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Laboratory Astrophysics in Europe

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On behalf of the PCMI community
that stated interest as written in section 4

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Abstract:

To make the best use of the infrastructures and observatories, laboratory astrophysics must be structured at the European level and maybe world-wide level. Based on 30 years of experience of structuration of the French community in the CNRS/INSU/PCMI framework, we propose a few ideas to get a successful structuration that is reactive and led by the broad community. We also describe the strengths of the French PCMI community with the hope that this will contribute to the European structuration of laboratory astrophysics. Among the outstanding astrophysical questions, we can find the formation of structures and its link with the stellar formation, the molecular complexity, and the cycle of matter, bridging the gap between galactic and extra-galactic studies of the interstellar medium. Federating astronomers, physicists, and chemists is required because the interstellar medium is often out of equilibrium, extremely cold or hot, and diffuse. The matter (gas and dust) appears under forms that are unstable on Earth because the kinetics of the interstellar medium is slow. Moreover, the extreme conditions of the interstellar medium imply physical processes that are unusual on Earth (ambipolar diffusion, hypersonic shocks, high UV illumination, ...). The interpretation of observational data from the interstellar medium thus requires that physicists and chemists bring their know-how and the access to big research infrastructures (SOLEIL, ...) to astronomers. In turn, observations of the interstellar medium with world-class observatories (ALMA, NOEMA, VLT, Herschel, Planck, JWST, ...) represent a unique laboratory for physicists and chemists.

1 Physics and Chemistry of the Interstellar Medium

Studies of the interstellar medium have undergone a spectacular development in the last 40 years, and they are now ready to take advantage of the unprecedented spatial and spectroscopic capabilities of current and future observatories. Will observations be matched on the theoretical side by physical insight into fundamental processes and supported by modelling tools and analysis methods appropriate to all accessible environments? The French PCMI (Physics and Chemistry of the Interstellar Medium) community addresses several facets of this vast issue, related 1) to the formation and evolution of dust grains in a magnetized and UV illuminated environment, 2) to the gas-phase, grain-surface chemistry, and their coupling, 3) to the inventory of organic molecules and its potential link with the prebiotic origin of life, 4) to the coupling of chemistry with magneto-hydrodynamical (MHD) turbulence (transport, dissipative structures, shocks). It offers a close connexion between extraordinary laboratory astrophysics, state-of-the-art numerical developments, and cutting-edge astronomical observations.

Almost 200 molecules have been detected so far in the interstellar medium and in circumstellar shells. Simple molecules are versatile tracers of diffuse matter in the universe, from high-z galaxies to proto-planetary disks, because their internal and external degrees of freedom bear the full signature of the physical conditions in their environment. To fully benefit from the diagnostic power of the molecular lines, the formation and destruction paths of the parent molecules must be quantitatively (and not just qualitatively) understood. A prerequisite is the theoretical understanding of state-to-state collisional rates for more and more complex species to be able to fine-tune a radiative transfer analysis that delivers reliable abundances. Understanding the relation of these abundances with the bulk of the gas made of mostly invisible H_2 molecules then requires powerful astrochemical models that, in turn, rely on in-depth studies of physical and chemical processes at play in both gas-phase and solid-state chemistries.

Moreover, this chemical activity is tightly coupled to the gas dynamics. Chemistry affects the gas motions because 1) the ionisation state controls the coupling to the magnetic field, and 2) the line radiation from polar molecules is the main cooling agent over a broad range of astrophysical environments, controlling the equation of state and therefore affecting the dynamics. Conversely, the gas dynamics affects the chemistry because the various perturbations lead to steep and time-variable density and velocity gradients, which change the rates of molecule formation and destruction by orders of magnitude. While the fields of astrochemistry and gas dynamics have initially evolved on parallel tracks, it is now recognized that combining existing sophisticated chemical codes with gas dynamics is a vital step to fully benefit from the versatility of molecular line data. It is also a tremendous challenge given the non-linearity of the fluid dynamics and the stiffness of the chemical reactions.

