reactions alone cannot match the observations. More recent models incorporate the dust component and include parameter values and even processes that are reproduced in dedicated laboratory simulations. Among the processes studied experimentally are the formation and characterization of dust analogs, the diffusion of species in the dust, the accretion, thermal and photon/ion-induced desorption of molecules in ice mantles, and other effects of irradiation on icy dust grains, in particular the formation of complex organic species that are searched for by radioastronomers and in cometary nuclei.

Small molecular clusters in astrophysical dust formation processes

Beate Patzer

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The transition from a molecular gas to solid particles takes place via the formation and growth of small clusters in the gas phase. The required thermodynamic and kinetic data of such microphysical processes are often not available. Theoretical computation is therefore in many cases the only means to obtain at least some information about the desired quantities. Consequently, the nature and physical properties of molecular clusters possibly involved in dust formation processes from the gas phase have been studied theoretically employing computational electronic structure techniques. The properties, thus obtained, are necessary prerequisites for the study of such phase transitions in astrophysical environments such as e.g. circumstellar surroundings of cool, late-type stars, nova and supernova ejecta, or substellar atmospheres. Implications regarding the formation of dust particles under astrophysical conditions are discussed focusing on the formation of carbide particles from the gas phase.

Solid H2 in the ISM: Gravitational Stability of Fluids in a Phase Transition

Andreas Füglistaler

Geneva Observatory, University of Geneva

Context We are studying solid hydrogen formation as a result of combining phase transition with gravity. Observations of various ices suggest that phase transition processes are happening in cold regions. H2 condensation conditions can be reached in dense regions such as molecular clouds and disks. Solid H2 might explain the low efficiency of star formation and help hiding missing baryons in spiral galaxies. Physics Linear analysis shows that fluids in a phase transition are gravitationally unstable at any scale, because compression does not increase pressure, but the condensed phase fraction. Using the intermolecular Lennard-Jones potential, the virial equilibrium study shows that there is an unvirializable density domain where H2 clumps can form at temperatures 600 K. For an initial gas phase collapse the geometry is essential. Contrary to spherical or filamentary collapses, sheet-like collapses starting below 15 K easily reach H2 condensation conditions because then they are fastest and both the increase of heating and opacity are limited. Simulations We study the non-linear dynamics of fluids in and out of a phase transition using the molecular dynamics code LAMMPS. Super-molecules are used to combine the Lennard-Jones and gravitational potential. The simulations confirm that fluids in

a phase transition are gravitationally unstable, independent of the strength of the gravitational potential. The instabilities produce a wide spectrum of ice clumps, from small multimers, to comets, to gravitationally bound planetoids. Conclusions Our work shows that the physics of cold self-gravitating fluids such as dark molecular clouds is much richer than usually assumed. The segregation in a gravitational field of small grains towards larger bodies such as comets and planetoids cannot be simulated with traditional hydrodynamical codes, but is possible with a super-molecular approach. Observations, linear and virial analysis as well as computer simulations suggest the possibility of substellar H2 body formation due to the combination of phase transition and gravity in cold regions. H2 phase transition is reached easily during plane-parallel collapses if the initial temperature is < 15 K .

Dust and ice in star forming regions.

Stephanie Cazaux

Aerospace engineering, Delft University of technology

Eighty years ago, dust was first identified in interstellar space as the something which can absorb the light coming from the stars. These small dust particles were originally thought to be only passive and annoying entities obscuring astrophysical objects that astronomers wanted to observe. However, it appears that dust is a powerful interstellar catalyst that is responsible for the presence of the simplest molecule, H2, as well as the most complex molecules in our Universe, like amino acids. In the environments where stars are forming, the catalytic activity of dust can dramatically alter the gas phase chemical composition and thermodynamics. In the inner regions of interstellar clouds, dust retains the chemical species captured from the gas phase to grow icy mantles. Dust becomes a reservoir of interstellar gas. These ices are hosts to a rich chemistry, driven by UV photons and cosmic rays, which can generate complex molecules essential for the formation stars, planets and even life itself. During this talk, I will show which different processes are involved in the formation of simple (H2) and more complex (H2O, H2O2, CH3OH) species on interstellar dust as well as the formation of ices. The different methods to account for grain surface chemistry in astrochemical models will also be discussed. At last, I will show the impact of dust (as catalyst or reservoir) on the chemical composition of star forming regions.

Modelling gas-surface processes : Theory and experiment for adsorption energies determination of nitrile/isonitrile isomers

Yves Ellinger
UPMC

The CN nitrile bond is the most widespread functional group among the 200 interstellar and circumstellar molecules detected to day. This functional group gives rise to the well-known cyanopolyynes R-CN and isocyanopolyynes R-NC series when R contains CC delocalized triple bonds that can spread on a terminal CN group, respectively. When R is a saturated group, the number of detected isomers is reduced to CH3CN, CH3CH2CN, n-C3H7CN and i-C3H7CN nitriles and only to CH3NC for isonitriles (not counting HCN and HNC). In this work we address the question whether a differential adsorption could be at the origin of a drastic selection of only one type of isomer. Among the various types of grains surfaces proposed by Greenberg (1976), we discarded the hydroxylated surfaces that could chemically interact with the nitrile group and focus instead on the carbonaceous aromatic grains often modeled by polycyclic aromatic hydrocarbon (PAH) molecules. The key features on this concerted approach. are: i) theoretically, using periodic DFT calculations often referred to as first principle simulations by means of the Vienna Ab initio Simulation Package (VASP); ii) experimentally, measuring the desorption energies E by means of temperature programmed desorption (TPD) of CH3CN and CH3NC on a Highly Oriented Polycrystalline graphite (HOPG) substrate (see Bertin et al. 2017 for details). Assuming a perfect HOPG surface, we considered both parallel and perpendicular orientations of these pseudo linear isomers with respect to the aromatic plane. For parallel orientations of CH3CN and CH3NC with respect to the graphite surface, a manifold of 24 different geometries were probed (counting rotations of the CH3 group). In both isomers we found a slightly tilted preference for geometries in which two of the CH3 hydrogens are closer to the CC nuclear frame. For each isomer, all adsorption energies are within a range of 50 meV, giving average values of 275 and 261 meV for CH3CN and CH3NC, respectively. In perpendicular situations, the strongest adsorptions occur in both cases when the CCN/CNC backbones are on top of a carbon atom, but E is 40% smaller. All these theoretical values are too small compared to experiments. However, it is well understood that there is no perfect surface for sure in the laboratory, neither in space most probably due to the radiation field or possible sputtering following collisions damages. Then, to further approach the model surface to more realistic ones, several types of imperfections were a priori introduced in the topmost layer. Local defects, as surface holes, have been considered. With the removal of two adjacent carbons in the topmost layer, leaving a localized hole the size of pyrene, E are increased by 10% for both CH3CN and CH3NC isomers. If the rim of the hole is saturated by H atoms, E are increased by 40% with respect to the pristine surface, giving still too low E values. Delocalized defects are provided by the existence of steps. In this case, part of the topmost layer is like a terrace laid on top of the layer underneath, which is typical of the making of HOPG samples in the laboratory. In view of the ubiquitous presence of hydrogen we have considered the hydrogenated step only. Here, both isomers are

most stable when stretched out in the trough of the step with adsorption energies of 478 and 442 meV to be compared to the TPD values of 440 and 430 meV for CH3CN and CH3NC respectively. This remarkable agreement shows the predicting dimension of the interdisciplinary approach to surface processes in the laboratory and hopefully in space. Notes Bertin; M., Doronin, M., Fillion, J.-H., et al. 2017, A&A, 598, A18; ibid submitted 2017 Greenberg, J. M. 1976, Astrophys. Space Sc, 39, 9

Theory of inelastic and reactive collisions

Laurent Wiesenfeld

Institute for Planetary Sciences and Astrophysics Grenoble (IPAG)

Physical conditions of interstellar matter are such that thermodynamical equilibrium is far from a good approximation in many circumstances, being it for internal degrees of freedom for molecules, and to a more general extent, to the chemical composition of the gases. The chemical composition of gases is mostly governed by chemical kinetics, not even always reaching steady-state conditions. In a similar way, excitation conditions of polar molecules result of a trade-off between collisional and photonic interaction. In the last decade, significant progress has been made in our understanding of molecular collisional excitation, which has contributed to molecular line diagnostic studies. We will review the theoretical efforts in obtaining state-to-state collisional rate coefficients for the excitation of diatomics and polyatomics. Examples will be presented for small molecules, like CO, NH_3, and H_2O in collision with atomic H, He and molecular H_2. Also, examples of collisions of higher mass molecules, like HNCO and $HCOOCH_3$ will be described, together with the difficulties associated with those collisions. Some insights towards ro-vibrational excitation will also be described. Recent comparisons with experimental results have demonstrated that collisional data have now reached such accuracy that they no longer limit the interpretation of molecular spectra. Numerous quantitative comparisons exist, with pressure broadening experiments at the forefront, because of the absence of any adjustable scale parameter in the measurement or theoretical computations. We also display comparison between observation and prediction of van der Waals complex vibrational levels as well as positions of collisional resonances at small collision energy.