About 60 molecules detected in the interstellar medium are organic compounds with more than 6 atoms with a straight-chain backbone. Two notable exceptions are fullerenes that are composed of cyclic chains, and the recent detection of the first branched molecule, i.e., iso-the iso-propyl cyanide (i-C_3H_7CN), raising again the degree of molecular complexity that can be reached in the interstellar medium. One can also point out propylene oxide, the first chiral compound observed in the ISM. More complex molecules, such as amino-acids have been identified in meteorites on Earth or in-situ in comets. It thus seems that interstellar chemistry is able to produce molecules of biological interest that could have played a role in the emergence of life on Earth. The first discovery of CH_3NCO on the Churyumov-Gerasimenko comet with the Philae mass spectrometer, followed by the first detection of this molecule in the interstellar medium, strengthens the idea of a close link between interstellar and cometary matter.

With the exception of in-situ missions in the solar system, the identification of interstellar molecules requires the spectral analysis of their electromagnetic emission. In particular, complex molecules have an extremely dense rotational spectrum with hundreds of lines in the millimeter (mm) and sub-millimeter (submm) spectral range. Searching for new molecules thus requires blind spectral surveys. Fortunately, the advent high spectral resolution, wideband spectrometers on many telescopes (IRAM 30-m, NOEMA, ALMA, APEX, ...) turns almost any observation in a sensitive line survey. Many observational projects thus contribute to the serendipitous detection of unexpected molecular spectral signatures. An obvious example is the detection of rare isotopologues of standard molecules (i.e., molecules containing D, ^{13}C, ^{15}N, ^{18}O or ^{34}S isotopes) that provides constraints on the molecule origin. Questions usually discussed inside the astrochemical community become of interest to a wider researcher audience. However, detection of new molecules and computation of their abundances require dedicated laboratory investigations to provide accurate spectroscopic data (rotational, torsional, and vibrational modes) for a broad range of conditions going from 10 to several hundred Kelvins.

Over the 5 last years, a major surprise has been the detection of complex organic molecules in unexpected environments, either in very cold dense cores where their presence challenges the usual ideas about their formation (thermal desorption from grain ices), or in photo-dissociation regions where the harsh UV illumination was thought to easily destroy them. Laboratory investigations finely characterizing the chemical routes are required to understand the chemical inventory in interstellar ice and gas phases. All this shows the incredible resilience of molecular complexity in space.

Dust is also a key player in the physics and chemistry of the interstellar medium. Dust is another tracer of the mostly invisible molecular hydrogen gas where star forms, both in our galaxy and in near and far external galaxies. But this assumes that dust and gas are well coupled, that the distribution of dust size and the composition of the grains are understood, and that the absorption and emission properties of grains are well characterized. The analysis of the data from the Planck, Herschel and Spitzer satellites has revealed the variation of the dust properties (size distribution through the core shine effect, grain composition, grain polarization…) according to the environments (kinetic and chemical histories of the clouds, metallicity, diffuse vs dense clouds). These observational results have brought new constraints on dust models. In particular, they shed light on their limited ability to reproduce the observations. Both the emissivity of the dust and its intrinsic polarization are not yet accounted for in dust models, leading to uncertainties in cloud mass determination, and in the foreground subtraction for cosmological studies.

The composition of dust is first constrained by its formation in shells around evolved stars or in the remnants of supernovae explosions. In these scenarii, the details of the processes leading to the nucleation of gas phase species to form seeds, the first solids on which the dust grains grow, are still poorly known. The combination of accurate observations, dedicated laboratory experiments, and theoretical modeling are all required to progress on this topic. The gain in spatial resolution and in sensitivity of the new instruments (such as NOEMA, ALMA, Matisse, etc.) allows us to observe candidate molecular seeds of grains at the very inner part of circumstellar shells.

Carbonaceous dust (PAHs or very small grains) undergoes a rich physical and chemical evolution at the interface of clouds illuminated by the stellar or interstellar radiation field. In this process, the nature of dust deeply changes, and the gas phase is either depleted or enriched in molecules. Such regions are found not only at the edge of interstellar clouds but also in protoplanetary disks or within circumstellar shells. PAHs are for example photo-dissociated and ionized, small hydrocarbons are released into the gas phase by the photo-evaporation of small carbon grains. A clear understanding of these processes allows astronomers to measure the UV radiation field from the observations of evaporating very small grains.

Finally, dust grains are also known to be a main agent of the coupling of the interstellar magnetic field and the gas. It is now well agreed that this coupling drastically changes the dynamic of the interstellar medium at all scales with a strong influence on its ability to form (multiple) stars and planets.

2 Laboratory astrophysics for interstellar studies

Gas-phase scattering and reactivity

Low temperature experimental kinetic data for only a few hundreds (KIDA database http://kida.obs.u-bordeaux1.fr/) of neutral-neutral or ion-neutral reactions have been determined while astrochemical networks have 1000s of reactions, forcing modellers to use rate coefficients estimated from various levels of theory when no experimental data are available. Furthermore, little is known about the products of reactions and their branching ratios. In many areas of the ISM deviations from thermal equilibrium (non-LTE regime[1]) are expected owing to the complex competition between the radiative and collisional processes. In this regime, the state-to-state reactivity and energy transfer state-to-state collisional rates (including nuclear spin states), far from being understood, become crucial for modelling the chemistry. Data valuable at high temperature are also very scarce while of great importance for modelling hot astrophysical environments (circumstellar envelopes, disks …) including the early universe where the knowledge of state-to-state chemistry is also essential. All these limitations have clear consequences for the provision of rate data for modelling chemical processes in the ISM. The development and combination of new experimental and theoretical techniques are essential.

It is only in the past 20 years that experimental tools have become available to explore quantitatively the product branching ratios of bimolecular reactions. Indeed, experimental measurements require either determining absolute concentrations or using a calibration reaction of known product yield(s). Various experimental approaches, including mass spectrometry, infrared or microwave spectroscopy, are currently in development. State-to-state reactivity, which is crucial for non-LTE chemistry, is even more challenging experimentally. For instance, if rate coefficients have been determined for reagents in quite low vibrational states less information is known about the influence of reagent rotational excitation on reactivity. One reason for the scarcity of such data is the ease with which rotational energy transfer occurs in molecular collisions. More generally, the reactivity of specific states, the assignment of the structure and internal quantum states of the products of reactive or non-reactive collisions and photodissociation are great experimental challenges. Another challenge is also to be able to address radical-radical reactivity experimentally.

Methods of quantum chemistry have reached a stage where it is now possible to build with very high accuracy ab initio potential energy surfaces (PESs). Large polyatomic systems (> 10 atoms) still require improvement of these methods, especially when dealing with excited states or relativistic (e.g., spin-orbit) effects. To reach for these large systems the accuracy achievable today for the small ones, the international theoretical chemistry community is working on the development of new methods and their incorporation in the main software packages (MOLPRO, GAMESS). Therefore, today the most challenging problems concern the study of the dynamic of the nuclei on the calculated PESs to determine rate constants and branching ratios. Nuclear dynamics approaches have considerably progressed during these last years in the treatment of non-reactive collisions occurring on ground electronic states, mainly due to increased computing power but also to reduced dimensionality approaches.

[1] LTE stands for Local Thermodynamic Equilibrium

One would like to reach the same level of progress for reactive processes involving ground but also excited electronic states.

For small systems (< 4 atoms) accurate quantum dynamics treatment are possible at the very low temperature of the ISM (10 - 100K). The challenge is for higher temperatures when accurate state-to-state collision rates are needed because of the large number of ro-vibrational states involved. For larger systems, quantum dynamics treatments are a challenge even for the low temperature of the interstellar medium, because of the number of molecular internal degrees of freedom involved. The developments based on the reduction of the dimensionality of the problem by ranking them (for instance, reactive versus non-reactive) are among the solutions being explored to meet these challenges. Mixed molecular dynamics methods are also being developped for treating at a quantum level certain degrees of freedom while the others are treated classically. More complication arises when dealing with excited electronic states (avoided crossings or conical intersections, spin effects ...) and the complexity of the dynamics of an excited state which can relax through various and sometimes competing processes (bond breaking, vibrational relaxation, isomerisation …)

A step ahead in this domain of reactive collisions would certainly benefit from a European network equivalent of the previous "MOLECULAR UNIVERSE" but dedicated to the development of nuclear dynamics tools for chemical reactions. Such a network would need to combine experts in the areas of laboratory kinetics, theoretical chemical physicists with experts of reactive and non-reactive processes in both fields of electronic structure and nuclei dynamic theories. Such a network would particularly benefit from the expertise of the theoretical chemistry community that develops original approaches to treat complex molecular systems evolving on several coupled PES's. From an experimental point of view, a European network would allow profitable exchanges of knowledge for the development and the diffusion of state-of-the-art experimental techniques producing experimental data in relevant physical conditions. There are a number of techniques such as molecular beams, free supersonic jets, CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme, i.e., Reaction Kinetics in Uniform Supersonic Flows, cryogenic ion traps) among others, that allow many gas-phase molecular processes to be studied at very low temperatures, down to 6 K. The expertise of these techniques could be shared through scientific collaborations and benefits to a significant number of European research groups as it can be coupled to various diagnostic tools (lasers, spectrometers, synchrotron radiation, ..) to tackle many of the current astrophysical challenges.