Astrochemistry in temperature variable ion traps

Dieter Gerlich
TU Chemnitz

In the introduction I will give a short historic overview over various instruments for studying gas phase processes under circum- and interstellar conditions. Experimental methods include discharges, molecular beam methods, flow systems, ion traps, and storage rings. The versatility and the sensitivity of the cryogenic 22-pole trap allowed the first systematic study of radiative association. Low temperature conditions result in isotope enrichment (e.g. H3+ + H2), in long lived reaction intermediates, or also in sig-nificant changes of the reaction rate coefficients (e.g. FeO+ + H2.). Combination of traps with radical beams extend the range of applications(H-+H, CH+ + H, NH+ + H). In addition to new high resolution spectroscopy methods (e.g. He-H3+), new strategies are needed to search systematically for carriers of the DIBs. First steps are the electronic spectra of C60+ recorded in a cryogenic linear quadrupole traps as well as IR spectra of multiply charged C60n+. A final example will mention results from a high temperature trapping experiment which can provide information on the formation and stability of fullerenes and other hydrocarbons. With an optimistic outlook I hope to motivate the next generation of experimentalists to apply and improve traps for exploring interstellar matter including interstellar dust.

Status on gas-grain chemical models for astrochemistry

Valentine Wakelam
Laboratoire d'astrophysique de Bordeaux, France

Chemical models for interstellar environments are complex tools in constant evolution based on new experimental and theoretical results on individual processes, but also on new astrophysical observations. Each of these results is a new stone to our understanding of interstellar chemistry. There are still many uncertainties in the gas-phase chemistry but more importantly in the chemistry occurring at the surface of interstellar dust. I will show in this presentation what we think we know and what are the predictions of such models for different types of environments (cold cores, protostars protoplanetary disks). I will also show what are the current limitations of these models and how we could go one step further.

The Gas Grain Chemistry of Translucent Molecular Clouds

Dominique Maffucci
University of Virginia

Recent absorption line surveys of the the translucent molecular clouds along the line of sight to Sagittarius B2 reveal chemical complexity including both small and large molecules in the gas phase. We model the abundances by parallelizing the chemical code Nautilus to produce grids of rate law solutions for the physical parameters spanned by the uncertainties in the observed conditions. Using both unweighted and weighted fitting methods, we highlight the strengths and limitations of each method and discuss the implications of the agreement between our models and recent observations using single dish and interferometric instruments.

Chemistry in young stellar objects with grain growth

Nanase Harada
Academia Sinica Inst. of Astronomy and Astrophysics

Although it is known that grain growth has occurred in the protoplanetary disks around the pre-main-sequence stars, recent observations suggest that it may have occurred already in the earlier stage, around Class 0/I protostars. Such grain growth can affect the surface area where grain-surface reactions can take place. We modeled the chemistry with the effect of grain growth with the physical conditions of protostars with the effects of grain growth. Our results show that sulfur-bearing molecules are most sensitive to the grain growth. By comparing modeled ratios of H2S, SO, and SO2, observed values agree best with the case where the maximum grain size has grown by a factor of 10-100.

Talks: Day 2 – Tuesday 18 July

Public astrochemical tools with dust surface processes and how to use them properly

Dmitry Semenov

Max-Planck-Institut fuer Astronomie

The interstellar medium (ISM) is surprisingly chemically rich, with more than 200 different molecules detected, including simple stable molecules and radicals, ions, and complex organics. Astronomers employ these molecules to infer the crucial information about the physical conditions, kinematics, and evolutionary stages of various ISM environments, ranging from diffuse clouds to dense clouds to proto-planetary disks to expanding shells of AGB stars. The recently completed ALMA and other upgraded radio facilities like eVLA and NOEMA provide unprecedented sensitivity at (sub)mm-wavelengths, allowing astronomers to detect more and more of cosmic species. According to our current theoretical and laboratory understanding, this rich molecular repertoire is a result of a multitude gas-phase, gas-grain, and dust surface processes. Thousands of these processes are included in several public databases, such as KIDA and RATE2012, albeit often without dust surface part. In addition, there are several publicly available gas-grain chemical codes that can be used together with these reaction sets to make predictions about abundances and evolution of various molecules in astrophysical objects. In my presentation I'll be talking about these tools and how a non-specialist can use them, including our ALCHEMIC and ANDES codes.

KROME: a tool for microphysics

Tommaso Grassi

Niels Bohr Institute / Starplan

A brief review on the code KROME and on its role in modelling chemistry and microphysics.

Photochemical-hydrodynamics with TORUS-3DPDR

Thomas Haworth
Imperial College London

I'll present TORUS-3DPDR, a code capable of multidimensional hydrodynamics, Monte Carlo radiative transfer and photoionisation/PDR physics. The code is unique in its ability to tackle dynamical problems where photoionisation and PDR physics are important using a direct treatment of the detailed microphysics. This is of course at substantial computational cost. In particular, I'll present results from an ongoing study into the external photoevaporation of protoplanetary discs, where the thermal properties are set by PDR physics. This will include photochemical-hydrodynamic benchmarks (Haworth et al. 2016, MNRAS, 463, 3616), identification of a disc being photoevaporated by an extremely weak UV field (Haworth et al. submitted) and multidimensional models of photoevaporating discs (Haworth et al. in prep).

Chemical Modelling with UCLCHEM

Jonathan Holdship
UCL

UCLCHEM is a gas-grain chemical code for cores, clouds and c-type shocks. I will present an overview of the now publicly available code and some of its applications. Further, I will show how bayesian inference methods can be used to do a sensitivity analysis to determine which reactions in a network with unknown reactions rates are the most important. Eg. knowing that grain surface reactions take place but not their rates, can we determine whether a small number of reactions are much more important than the others to focus experimental efforts?

Hot chemistry in PDRs & the Interstellar Medium DataBase

Frank Le Petit

LERMA - Observatoire de Paris

Our understanding of the chemical structure of PDRs is evolving significantly. Herschel has provided many observations of CO ladders in Galactic and extragalactic regions. In famous PDRs as the Orion Bar and NGC 7023, CO is detected up to J 20. The first interpretations of these CO ladders in PDRs were puzzling and several hypotheses have been suggested to heat the gas and excite CO such as mechanical heating, shocks, cosmic rays, ... Today, it starts to be recognized that UV photons can induce a hot chemistry that leads to the formation of excited molecules at the H/H2 transition. This view is confirmed by the recent ALMA observations of the Orion Bar (Goicoechea et al. 2016). This hot chemistry is difficult to simulate properly because it is the result of many interlinked complex processes. In this talk, I will present how we simulate these key processes in the Meudon PDR code and their impact on the hot chemistry at the edge of PDRs. In particular, I will show why it is important, to interpret these observations, to solve simultaneously and in detail the chemistry, the individual heating and cooling mechanisms as well as level excitation. I will focus on 1) how detailed modelling of H2 formation on warm grains impact the formation and the excitation of CO and other molecules, 2) how some state-to-state chemical reactions are critical to simulate properly the enhancement of the production of some key molecules, 3) why it is mandatory to consider properly H2 excitation in vibrational states to explain the intensity of other molecules in PDRs. This will be illustrated by the interpretation of the Herschel observations of Orion Bar, NGC 7023 and Carina. Such detailled PDR models require years to be developed. In a second part of the talk, I will present ISMDB (the Interstellar Medium DataBase) that gives access to thousands of pre-computed PDR models. More than just a database, ISMDB is an architecture that helps to solve inverse problems. I will show how ISMDB can provide a first order interpretation to complex observations with the example of the interpretation of H_2 observations ($\sim$70 levels) in NGC 7023. ISMDB is one of the applications used by IVOA to define Virtual Observatory standards for theoretical data.

Complex Deuterated Species in the Interstellar Medium

Ankan Das
Indian Centre for Space Physics

Despite the low elemental abundance of atomic deuterium in the interstellar medium (ISM), observational evidence suggests that several species, both in the gas phase and in ices, could be heavily fractionated. The high abundance of some abundant and simple interstellar species could be explained by considering the chemistry that occurs on interstellar dust. Because of its simplicity, the rate equation method is widely used to study the surface chemistry. However, because the recombination efficiency for the formation of any surface species is highly dependent on various physical and chemical parameters, the Monte Carlo method is best suited for addressing the randomness of the processes. We carry out Monte-Carlo simulation to study deuterium enrichment of interstellar grain mantle under various physical conditions. Moreover, we explore various aspects of deuterium enrichment by constructing a chemical evolution model in both gaseous and granular phases (by considering the rate equation method). Depending on various physical parameters, gasses and grains are allowed to interact with each other through the exchange of their chemical species. Obtained deuterium fractionation of some abundant interstellar ions is then used to predict the ionization degree around the various region of a molecular cloud. This gas-grain model is further utilized to predict the abundances of some new complex deuterated species. Quantum chemical calculations were implemented in our computation to prepare the reaction pathways of these deuterated species and supplement our results with the observation-specific information. The simple radiative transfer method is also used to justify our results.