Gas Phase Spectroscopy

Accurate knowledge of the energy levels of molecules is a pre-requisite to the unambiguous identification of new species in the interstellar medium. Molecular spectroscopy at high spectral resolution in the (sub-)millimeter spectral range delivers the required accuracy. The astrochemical power of the numerous spectral surveys, that ALMA, NOEMA and SOFIA deliver, will thus rely on these high resolution spectroscopy experiments. In the last decade, a revolution has occurred in these experiments which can now measure sensitive, high resolution spectra in the entire frequency range of interest, from the millimeter (50 GHz) to the far infrared (5 THz), where a large fraction of the interstellar gas emits. This included the advent of new solid sources in the frequency multiplication chains to produce the local oscillator signal used in heterodyne techniques. Recently, chirped-pulse technology became commercially available up to 110 GHz. This is a new revolution that will facilitate recording the spectra of reactive species. In parallel, theoreticians need to improve their models to match the experimental accuracy for the high quantum numbers that are now routinely achieved in the Terahertz range. One such example is the large amplitude motion code used for molecules that exhibit internal rotation of the methyl rotor. This is the case for numerous complex organic molecules in the ISM (methanol, methyl formate, dimethyl ether, acetaldehyde, ...)

In the vacuum ultraviolet (VUV) wavelength range, there are also important needs for accurate measurements of fundamental molecular parameters such as absorption line positions, widths and absolute cross sections, as well as ionization/fluorescence yields for the understanding of the relaxation processes of molecular excited states. The last ten years have been marked by the development of a Fourier Transform Spectrometer for the VUV (VUV-FTS at SOLEIL/DESIRS), enabling absolute absorption cross section measurements of a large array of stable molecules. These cover a wide range of wavelengths and with unprecedented resolving power at the shortest VUV wavelengths (10^6 at 10 eV, 1.5 10^6 above 15 eV), in excellent complementarity with the high-resolution laser-based approach focused on narrower spectral ranges. Current new challenges consist in developing appropriate techniques for producing small radicals and other unstable species (via discharges, flow tubes), ubiquitous in the ISM as well as in comets. Also the development of very-high resolution spectroscopy with VUV lasers combined with photoelectron spectroscopy techniques (PFI-ZEKE, Mass Analysed Threshold ionization MATI) is very promising for the spectroscopy of molecular ions.

Another aspect linked to the study of molecular relaxation processes after VUV excitation is the question of the stability of large molecular systems, from elementary "complex organic molecules" to pre-biotic molecules and clusters undergoing a rich photochemistry. Exposed to VUV radiation, the photolysis of such systems can produced multiple fragments. The determination of absolute branching ratios is crucial for gas phase astrochemical models but extremely difficult to measure accurately in the laboratory. This can be solved by using complementary approaches based on state-of-the-art UV/VUV laser spectroscopy (often in a pump/probe arrangement) and synchrotron radiation (SR) techniques such as electron-ion coincidence techniques (PEPICO) providing state-to-state photochemical data for dissociative ionization processes. Also the coupling of ion traps to synchrotron beam lines or to lasers offers additional perspectives for the study of PAHs and other model systems of very small grains in the context of their identification and survival in space. VUV photodynamics studies in the gas phase may also address the question of the origin of biomolecular asymmetry in space, with the study of chiral asymmetry in the photoionization of gas phase enantiomers.

In summary, recent developments in spectroscopic techniques are opening a new area in the study of complex systems. It is essential to share the expertise from different leading groups in Europe for the production of exotic species and adapt them to the different spectroscopic schemes to ensure the maximum return for laboratory astrophysics, and therefore towards the whole field of astrophysics. Among the great variety of molecular model or actual systems that need to be studied, a strategy for defining key molecular species that have to be studied should be established in close collaboration with astronomers. Therefore, the European Infrastructure should be able to support collaborative projects and define a common strategy for studying systems gradually: in the laboratory (of course) but from the beginning targeting actual issues that should be defined with astronomers, in full synergy with the analysis of astronomical spectra and the developments of astrophysics models.

Ice mantles: formation/destruction, processing, ice chemistry

Ice mantles covering interstellar dust grains are present in the molecular clouds of our galaxy. In such clouds, gaseous atoms/radicals and molecular species accrete efficiently on the cold surfaces of dust grains which act as micro-reactors able to gather the reactants and to dissipate the extra energy. These grain surfaces, where radical-radical reactions take place, can boost the efficiency of the formation reactions for some species with respect to pure gas phase reaction processes. These properties make dust grains efficient catalytic agents that laboratory experiments must closely investigate to quantify these mechanisms under controlled temperatures mimicking the interstellar medium environments. The physical state of the ice is extremely important so that surface physicists can perform pertinent experiments on realistic surfaces for a better understanding of interstellar chemistry. The ice physical state (e.g. amorphous, crystalline, metastable) and chemical composition are the direct consequences of the bulk and surface reactions, thermal history, and also the interaction with swift heavy ions and photons. Astrophysical environments are exposed to UV and cosmic ray radiations that can be simulated in the laboratory for a better understanding of astrophysical processes. This includes the photo-synthesis of complex molecular structures, such as polymers of elementary bricks of life, from basic precursors, and even sometimes their asymmetric synthesis allowing the production of enantio-enriched chiral compounds. These processes provide not only a rich photochemistry and radiolysis evolution of the ISM solid phase, but also desorption processes of the newly formed molecules to enrich the gas phase. As an example ultraviolet (UV) ice photodesorption is an important non-thermal desorption pathway in many interstellar environments that has been invoked to explain observations of cold molecules in disks, clouds, and cloud cores. Hence, systematic laboratory studies of the UV photodesorption rates are of utmost importance to constrain their impact in astrophysical models.

Many important challenges have to be overcome in the next decade. Among them is the ability to accurately predict the physical-chemical behavior of more realistic interstellar complex mixtures that will be routinely observed by space telescopes (JWST). This effort is compulsory to solve the increasing amount of puzzling questions brought to us by the always-increasing resolution and sensitivity powers of the current generation of telescopes (ALMA and NOEMA). A good example is the still unexplained high abundances of complex organic molecules observed in the gas phase. The desorption of solid mantles certainly plays an important role here. The discovery of potential synthesis routes for pre-biotic molecules is also required to understand the potential limit of the chemical complexity in the interstellar medium. Finally, a detailed understanding of very basic and fundamental processes such as the nuclear spin conversion of small molecules (such as H2, H2O, NH_3,…) in the ice also represents a challenge for future laboratory astrophysics investigations considering the fact that out-of-equilibrium nuclear spin temperatures in comets and in star forming regions of the ISM remain unexplained.

Laboratory astrophysics sheds light on the molecular processes, under template simulated astrophysical experiments (gas phase, ice surface, ice bulk). At the European level, a consortium of solid state and surface astrochemical research groups (LASSIE-ITN involving 13 institutions across Europe) has been very successful in developing interdisciplinary approaches in the field, creating a network of sophisticated laboratory experiments on surface preparation and experimental practices. This common initiative has proven a powerful tool for a better understanding of the physics and chemistry of the ice mantles. However, the great complexity of these systems implies that many elementary mechanisms still need to be identified or quantified, before they can actually be included into models (e.g. processes driven by X-ray photons, reactive desorption from ice mantles, surface reactivity). A better understanding of molecular mechanisms is mandatory to model such processes. This requires dedicated experiments, as mentioned above, but also a better coupling with theoretical physicists that need to be fostered in the future.

In this context, the research groups involved in solid state and surface science across EU need to further coordinate their actions. Operative state-of-the art equipments need to be maintained and the EU network should support collaborative projects between theoretical and experimental approaches, with the aim to gain progressively on our ability to predict the behavior of more and more complex ices. Beyond this effort in laboratory astrophysics, it will naturally open new concerted approaches with astronomers in order to solve the difficulty to interface solid and gas phases in a same astrophysical model.