Astrophysical multiscale modeling with AMUSE

Simon Portegies Zwart
Leiden Observatory

Astrophysical phenomena cover many order of magnitude in spatial and temporal scales. An additional complexity is introduced by the multi-physics aspects of the Universe. We present the Astrophysical Multipurpose Software Environment (AMUSE), which was designed specifically to allow researchers to simulate these processes on high-performance architectures. In AMUSE subgrid physical phenomena can be taken into account explicitly. The coupling across scales and across physical domains is realized by means of operator splitting. In multi-scale simulations, when the underlying physics shares the same Hamiltonian, we demonstrate that this coupling strategy captures the right physics to second order. When employing the operator splitting strategy across discipline we validate the results by comparison with historic results.

Simulation projects can be setup in AMUSE in a declarative fashion in which the coupling strategies are described at a meta level. These descriptions allow for the strict separation of individual modules for multi-scale and multi-domain simulations in the form of patterns. In this study we describe how these patterns are implemented in AMUSE and where they can be used to help the modeling celestial phenomena.

Chemistry/Microphysics in hydrodynamical simulations

Paul Clark
Cardiff

We review the current state-of-the-art in chemical / ISM modelling. The first half of this talk will focus on the advances that have been made over the last 10 years, and how they have shaped our current understanding of star formation and molecular cloud formation. In the last part of the talk, we will focus on the major issues that we face in numerical modelling, and highlight several paths for future research.

Primordial star formation using GRADSPH-KROME

Rafeel Riaz
University of Concepcion, Chile

Primordial chemistry is known to be important during primordial star formation, as it regulates the formation of molecular hydrogen via gas-phase chemistry, which is the main cooling agent and regulates how fragmentation occurs. We present here a new numerical approach where the MPI-parallel smoothed particle hydrodynamics code GRADSPH (Vanaverbeke et al. 2009) has been combined with the chemistry package KROME (Grassi et al. 2014). We employ the new KROME-GRADSPH framework to investigate the collapse of primordial clouds in the high-density regime, exploring the fragmentation process and the formation of binary systems. In this talk, I will present the results from a parameter study investigating the effect of rotation and different Mach numbers on the interactions of the dynamics with the chemistry, and quantifying the outcome of the simulations under different conditions. I will conclude with a short outlook on the implications of radiation backgrounds and metal cooling.

Non-ideal MHD in star formation

Pierre Marchand
CRAL - ENS Lyon

Non-ideal MHD effects play a major role in the regulation of angular momentum during the early stages of star formation. Their strength is defined by their associated resistivities, whose values depend on the chemical environment. First, we present how we computed these resistivities from our chemical network, then what are the consequences of non-ideal MHD effects on the formation of structures.

The intricate interplay of physics and chemistry: an AGB story

Jels Boulangier
KU Leuven

Mass loss of evolved stars, such as AGB stars, is one of the most dominant sources of chemical enrichment of the ISM. The chemical mixture of the ISM eventually determines the composition of molecular clouds, stars and even planets. As these new stars evolve, almost all of them go through the AGB phase thereby completing the chemical life cycle. Understanding the transport by and composition of the AGB stellar winds, from the star itself to the ISM, is a crucial stage in the cycle. The physical and chemical conditions of AGB winds, which contain shocks, are poorly understood due to i) lack of high resolution observations, ii) simplifying assumptions in theoretical models and iii) lack of laboratory data. We strive towards developing a self-consistent hydro-chemical model, improving on the current wind models. This approach is needed because of the intricate interplay between dynamics and chemistry, caused by shocks and cooling/heating. The chemical composition determines which cooling mechanisms (e.g. H2, CO, metal lines) influence the thermal evolution of the gas. In turn, the temperature acts on the dynamical behaviour of the wind which again will impact the rate of chemical reactions. Therefore, we take into account all important chemical reactions and thermal mechanisms. A future prospect is to include dust, aiming for a more complete picture of dust-driven AGB winds. Our self-consistent hydro-chemical model will help us answering questions such as: What is the dynamical/chemical structure in AGB winds? How important is the chemical-dynamical feedback loop? Do chemical instabilities exist?

The influence of dynamic evolution on the chemistry of protoplanetary discs

John Ilee

Institute of Astronomy, University of Cambridge

Protoplanetary discs are one of the most extreme environments in astrophysics, spanning a huge range of temperatures and densities. As such, modelling their chemical evolution is challenging, and has often been reduced to the study of 2-dimensional, axisymmetric discs. However, the advent of ALMA has shown that many protoplanetary discs do not conform to this axisymmetry. Dust traps, warps, embedded planets and spiral arms have all recently been observed in discs, complicating matters further. In particular, the influence of the dynamic evolution of the disc on the chemical evolution has not been well studied. In this talk I will discuss our groups work on some of the first calculations of chemical evolution in protoplanetary discs in three-dimensions (Ilee et al. 2011). In discs which a sufficiently massive, the spiral shocks induced by the self gravity of the disc can have a large effect on the chemistry. Species are desorbed from dust grains at much further radial locations than they would otherwise exist. In addition, the increased temperatures and densities caused by the shocks leads to gas phase reactions in warm, shocked regions that would not otherwise occur. Additionally, if these discs are massive enough to fragment, then our results suggest that these fragments should possess unique chemical signatures which will enable us to characterise them (Ilee et al. in prep.). We have shown that ALMA will be essential in being able to characterise these phenomena in the wild (Douglas, Caselli, Ilee et al. 2013; Evans, Ilee et al. in review). Such discs are not confined to existing around more massive stars, and in fact may have preceded the formation of the Solar System, leading to changes in the initial chemical conditions that should be adopted when considering chemical models of more evolved protoplanetary discs (Evans et al. 2015).

Talks: Day 3 – Wednesday 19 July

Towards a complete model for H-C-O chemistry in the ISM

Troels Haugboelle
STARPLAN, National History Museum of Denmark and the Niesl Bohr Institute, University of Copenhagen

I will present a new model for H-C-O chemistry including photo-chemistry, ices, and dust, which is coupled, using KROME, to deep adaptive mesh refinement models of the ISM.

Chemical signatures in magentized cores

Seyit Hocuk
MPE

Magnetic fields are thought to play a notable role on the dynamics of evolving interstellar clouds. Various independent studies recently suggested the significance of magnetic fields on simple gas-phase chemistry (e.g. Seifried & Walch 2015), and vice versa (e.g., Zhao et al. 2016). In this work, we test the interplay between magnetic fields and chemistry by utilizing a detailed gas-grain chemical network. Our focus lies on the chemical imprints that magnetic fields leave behind, especially on interstellar ices. We investigate the role of magnetic fields by simulating magnetized clouds with various field strengths, B = 0,5,10 μG, during the evolution of an interstellar cloud from the diffuse atomic to the dense molecular phase. We find that with ideal magnetic fields, the cloud contraction is delayed around the trans-critical phase where C+ converts to C and CO, and where the freeze-out process commences. Due to the time-dependent nature of chemical reactions, especially for surface species, this delay leaves an imprint on the chemical abundances. While the gaseous species are not strongly affected, aside from an enhancement of atomic carbon during the early phases of cloud evolution, ices show a stronger signature of magnetic fields. As the molecular oxygen ice abundance drops, carbon dioxide, formaldehyde, and methanol ices increase. The effect grows stronger with increasing magnetic field strength. We also reproduce the magnetic scaling relation that is inferred from

the Zeeman observations of Crutcher 2010,2012. This includes the consideration of OH freeze-out. We predict that at column densities above a few 10^{23} cm^{-2}, the line-of-sight magnetic field strength inferred from OH molecules should display a flatting toward higher column densities due to OH freeze-out. We also predict that due to the orientation of field lines towards the observers line-of-sight, the magnetic field strength can be misinterpreted as having very a low field strength at column densities below 10^{22} cm^{-2}.

Deuterium fractionation and H_2D^+ evolution in magnetized and turbulent filaments and their substructures

Bastian Körtgen

Hamburg Observatory

High-mass stars are expected to form from dense prestellar cores. Their precise formation conditions are widely discussed, including their virial condition, which results in slow collapse for supervirial cores with strong support by turbulence or magnetic fields, or fast collapse for subvirial sources. To disentangle their formation processes, measurements of the deuterium fractions are frequently employed to approximately estimate the ages of these cores and to obtain constraints on their dynamical evolution. We here present 3D magnetohydrodynamical simulations including for the first time an accurate non-equilibrium chemical network with 21 gas-phase species plus dust grains and 213 reactions. With this network we model the deuteration process in fully depleted interstellar filaments and prestellar cores in great detail and determine its response to variations in the initial conditions. We find qualitatively good agreement with recent observations of deuterium fractions in quiescent sources. Our results show that deuteration is rather efficient, even when assuming a conservative ortho-to-para ratio of H_2 of 3.

Effect of Grain Size & Freeze-out on Non-ideal MHD Diffusivities.