Refractory material

Understanding astrophysical phenomena may depend on the precision reachable to infer the physical quantities from the observations. In some cases, a precision better than 50% is required to reach astrophysical goals. For instance, H_2 usually cannot be detected, implying the use of tracers like dust to determine the mass of clouds. However, the optical properties of the dust must be known at a precision better than 20% so that dust can trace molecular gas as well as the HI line can trace atomic gas. An accurate knowledge of the optical constants of dust is also required for the subtraction of the galactic foreground for studies of the cosmic microwave background.

Determining the optical constants of interstellar dust is a challenging task for several reasons. First of all, it is necessary to define what are the interstellar dust analogues (composition, structure) and to synthesize them. Even though spectroscopic astronomical observations of dusty environments combined to the analysis of collected pre-solar grains help to define the dust analogues, it leaves a large variety of materials. The production of dust analogs is a complex task because it requires controlling the structural and chemical homogeneity at nanometer scale.

Another challenge is to measure the absorption/emission coefficient on a wide spectral range, ideally from the X-ray domain (important for the scientific exploitation of space missions such as the future Athena mission) to the far infrared and millimeter domain (see the Herschel and Planck missions and the ground based radio antennas and interferometers). Work, mainly on silicate dust analogues (efforts have now to focus on carbonaceous dust) and in the near, mid and far-infrared spectral domains, has been done by several teams in Europe, and in France in particular. Other groups are beginning to characterize dust in the X-ray domain. Even though these (European) teams are in contact and sometimes collaborate efficiently, coordination at the European level would be good to gather, exchange expertise. Modeling the optical constants from the experimental data in such a way that they may be used in ISM, planet, and atmosphere studies, is another necessary and important goal. The delivery of these data to the scientific community is crucial, this is for instance the goal of the SSHADE database developed within the Europlanet H2020 European project. Another goal difficult to address is the ionization properties of dust grains particles, a central question in astrophysics.

The study of the dust life cycle requires state-of-the art experiments able to simulate the astrophysical conditions and the physical processes occurring in circumstellar shells and in the various ISM phases. First, understanding the chemical and physical processes leading to the formation (nucleation and growth) of cosmic dust in circumstellar shells and in supernovae remnants constitutes a challenging task for laboratory astrophysics. Refractory dust analogs are usually produced in conditions different from the formation of cosmic dust. Producing relevant dust analogs in controlled conditions as close as possible to those found in astrophysical environments requires high temperature, surface free environment, and circumstellar-shell-like composition of the gas phase. Second, interaction with photons (UV and X-rays) and cosmic rays deeply alter the composition and structure of the dust grains in particular carbonaceous dust (PAHs, amorphous hydrogenated carbon dust). Irradiations experiments of dust analogs, performed on dedicated experimental setups coupled either to internal light sources or to light sources such as synchrotrons and particle accelerators (to reach high energies and fluences), are essential to address questions such as the photo-stability of PAHs, the destruction of the silicate and carbonaceous grain or its amorphization. Third, shocked regions modify the size distribution of grains and release some heavy element into the gas phase. Finally, dust grains are expected to coagulate in dense regions and the gas phase is known to deplete on cold grains when the density increases.