Bo Zhao

MPE

We developed a chemical network for calculating non-ideal MHD diffusivities in star formation, including 13 molecular, 23 ion species, charged grains and above 200 reactions. The freeze-out and thermal desorption of molecules on grains are also included. We find that all three non-ideal MHD diffusivities (ambipolar, Hall and Ohmic) are generally very sensitive to the grain size distribution, especially to the very small grains (VSGs) of few to tens of nanometers. Removing the large population of VSGs from the standard MRN distribution that dominate the coupling of bulk neutral matter to the magnetic field increases ambipolar diffusivity at densities below 10^{10} /cm^3, as well as Hall diffusivity at densities above 10^{10} /cm^3 by $\sim$1-2 orders of magnitude. In particular, the AD diffusivity reaches an overall optimum level when choosing a$_{min}$=0.1 μm and Hall diffusivity a_{min}=0.04 μm. The Ohmic diffusivity only becomes important at densities above 10^{13} /cm^3. Furthermore, we find that freeze-out of molecules replaces HCO+ with H3+ as the dominate ion species at the density range 10^6–10^{10} /cm^3. However, the change of ion weight by freeze-out has limited effect on the magnetic diffusivities at low densities.

Chemo-dynamical simulations of HII regions with non-frozen dust

Maria Kirsanova

Institute of Astronomy of the Russian Academy of Sciences

Sites of massive star formation are marked by expanding HII regions surrounded by photodissociation regions (PDRs) and further away by shocked molecular gas. We have developed a chemo-dynamical model of an expanding HII region and its environment in order to study impact of massive stars on molecular clouds and how far this impact extends. The model accounts for dynamics, dust microphysics, molecular evolution, and all relevant heating and cooling processes. We explain the very specific observational appearance of HII regions and PDRs in Spitzer's images: ring-like emission at 8 mkm surrounds areas bright at 24mkm (as well as at WISE 12 and 22 mkm bands). To do this we consider dust drift under the influence of stellar radiation pressure during the expansion of the HII region (see Akimkin et al.-2015, Akimkin et al.-2017, in press). Dust is represented by polycyclic aromatic hydrocarbons (PAHs) and an ensemble of silicate and graphite grains of larger sizes. We present calculations where the radiation pressure on dust, Coulomb drag, dust drift, and the lug of gas by dust are considered simultaneously to describe the

dynamics of the HII region. Big grains are effectively swept out of the HII region. PAHs and smaller graphite grains are mostly coupled to the gas. The time-scales of the dust blow-out from the HII regions are 20, 100 and 250 kyr for the models with star effective temperatures Teff of 30 000, 35 000 and 40 000 K, respectively. Notably, the dust-to-gas ratio inside HII region is larger for an ionizing star with a higher temperature since the dust grains have a larger electric charge and are more strongly coupled to the gas. While the radiation pressure expels 5090 per cent of the dust mass from the HII region into the neutral shovelled envelope, the dust drift in the molecular region is inefficient. So, it is reasonable to use dust grains of a single size for chemical modelling of molecular cloud around an expanding HII region. We produce synthetic observations of HII regions with Spitzer/Herschel and compare them with the HII region RCW120 which has an almost round shape (see Pavlyuchenkov et al.-2013). Spatial distribution of emission at wavelengths larger than 24mkm is explained by selective dust extraction from the HII region, but 8-mkm emission could only be explained with hypothesis of PAH destruction inside the HII region by UV emission. We show how chemical composition of PDR and shocked molecular gas as well as the spectral energy distribution toward the HII region and PDR change with time.

Constraining the accretion regions of meteorites via astrochemical modelling of protoplanetary disks

Jon Ramsey

STARPLAN, National History Museum of Denmark and the Niesl Bohr Institute, University of Copenhagen

Meteorites are the best available empirical record of the formation and early evolution of our Solar System. They originate from asteroid-sized parent bodies (i.e. planetesimals) that have experienced an energetic collision, ejecting material into interplanetary space. While roughly thirty thousand meteorites have so far been discovered on Earth, the meteoritic record remains very far from complete. Indeed, in many cases, interpretation of meteorite data is degenerate in regards to space and time. I will present astrochemical and radiative transfer models of protoplanetary disks which attempt to constrain the accretion space-time of meteorite parent bodies. Through the inclusion of molecular ices and isotopologues of hydrogen and nitrogen, it is possible to make comparisons with meteoritic data, and therefore make inferences about parent body accretion within the early Solar System.

Molecular gas chemistry and radiation transport with mesh-less hydrodynamics

Alessandro Lupi
Institut d'Astrophysique de Paris

Recent developments of numerical simulation techniques and sub-grid modelling have allowed to investigate in more detail the galaxy properties and the role of star formation and feedback from stars and AGN on the host evolution. However, many studies on galactic and cosmological scales still lack a detailed treatment of the chemistry, a necessary ingredient to compare the simulation results with observations, in particular after the advent of the ALMA telescope. I will present a model to follow the chemical species abundances, via the chemistry package KROME, which also takes into account gas and dust shielding, self-shielding of molecular gas, and HII region formation (both as a sub-grid model and with on-the-fly radiative transfer calculations). I will discuss the results of a suite of idealised simulations of an isolated gas-rich galaxy using this model, implemented in the new hydrodynamic code GIZMO, which has proved to capture the advantages of both standard techniques, SPH and AMR, avoiding their main limitations. I will also show how this model can recover the Schmidt-Kennicutt law and naturally predict the correlation between molecular gas density and star formation rate. I will finally discuss how this model can be easily extended to include additional species and I will introduce the future works we are working on, aimed at following the dynamics of molecular gas in high-redshift quasars and the formation of CII in high-redshift dwarf galaxies.

Hydrodynamics with gas-grain chemistry and radiative transfer: comparing dynamical and static models

Olli Sipilä
Max-Planck-Institute for Extraterrestrial Physics

Chemical models have been invoked to try to reproduce the abundances of various molecules observed toward starless and prestellar cores. In such studies a static physical model is often adopted to represent the object, and the chemical model is run assuming that the physical structure remains fixed as the chemistry evolves. This assumption is inherently incorrect, as we know that the time-dependent gas-grain chemistry affects the temperature structure, and thus also the density structure, of the object owing to depletion onto grain surfaces which modifies the abundances of the cooling molecules. In the present study we discuss a new 1D hydrodynamical model that integrates the basic equations of hydrodynamics (no magnetic fields) with gas-grain chemistry and radiative transfer. We compare the chemical abundance profiles predicted by the hydrodynamical model to those given by a static model,

and simulate some commonly observed lines. It is found that at late times, the two types of model give clearly different predictions, indicating that the use of a static model can indeed be a very inaccurate assumption. Our new model is very versatile as it includes extensive descriptions of deuterium and spin-state chemistry, increasing the number of tracer species whose line emission profiles can be self-consistently modeled.

Modeling observations

David Neufeld

Johns Hopkins University

Observations at far- and mid-infrared wavelengths provide a wealth of information about the molecular inventory of interstellar gas clouds. Because of the different chemical pathways responsible for their formation and destruction, different molecules probe specific aspects of the interstellar environment. Carefully interpreted, they provide unique information about the molecular fraction, the UV radiation field, the dissipation of energy within the turbulent ISM, and the cosmic-ray density in the Galaxy. This talk will include a general overview of astrochemical probes of the interstellar medium, along with new estimates of a key parameter in astrochemical models: the cosmic-ray ionization rate.

Chemistry in high line-mass filaments

Amelia Stutz
UdeC

Star formation takes place in a broad range of filamentary gas environments. The filament gas volume density is a critical parameter for chemical modeling and is the starting point for more detailed theoretical and numerical investigations into e.g., high density tracers such as N2H+, deuteration, electron densities, and other chemical properties of the typical yet extreme filamentary environments leading to massive star and cluster formation. By scrutinizing the nearest example of a high line-mass filament (Orion A's Integral shaped filament; ISF) and cluster in formation we gain new insights into the physical conditions the gas that lead to star cluster formation. Based on Herschel submm data at ∼10000 AU resolution, we have shown that the gas in the ISF has a high volume density, with a radial profile that is distinct from the nearby low mass filaments that have been studied to death. Our investigation reveals that the magnetic field in the ISF plays a central role in the dynamics of the gas. Moreover, previous studies have revealed that the cloud is enveloped in a helical B-field. Circular (or more generally, helical) fields have the form necessary to confine filaments and squeeze them to higher densities. Furthermore, our recent ALMA observations at ∼1000 AU resolution show that this high density filament exhibits gas fragmentation properties that are very different from equilibrium models of low line-mass filaments. Despite the growing wealth of observational evidence that the ISF represents a different and distinct environment than those probed in "Taurus-like" filaments, we currently have almost no knowledge of how these differences in conditions may manifest as chemical differences in the gas.

Gas phase elemental abundances in molecular clouds (GEMS)

Asuncíon Fuente
Observatorio Astronmico Nacional

Simulations with an increasing level of complexity are being developed to model the chemistry and dynamics of collapsing clouds. The pioneering one-dimensional models have been overtaken by 3D-radiation-hydrodynamical (3D-RHD) and magneto-hydrodynamic (3D-RMHD) simulations coupled with a full gas-grain chemistry. But all these sophisticated simulations share the problem of the uncertain initial conditions (turbulence, ionization degree, elemental abundances, magnetic field) and geometry. Our project aims at determining the S, C, N, O elemental abundances and the gas ionization fraction as a function of visual extinction in a selected set

of prototypical star forming regions. These parameters determine the cloud evolution and future star formation activity and are the essential ingredients of any 3D-R(M)HD simulations. We present preliminary results TMC 1 and Barnard 1, prototypical dark clouds with low and moderate star formation activity, respectively.

Phosphorus: the missing prebiotic element. How to detect and model it.

Victor M. Rivilla

Osservatorio Astrofisico di Arcetri, OAA-INAF

Phosphorus (P) is one of the key chemical elements for the development of life. Along H, C, O, and N, Phosphorus is one of the constituents of the macromolecule of DNA. The extreme structural stability and functional reactivity of P-bearing compounds (phosphates) make them unique in many biochemical processes. For this, we think that Life on Earth may have originated in a solution rich on P-bearing compounds. Therefore, the study of the chemistry of P in the ISM, and in particular in planet- and star-forming regions is mandatory to understand the formation of the building blocks of life. However, our knowledge about Phosphorus in the ISM is still in the dark. With the goal of better understanding the interstellar chemistry of P, our group in the Arcetri Observatory started a project to detect P-bearing molecules in star-forming regions. I will present the results of a survey of 30 galactic massive dense cores searching for P. We have detected the molecule PN in 10 of them, which doubles the number of detections so far. Moreover, we have also detected for the first time in star-forming regions, the chemical bond P-O, which is essential to build-up the backbone of DNA. With the aim of understanding the origin of P in star-forming dense cores, our group at MPE is currently developing a chemical network focused in the P-chemistry. Our preliminar modelling indicates that PO and PN are chemically related and form purely in a sequence of gas-phase ion-molecule and neutral-neutral reactions during the cold collapse phase. However, due to the lack of observational and laboratory data, the theoretical modelling is still in its infancy. We are currently upgrading our chemical network to include more P-bearing molecules with the aim of better understanding the first steps of phosphorous chemistry in the ISM.

Post-processing of existing hydrodynamic simulations with chemical networks

Tom Douglas
University of Exeter

In order to calculate chemical abundances for regions of interest in hydrodynamic models detailed histories of density, temperature and radiation intensity are needed for parcels of gas. This is usually accomplished by using tracer particles which follow the flow of the gas and record the gas properties at a much higher frequency than the rest of the model. This has the disadvantage of needing to be included when the model was started and gives little control over which regions of the model are adequately sampled, particularly if low density regions are of interest. Here we present an alternative method where radial basis functions are used to create an interpolant of the gas properties in space and time from the points saved as a matter of course in creating the simulation. This interpolant is then used to recreate approximate paths for gas parcels originating from any point in the simulation. This allows an arbitrary number of parcels to pass through regions of interest. We present an example 2d radiation-hydrodynamic simulation of star formation and use it to explore how accurately paths are recreated with varying times between recorded gas states.

Synthetic observations of the transition to coherence: the role of turbulence, magnetic fields and initial conditions

Rachael Spowage
Cardiff University

The observed transition to coherence in molecular clouds has been at the forefront in the discussion of the dissipation of turbulence. Typically observed as a near-constant, trans- or sub-sonic velocity dispersion within the confinements of a dense core, previous observations in dense gas tracers have shown a sharp drop in velocity dispersion over the core boundary. We will present an investigation into the physical triggers of the transition to coherence. Utilising a combination of simulations and radiation transfer modelling, we produce synthetic images in a multitude of molecular lines, including NH3, C18O, HCO+ and N2H+. Initially probing the effects of the mode of turbulence on the presence of a transition to coherence, we find that the predicted transition occurs in all environments, for all molecular tracers. We find compelling evidence that temperature plays a significant role in producing the observed coherent region, not the dissipation of turbulence. Using the typical simulation approach of a uniform density sphere, we find an abundance of multiple peaks along each line of sight otherwise not seen in observations. This highlights the current concerns about the impact of initial conditions on the resulting evolution of

the molecular cloud. We will highlight this discrepancy by considering the presence of a transition to coherence in a set of cloud-cloud collision simulations, and role of magnetic fields.

Synthetic observations of filaments: the problems of mapping from PPV to PPP

Seamus Clarke
University of Cologne

We present moving-mesh simulations of filament fragmentation which include time-dependent chemistry and coupled thermodynamics. From these simulations we produce synthetic observations of C18O, J 1-0, with spatial and velocity resolution comparable to the observations of fibres presented in Hacar et al. (2013). We show that there are multiple velocity components throughout the filaments. Furthermore, we detect numerous velocity coherent sub-filaments in position-position-velocity (PPV) space. However, the mapping of PPV structures to position-position-position (PPP) space shows much confusion along the line of sight: the merging of separate PPP structures, the blending of true PPP structures with unconnected gas, and the artificial separation in PPV space of PPP structures due to shocks.

Abstracts: Poster

Reproducing small scale chemical segregation in the hot core G35.20-0.74 B

Veronica Allen

Kapteyn Astronomical Institute

Chemical differentiation at the scale of thousands of AU has been observed in several hot cores (chemically rich high-mass protostars) including Orion KL, W3(OH) and W3(H2O), and AFGL 2591 VLA 3. Using ALMA cycle 0 observations, we have detected a difference in chemistry within Keplerian disk candidate G35.20-0.74N core B (G35.20B) on a scale of 900 AU (Allen et al. 2017 submitted). In this source, all observed nitrogen-bearing species have higher abundances toward the south-east and cyanide abundances are at least one order of magnitude less toward the north-west. We used a time-dependent chemical model with gas and grain surface chemistry to determine what factors could lead to the chemical differentiation seen in G35.20B. We vary initial ice conditions, warm up speed, and density to successfully reproduce our observations. We find that the initial ice conditions have little effect on the observed abundances at the end of the warm up. The model temperatures at which our observations are reproduced indicate a temperature gradient where the south-east is warmer than the north-west which is aligns with the conclusions of Allen et al. 2017.

Chemical composition of three new hot cores discovered in Sagittarius B2(N) with ALMA

Melisse Bonfand

Max Planck Institute for Radio astronomy

Observations of star forming regions at (sub)millimeter and centimeter wavelengths have allowed astronomers to detect numerous molecules including some of the most complex molecules ever observed in the interstellar medium (ISM). One of the best targets to study these complex organic molecules (COMs) is the Sagittarius B2 molecular cloud. Sgr B2 is one of the most prominent regions forming high-mass stars in our galaxy. In order to extend the inventory of interstellar COMs and improve our understanding of the chemical processes occuring in the ISM, the EMoCA survey (standing for Exploring molecular complexity with ALMA) has been conducted with ALMA in its cycles 0 and 1. The observations target Sgr B2(N), one of the main centers of activity in Sgr B2. We present the discovery of three new hot cores in this region, made possible thanks to the high sensitivity of the EMoCA survey. The chemical composition of these new sources and the column densities of the detected molecules are derived by modelling their spectra. The association of the hot cores embedded in Sgr B2(N) with class II methanol masers, outflows, and/or ultra-compact HII regions suggest an age sequence that we wish to better constrain by comparing the chemical composition of the sources with the predictions of the chemical kinetics model MAGICKAL (Garrod 2013).

An imaging line survey from OMC-1 to OMC-3 in the 1mm window

Nina Brinkmann

Max Planck Institute for Radio astronomy

The northern part of the Orion A molecular cloud is one of the most prominent regions of low to high-mass star formation, whose close proximity of just 414 7 pc enables us to spatially resolve its physically and chemically different regions. Continuum maps show sub-structures which divide Orion A into morphologically different regions: the bright OMC-1 in the south, with a group of filaments radiating away from its central region and the less prominent OMC-2/3 in the north. OMC-1 contains two high-mass star forming sites and is heavily influenced by intense UV radiation from the young massive 'Trapezium' stars. It also includes the prototypical photon-dominated region (PDR) Orion Bar, outflows, a hot core containing a rich chemistry of complex molecules, but also more quiescent gas. In contrast, there are no massive O/B stars in OMC-2/3, but a large number of pre-stellar cores and protostellar Class 0/I objects, resulting in a very different environment with outflows

driven by young embedded stars, but without extreme UV radiation. Our unbiased dataset obtained with the APEX telescope covers the area of OMC-1 to OMC-3 from 200.2 GHz to 281.8 GHz, enabling us to examine the characteristics of low to high-mass star formation in a variety of environments within a contigous molecular cloud, helping to understand the influence of star formation on the sourrounding material and vice versa. We cannot only compare regions in terms of their molecular content and excitation, but also infer temperatures, optical depths, column densities and abundances for a variety of molecular species.

Impact of radiation backgrounds on the formation of massive black holes.

Vanesa Diáz & Camila Olave

Universidad de Concepción

The presence of supermassive black holes of a few billion solar masses at very high redshift has motivated us to study how these massive objects formed during the first billion years after the big bang. The most promising model that have been proposed to explain this is the direct collapse of protogalactic gas clouds. In this scenario, we need very high accretion rates of 1 $M_\odot$/yr to form these objects, which is something very unusual in astrophysics, and important to understand the conditions under which it may still occur. The main coolant of the primordial gas is the molecular hydrogen which forms via gas-phase reactions, so it is important in regulating cooling and therefore fragmentation. Recent studies have shown that if we use a strong radiation background, the hydrogen molecules are destroyed, regulating the amount of available cooling, favoring the high accretion rates and therefore producing objects of very high mass ($\sim 10^5$ $M_\odot$). So, in this project I explore the impact of external UV radiation fields on the formation of the first supermassive black holes using the astrochemestry package KROME combined with the smoothed-particle-hydrodynamics code GRADSPH in which my goal is to add radiative background to explore the fragmentation in collapse simulations and then probe if more massive objects will form, leading to the formation of a massive black hole.

Metal poor chemistry during high-redshift star formation

Patricio Fibla & Felipe Navarrete
Universidad de Concepción

The first stars are expected to form in the early Universe were the main coolant is the molecular hydrogen, which is efficient down to temperatures of 300 K. Metal enrichment changes the chemical and thermal conditions, and allows to cool the gas to lower temperatures where fragmentation may be enhanced. So far, however, only a few studies have been pursued with 3D simulations where these effects were taken into account, often employing an approximate model for the cooling and following the dynamical evolution just for a short time. I will present here three-dimensional cosmological hydrodynamical simulations during the early stages of the collapse process including a detailed treatment of the chemical networks involved, focused on the impact of the presence of O, N and Si on the temperature during the collapse. For the later, I will employ the astrochemistry package KROME coupled with the hydrodynamical code GRADSPH.

Formation of Resonant Moons in Weakly Accreting Circumplanetary Disks

Yuri Fujii
Nagoya University

During the formation phase of gas giants, circumplanetary gaseous disk form around the planets. Circumplanetary disks are important not only for mass supply to gas giants but also for formation of regular satellites. Because of the comparatively small size-scale of the disk, quick magnetic diffusion prevents the magnetorotational instability (MRI) from being well-developed at ionization levels that would allow MRI in the parent protoplanetary disk. In the absence of significant angular momentum transport, continuous mass supply from the parental protoplanetary disk leads to the formation of a massive circumplanetary disk. We have developed an evolutionary model for this scenario and have estimated the orbital evolution of moons within the disk. In a certain temperature range, we find that inward migration of a moon can be stopped by a disk structure resulting from the opacity transitions. We also find that the second and third migrating moons can be captured in mean motion resonances. In this way, a compact system in Laplace resonance, which are similar to inner three bodies of Galilean satellites, can be formed in our disk models. It may be difficult to form icy moons in situ in our disk models, but the temperature range is favorable to induce high-temperature chemical reactions, such as CAI formation.

Representative and calculable DFT models of the mesoporous silicas

Maciej Gierada

Cracow University of Technology

Among a large number of amorphous materials that are used nowadays as a support for nano-objects, mesoporous structures play an important role due to their specific parameters. However, theoretical investigations involving these materials are significantly limited due to the lack of appropriate models that well and accurately describe structure of the walls at different conditions (p, T) and enable effective computation at the same time. In this work, we present DFT models which resolve that issue. In particular, we focus on the material known as MCM-41. The models developed [1] show good agreement with experimental data, as evidenced comparing pore size diameter, wall thickness, wall density, T-site density, T-site density of the wall, Si-O-Si distances and angles, as well as number and type of silanols at different conditions. IR spectra were also computed confirming that our models are realistic. AIMD simulations of the model with water inside the confined spaces show low mobility of H2O molecules indicating their strong adsorption. As the models developed are easily applicable in future investigations, we believe that they will be widely used, for example as a support for modelling active sites or to study adsorption and other phenomena occurring in the interstellar medium. Hence, this contribution opens new perspectives in theoretical studies of amorphous silica materials. Acknowledgments This work was supported in part by the National Science Centre, Poland, Projects No. 2015/19/N/ST4/00007 and 2015/19/B/ST4/01836, and by French state funds managed by the ANR within the Investissements d'Avenir programme under reference ANR-11-IDEX-0004-02, and more specifically within the framework of the Cluster of Excellence MATISSE led by Sorbonne Universit. HPC resources from GENCI-[CCRT/CINES/IDRIS] (Grant 2015-[x2015082022]) and the CCRE of Universit Pierre et Marie Curie are also acknowledged. Other computational resources from PL-Grid Infrastructure are acknowledged as well.

The Possibility of Forming Propargyl Alcohol in the Interstellar Medium

Prasanta Gorai
Indian Centre for Space Physics

Propargyl alcohol (HC2CH2OH, PA) has yet to be observed in the interstellar medium (ISM) although one of its stable isomers, propenal (CH2 CHCHO), has already been detected in Sagittarius B2(N) with the 100-meter Green Bank Telescope in the frequency range 18 26 GHz. In this work, we investigate the formation of propargyl alcohol along with one of its deuterated isotopomers, HC2CH2OD (OD-PA), in a dense molecular cloud. Various pathways for the formation of PA in the gas and on ice mantles surrounding dust particles are discussed. We use a large gas-grain chemical network to study the chemical evolution of PA and its deuterated isotopomer. Our results suggest that gaseous HC2CH2OH can most likely be detected in hot cores or in collections of hot cores such as the star-forming region Sgr B2(N). A simple LTE (Local thermodynamic equilibrium) radiative transfer model is employed to check the possibility of detecting PA and OD-PA in the millimeter-wave regime. In addition, we have carried out quantum chemical calculations to compute the vibrational transition frequencies and intensities of these species in the infrared for perhaps future use in studies with the James Webb Space Telescope (JWST).

On Hydrogenation Reactions of Precursors of Amino Acids in the Interstellar Medium: Theoretical Study

Soledad Gutiérrez-Oliva
Pontificia Universidad Católica de Chile

Based on the experimentally determined network of hydrogenation processes of hydrogen cyanide HCN into methylamine CH3NH2 , in this research we studied the mechanisms of hydrogenation of precursors needed in the amino acids formation reactions that takes place in the interstellar medium. Using high level ab-initio calculations and theoretical descriptors of the electronic and structural activity taking place during a chemical reaction, a detailed characterization of the mechanisms involved in the different steps of the hydrogenation are provided. The study is based upon the reaction force analysis and takes advantage of the partition of the reaction coordinate into reaction regions where different mechanisms might be taking place. The reaction mechanisms are elucidated through the characterization of the evolution along the intrinsic reaction coordinate of various structural and electronic properties. Transition states structures, the physical nature of activation energies and the specific interactions driving the reaction mechanisms are analyzed and discussed.

The LEGO Survey: Unique Constraints on the ParsecScale Chemistry of Molecular Clouds

Jens Kauffmann
Max Planck Institute for Radio astronomy Bonn

I am reporting on first results from the LEGO survey, a widefield mapping project at the IRAM 30mtelescope that was allocated ∼200h to date. Until now, LEGO covers molecular line emission from the entire 3mmband in about 10 molecular clouds. This work spatially resolves the lineemitting regions in two molecular clouds (Orion A and Rosette). These data enable detailed explorations of the astrochemical processes producing molecules, and of the excitation mechanisms controlling line emission. This work is critically complemented by a study of more distant molecular clouds spread throughout the Milky Way. This second data set reveals a fascinating diversity in line emission properties that questions to what extent any given individual molecular cloud can serve as a template for the general line emission properties of molecular clouds. First results of LEGO (Kauffmann et al., subm.) focus on the role of molecules as tracers of dense gas. We in particular show that transitions used as "dense gas tracers" including the HCN (10) line generally trace gas at densities 1000 cm^{-3}. This is a consequence of high chemical abundances, but it might also result from the easy excitation of molecules like HCN by electrons (Goldsmith & Kauffmann, accepted).

Grain charge distribution in the ISM

Juan Ibanez-Mejia
Universität zu Köln

Dust grains play a critical role in the thermal and chemical properties of the interstellar medium. However, little is still known about how well coupled the dust grains are to the gas, and it is commonly assumed to have a constant dust-to-gas ratio and universal particle size distribution. In order to understand the dynamics of dust grains in plasmas, we review the dominant charging mechanisms, investigate the charge distribution of a population and investigate how charge fluctuations can affect the dynamical evolution of dust particles in the multiphase, turbulent, interstellar medium.

Exploring Out of Equilibrium Chemistry Composition of Planetary Atmospheres

Karan Molaverdikhani

Max Planck Institute for Astronomy - Heidelberg University

Chemical composition and temperature structure of most of the studied planetary atmospheres have been explored by using retrieval and/or self-consistent models, assuming thermochemical equilibrium dominates at all pressures. This assumption has been shown to be a plausible approximation for several hot-Jupiter cases. However, photochemistry influences the low-pressure region at the top of atmospheres and mixing/vertical transport maintain the chemical composition of mid-pressure regimes of atmospheres out of equilibrium. Consequently, investigation of non-hot-Jupiter atmospheres demands the consideration of kinetic models where thermochemical equilibrium is no longer valid. We present the results from our recently developed 1D non-equilibrium chemistry model that is radiatively self-consistent. We compare the results from our model with other chemistry models to explore the diversity of atmospheric regimes and to determine dominant processes in the atmospheric regimes of these planets.

Chemical modeling of protoplanetary disks ensemble

Tamara Molyarova

Institute of Astronomy of the Russian Academy of Sciences

Chemical composition of interstellar gas depends on many parameters, such as initial elemental composition, local temperature, density, radiation field and amount of available dust surface. In protoplanetary disks all these conditions change in a wide range, depending on global properties of the disk: mass, density profile, size, luminosity and mass of the central star. We calculate chemical evolution of 1500 protoplanetary disks with varying physical structure and star parameters. Our grid of models comprises gravitationally stable disks ($<0.1\ M_{\odot}$) of different masses and density distributions around T Tauri stars of various masses. We use ANDES code, developed by Akimkin et al. (2013), a model of chemistry and dust properties of protoplanetary disk, which employs modified ALCHEMIC chemical network (Semenov & Wiebe (2011)). We analyze obtained disks ensemble to find out how disk properties influence concentrations of chemical species. Abundances of the majority of species, especially volatiles, vary strongly with disk structure and star parameters. We provide the so-called CO X-factor for disks, that in our study accounts not only for CO freeze-out and photodestruction, but also for the carbon redistribution into the other molecules (primarily into CO_2). The average X-factor is one magnitude smaller, than is expected if all carbon goes into CO, with a considerable dispersion

of ∼0.5 magnitude. We also seek for other gas mass tracers, that have the smallest relative abundance dispersion due to different disk parameters. That is useful in the context of protoplanetary disks surveys with modern observational facilities.

Physico-chemical evolution of the ptoroplanetary disk

Hiroko Nagahara

Earth-life Science Inst., Tokyo Inst. Tech.

Protoplanetary disk is one of the most well studied filed in astrophysics, however, our knowledge about its evolution is poor and we have not yet fully understood how it evolves, how planets are formed, and how it is chemically diverse. Chemistry is the most powerful tool to combine observation and theory, and various exciting results are obtained with ALMA. The chemical information with ALMA is, however, mostly about gas, and therefore, way to understand the counterpart, dusts, should be considered along with gas chemistry. We have been working on chemical evolution of protoplanetary disk by combining fluid dynamics and chemical equilibrium, which is applied to the protosolar disk to simulate chemistry of chondrites and comets. Our model stands on an advection-diffusion equation with the Lagrangian expression, where transportation of individual particles are tracked and where chemistry of the disk is shown by the summation of particles with different chemistry depending on their thermal history. High temperature dusts condensed in the inner region of the disk are transported outward, whereas, most of dusts originated in the outer region including ice and organics are transported inward. Mixing of various particles results in temporal and spatial variation of chemical composition of the disk. We show that the disk chemistry is strongly dependent on the initial condition, whether it was small or extended to hundreds of au, or how much the disk mass was, all of which affects the temperature evolution of the disk. We conclude that our solar system was initially as small as 10au in order to explain the chemistry of chondrites and solid materials observed in comets. The model is applicable to disks with the size different from our solar system.

The impact of chemistry and feedback on internal structure of z 6 galaxies

Andrea Pallottini

Centro Fermi (Rome, IT), Cavendish Laboratory (Cambridge, UK)

The discovery and characterization of primeval galaxies represent some of the biggest challenges of current observational and theoretical cosmology. This kind of studies recently entered a golden era, thanks to the unprecedented capabilities of the Atacama Large Millimeter Array (ALMA). Far infrared fine structure lines – [CII]158um in particular – are exquisite tools to search for and characterize the most remote system in the Universe. These experiments can be combined with detailed galaxy simulations to achieve a solid theoretical understanding. I will present zoom-in, AMR, high-resolution (30 pc) simulations of high-redshift (z 6) galaxies with the aim of characterizing their internal properties and interstellar medium. Comparing our simulations with observations allow us to draw novel and unique conclusions. Such comparison is fundamental to (i) assess the impact of chemical network on the internal structure and morphology of high-z galaxies and to (ii) constrain feedback prescriptions in simulations, which are a far cry from being fully understood.

Modelling reactivity in the bulk of cometary ices

Francoise Pauzat

CNRS/UPMC

The search for O2 in space has been carried out for years to no avail, contrary to S2 which has been observed for decades in comets. But both suddenly arose a new interest following their observation in comet 67P/Churyumov-Gerasimenko (Bieler et al 2015 ; Le Roy et al 2015). As a matter of fact, the nature of their source is still unknown for both of them. Assuming that both, O2 and S2, should have similar ways of formation, storage and release, we propose that these dimers were formed inside the icy grains precursors of comets by irradiation (photolysis and/or radiolysis) of respectively, the H2O molecules of the ice itself and the S-bearing molecules embedded in the ice, in particular SH2 which could exist scattered or as clumps in the middle of the bulk of H2O ices. In this scenario, the irradiation is assumed to create simultaneously voids in the compact ices, voids within which the molecules so produced can accumulate. We have investigated the stability of O2 and S2 molecules in such cavities, assuming that the surrounding ice is made of H2S or H2O and testing different shapes of cavities. For this purpose, we have used theoretical chemistry numerical models based on first principle periodic density functional theory (DFT). These models have shown to be well adapted to the description of compact ice and are capable to describe the trapping of volatiles in

the ice matrix (Ellinger et al 2015). We showed that the stabilization energy of O2 or S2 molecules in such voids is close to that of the H2O ice binding energy, implying that these molecules are well trapped in the ices without disturbing the icy matrix. The net consequence is that they can only leave this icy matrix when this latter sublimates, validating our scenario of a roughly common history for O2 and S2. Nevertheless, some differences between O2 and S2 are observed which can also be interpreted. Unlike O2 whose abundance correlates to that of H2O, our scenario implies that no global trend should be drawn between the variation of S2 and H2O abundances as S2 can accumulate in both S-bearing and H2O ices. Such results are supported by the ROSINA data collected between May 2015 (equinox) and August 2015 (perihelion), showing that there is no clear correlation of S2 with H2O or H2S in 67P/C-G (Calmonte et al. 2016) contrary to O2.

CO line ratios in molecular clouds: the impact of environment

Camilo Penaloza
Cardiff University

The use of CO line intensity ratios in Giant Molecular Clouds (GMCs) can help determine the excitation conditions of the molecular gas. Specifically different environments produce variations in the line intensity ratio, low ratios ($\sim$0.5) are found within the Galactic disc, those closed to unity ($\sim$0.9) are identified with the central molecular zone (CMZ) and high values ($\sim$1.5) are correlated with high radiation fields from feedback. In this work we focus on mimicking the CO emission for simulated GMCs. We perform a set of smooth particle hydrodynamics (SPH) simulations with time-dependent chemistry, in which environmental conditions such as mass, density, size, metallicity and the Interstellar Radiation Field were systematically varied. The simulations were then post-processed using radiative transfer (via RADMC-3D) to produce synthetic emission maps. These are created for different lines of CO's rotational ladder as well as different CO isotopes. We present results on how environment has a direct effect on the tracing potential of CO line ratios, as well as the limitations and accuracy of using synthetic observations.

Chemical modelling of formamide and methyl isocyanate in star-forming regions

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Comets are thought to contain relatively pristine material from the origin of the solar system, having condensed directly out of the pre-solar nebula (e.g., Mumma & Charnley 2011). It is postulated that comets may have even delivered some of the water and organic matter found on the Earth via impacts (e.g., Hartogh et al. 2011). Over 22 molecules have been identified in comets via radio observations (Crovisier et al. 2004), including organic species such as formamide (NH2CHO, Biver et al. 2014). Formamide and methyl isocyanate are particularly interesting for their potential role in prebiotic chemistry (Saladino et al. 2012). Formamide has been detected in a large variety of star-forming environments, as well as in Solar System comets, thus supporting the hypothesis that molecules with a strong prebiotic potential could have been delivered to Earth by comets after being synthesized in prestellar environments (e.g. Caselli & Ceccarelli, 2013). Recently, the Rosetta spacecrafts Philae lander detected methyl isocyanate (CH3NCO) in the comet 67P/ChuryumovGerasimenko (Goesmann et al. 2015). Methyl isocyanate has been detected for the first time recently towards SgrB2(N) (Halfen et al. 2015) and most recently towards Orion KL (Cernicharo et al. 2015). Finally, using all the available ALMA data, CH3NCO has been detected for the first time towards a low-mass proto-star, IRAS16293-2422 (Martin-Domenech et al. 2017; Ligterink et al. 2017). The chemistry of formamide and methyl isocyanate in the ISM, and of its precursors, is highly uncertain. This chemistry has theoretically been explored only for massive hot cores at high temperatures (Garrod et al. 2013) but only a few modellings has been done for the chemistry of these molecules under the physical conditions found in pre-stellar cores or low-mass proto-stars. There is increased evidence that chemical processes unaccounted for in past theoretical modelling (e.g. UV photo-desorption, cosmic-ray-induced diffusion, and/or chemical reactive desorption) are required to explain the formation, and detection, of complex organics in those regions. In this talk, I will present a detailed modelling of the chemistry of formamide and methyl isocyanate in star-forming regions such as pre-stellar cores (L1544) and hot corinos (IRAS16293-2422). This chemical modelling aims at fully characterising the main formation/destruction routes of these two species, establishing their expected abundances, and compare them to available observations. This study identifies their precursors and other related species, providing good molecular targets to test our models against observations.

Study of the Hydrogenation of Nitrogen ions (towards ammonium cations) Using 22 Pole Ion Trap at Low Temperatures, Relevant for Astrochemistry

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Ionic hydrides of nitrogen NH+, NH2+ and NH3+ are involved in the formation of ammonia in the interstellar medium [1, 2]; consequently, low-temperature studies of ion-molecule reactions with nitrogen-containing compounds may provide us with important information for understanding processes in the interstellar space. In the present work, the kinetics of NH+ + H2 NH4+ + H reactions has been studied using a linear RF 22 pole ion trap at temperatures down to 10 K. For instance, the reaction rate coefficient for NH2+ formation at 105 K, obtained from the fit of the measured data, is 1.210 9 cm3s-1. The measurement results are also in a good agreement with previously published results at 300 K [3, 4]; however, at low temperatures the values of the reaction rate coefficients differ from the Langevin rate coefficient. [1] Dislaire V., Hily-Blant P., Faure A., Maret S., Bacmann A., and Pineau des Forts G., Nitrogen Hydrides and the H2 Ortho-to-Para Ratio in Dark Clouds. Astronomy and Astrophysics, 537, A20, 2012. [2] Herbst E., The Chemistry of Interstellar Space. Chemical Society Review, 30, 168, 2001. [3] Adams N., Smith D. and Paulson D., An experimental survey of the reactions of NHn+ (n = 0 to 4) with several diatomic and polyatomic molecules at 300 K. The Journal of Chemical Physics, 72, 288297, 1980; [4] Kim J., Theard L. and Huntress W., ICR studies of some hydrogen atom abstraction reactions: X+ + H2 XH+ + H". The Journal of Chemical Physics, 62, 45-52, 1975.

The chemistry at low metallicity

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In low-metallicity environments, the chemistry is important in regulating the cooling, and therefore determines the mass scale of the first generations of stars in the Universe. O ne can broadly distinguish two main cases: Chemistry where the main contribution to the cooling is due to the presence of dust, such as during the formation of the Caffau star, as well as situations where the main contribution is due to metal line cooling, such as the carbon-enhanced metal poor stars. In this talk, I will discuss both situations and presen t 3D simulations in which both the effects of metal line cooling and dust cooling are treated in detail. I will discuss how these mechanisms affect the mass scale of the first gen erations of stars after metal enrichment.

Modelling the chemistry and dynamics of molecular clouds: What is needed?

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We present novel zoom-in simulations, modelling the self-consistently evolution of molecular clouds from their formation out of the diffuse ISM down to filamentary structures of about 0.1 pc within the SILCC collaboration (Seifried et al., 2017). These simulations incorporate a chemical network for H_2 and CO formation and all relevant heating and cooling mechanisms. This combined approach allows us to model the chemical, dynamical, and thermal evolution of molecular clouds simultaneously. We will discuss the indispensable necessity to model the chemical evolution in order to be able study the full complexity of molecular clouds.

We will present detailed criteria which are required to accurately model molecular clouds with such a zoom-in technique. In particular we will show that a high spatial resolution of better than 0.25 pc is required to obtain reliable dynamical and chemical properties like the velocity dispersion and the H_2 and CO content. Our simulations also show that different cloud definitions (by a threshold in density, H_2 or CO mass fraction) significantly change the predicted cloud properties. The differences also vary with the evolutionary stage as e.g. molecular hydrogen becomes present in gas with increasingly lower density over time ($n < 100$ cm^{-3}). We also demonstrate that the formation of H_2 is a highly dynamical process enhanced by turbulent mixing, which can hardly be accounted for with chemical post-processing.

Overall these results clearly demonstrate the necessity to model the chemical evolution along with the hydrodynamical evolution in order to be able study the full complexity of molecular clouds.

Following the gas-grain chemical evolution of pre-stellar cores in a hydrodynamic simulation

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Observational studies of low mass pre-stellar cores rely on chemical tracers to determine their physical properties. Furthermore, observations revealed core-to-core chemical variations and chemical differentiation within cores, e.g. the anti-correlation between carbon chain- and complex organic molecules. Theoretical interpretations of pre-stellar core chemistry often assume time independent physical conditions and are typically restricted to single cell or one dimensional models. In contrast, the explanation of the observed chemical features may require direction dependent irradiation and variations in the density and the temperature of the core material

on comparable to chemical time scales. On the other hand, pre-stellar core like objects form naturally in gravito-turbulent hydrodynamic simulations of molecular clouds. These simulations contain both the physical history and the three dimensional distribution of the core material. The self-consistent inference of chemical signatures from these simulations (especially those of nitrogen bearing and complex species), however, so far proved to be difficult due to computational limitations. In this contribution an efficient chemical post-processing method is presented that takes into account the complete physical history of the core forming material and utilises a state-of-the-art gas-grain chemical network. This allows the assessment to what extent the chemical history of the gas is erased during core formation, thus whether steady state physical conditions are appropriate in chemical models of the pre-stellar cores. Simple recipes for CO chemistry used in hydrodynamic simulations are also tested against the detailed model. Finally, cores with varying environments are compared in order to search for systematic chemical differences between them.

Hot grain surface chemistry applied to H2 and the origin of chemisorbed H2O in protoplanetary disks

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MPE

The origins of the reservoirs of water on Earth are debated. The Earths crust may contain at least three times more water than in the oceans. This crust water is found in the form of phyllosilicates, whose origin probably differs from that of the oceans.We wish to test the possibility to form phyllosilicate in molecular could and protoplanetary disk temperature and density environments. We developed an exploratory warm surface chemistry model where water from the gas-phase can chemisorbed on dust grain surfaces and subsequently diffuse into the silicate bulk. In this model H2 can form from the encouters of chemisorbed H-atoms. We apply the phyllosilicate formation model to a zero-dimension gas and chemical model and in a 2D protoplanetary disk model. Despite the high energy barrier for water chemisorption on silicate grain surfaces and for diffusion in the bulk the chemisorption sites can be occupied by a hydroxyl bond at all gas and dust temperatures from 80 till 700 K, at which point thermal desorption of chemisorbed water occurs. The occupation efficiency is only limited by the maximum water intake of the silicate. Phyllosilicate can be formed on dust grains at the dust coagulation stage in protoplanetary disks. It is however not clear whether the amount of phyllosilicate formed by warm surface chemistry is sufficient compared to that found in solar system objects.

Exploring the nature of first hydrostatic core candidates with synthetic observations

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The first hydrostatic core (FHSC) is the first stable object to form in simulations of star formation. Although several candidate FHSCs have been reported, this stage has yet to be observed conclusively. We have produced synthetic spectral energy distributions (SEDs) from 3D hydrodynamical simulations of evolving pre-stellar cores for a variety of initial conditions, such as different rotation rates and core masses, and examine the differences between the corresponding SEDs. I will present the results of fitting model SEDs to the SEDs of ten FHSC candidates and discuss the constraints this may place on the properties of the sources. Most of these FHSC candidates were fitted well by model SEDs from our set of 1440, which includes different rotation rates, inclinations, evolutionary stages and dust properties. By examining the consistency of model properties between the best fitting SEDS for each source we find that SEDs can indicate the likely age and rotation rate of the source, and can differentiate between young FHSCs and less evolved, collapsing pre-stellar cores. From this we suggest which of the FHSC candidates are most likely to contain a FHSC and what rotational structures may be observed. We also simulate CO observations and examine variation in the line profiles as the core evolves. We will then discuss the use of CO lines in identifying the kinematics associated with the FHSC, as well as the FHSC itself.

Impact of dust cooling on the formation of supermassive black holes

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Supermassive black holes are expected to form in the early Universe through the collapse of massive primordial gas clouds. While previous simulations have shown that warm atomic gas can collapse into quite massive objects of 10^4 - 10^5 solar masses, therefore potentially forming the seed of the observed supermassive black holes, the thermodynamics can be strongly modified in the presence of dust grains, cooling the gas from around 8000 K to 100 K. The resulting transition in the gas pressure allows the gas to fragment, leading to the formation of stellar clusters instead of a massive black hole. I will present here the first 3D simulations on the formation of supermassive black holes including a detailed chemical model for the impact of dust, showing the resulting decrease of the gas temperature and how the additional cooling triggers fragmentation. As a result, we find that the presence of dust may inhibit the formation of very massive objects.

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