3 Towards a European network on Laboratory Astrophysics

The PCMI model

PCMI stands for Physique et Chimie du Milieu Interstellaire (Physics and Chemistry of the Interstellar Medium). Formally, PCMI is an « action sur projet » from CNRS-INSU (Institute of Universe Sciences). It is also supported by the CNRS-INP (Institute of Physics), the CNRS-INC (Institute of Chemistry), and CNES (Centre National d'Etudes Spatiales).
The main motivation of the PCMI network is an astrophysical one, namely understanding the interstellar medium near and far. However, this goal requires cutting-edge expertise in laboratory physics and chemistry. The network has thus been conceived as an interdisciplinary structure. PCMI organizes every two years a general colloquium gathering of about 150 participants (about half of the community) to discuss recent successes and near term prospects. The PCMI community also delivers a written road map every four to five years to its funding agencies, which gives a framework to the community for the next few years.
PCMI has a yearly budget (200 to 300 keuros/year) that is mostly distributed among proposals written by the community (typically 40 requests/year). The goal is to support well-focused science projects by individual teams or groups of teams. Projects are reviewed by a scientific council composed of experts from the different scientific fields. Progress in the delivery of the science goals is monitored. There is a large and flexible variety of funding possibilities (laboratory equipments and consumables, observation missions, campaign of measurements in large physics facilities, collaborative missions, organization of workshops or schools ...) to ensure that science goals can be achieved. In view of the yearly budget, PCMI does not fund salaries, or medium or large infrastructures.
The PCMI working scheme has many advantages. It allows PCMI to support blossoming ideas up to the moment they become mature. PCMI funding is also a way to deliver a scientific label by peer referees in the domain. This label is then often used to compete for larger (regional, national, or even international) grants. For instance, in the last 3 years, two experimental groups that have been supported by PCMI for more than one decade have been succesful in obtaining the largest grants of the ERC (NANOCOSMOS, co-PIs: J. Cernicharo, C. Joblin, and J.-A. Martín-Gago, and CRESUCHIRP, PI: I. Sims). The yearly scheme also gives enough flexibility to quickly encourage new ideas. For instance, PCMI recently started to support the installation of a high resolution VUV laser at ISMO (PI B. Gans). In addition, one strength of PCMI is to foster collaborations between astronomers, physicists and chemists around a common scientific challenge. The first seeds of the PCMI network started in 1983, and it evolved in its current institutional form ("action sur projet") in 1999. Its longevity testifies that the organization described above answers both the needs of the French community that study the interstellar medium, and the prospective needs of its French funding agencies. Nevertheless, the outstanding science questions raised by current observations of worldwide observatories require matching means in laboratory astrophysics. This calls for an organization of groups working in this area at the European level.
We argue here that it would be interesting to generalize at least some of the PCMI working schemes to the organization of one of its topics, namely laboratory astrophysics applied to the study of the ISM, at the European level.

Concrete actions at the European level

Based on our PCMI experience, we here propose a few concrete actions that would directly benefit from an organization at the European level. We favor concrete actions that delegate the role of proposing to the community (e.g., through yearly call for proposals) because bottom-up approaches are much more innovative than top-down ones.

Diffusing experimental know-how and associating technology expertise

Understanding the ISM requires large databases of micro-physics parameters at low temperature and pressure. These are difficult to acquire because they require complex research apparatus. Diffusing experimental know-how is one of the keys to secure the filling of databases. For instance, the CRESU technology first developed in Meudon and Rennes was exported to Bordeaux, and very recently to Ciudad Real. Another key is to associate technology expertise from different groups to build more complex experiments. For instance, S. Schlemmer is helping C. Joblin's team to set up a new ion trap in the framework of NANOCOSMOS. A European network should encourage both practices.

Open the use of PI experiments to other groups

Setting up a cutting-edge physical and chemical experiment often requires 5 to 8 years to become mature with large funding requirements. Organizing a network whose goal would be to open the use of the experiments of willing PIs to other European groups would permit a better use of the investment and expertise. It would also offer the opportunity for long term sustainability of equipments developed under large research programs funded bay national and/or European agencies (ANR, ERC). It would also increase network connections, opening possibilities to develop more complex experiments.

Supporting the use of large infrastructures

Large infrastructures contribute to the networking and structuring of a community. Indeed, they allow teams from different origins (cities/countries) to meet and sometimes collaborate when they gather to set up an experiment on a given large infrastructure. This is an opportunity to provide experimental solutions to common problems.

In European networks, the use of large infrastructures is usually open through the Trans-National-Access funds delivered to and managed by the infrastructures themselves, opening the possibility to support typically up to one user per project from foreign institutions, which is not sufficient. This financial support could be reinforced in the framework of a European Laboratory astrophysics network. In addition to this useful system, a European network on laboratory astrophysics would also benefit from the possibility to attribute funds on a yearly basis to both set-up new experiments and allow them to be installed on large infrastructures. Indeed, our PCMI experience indicates that this is a powerful way to allow new ideas to emerge and thus to boost new scientific momentum, independent of a priori list of infrastructures and much before the project has a chance to be accepted by the review panel that evaluates the proposals to get time on a specific instrument. We finally note that efforts to provide access to computing resources across Europe exist, see in particular the European Grid Infrastructure (EGI) project (www.egi.eu).

Meeting, workshops, and conferences

Astrophysical studies are more and more done in consortia gathering people with quite different expertise from laboratory experiments to astrophysical observations through modeling. These are often geographically spread out, requiring short to medium or long visits to make progress on the interpretation of data. These meetings are often decided depending on the arrival of observational or experimental data. A flexible mechanism of funding open all year long would be desirable.
On the same idea, there could be a yearly call for workshop proposals on the main themes of the network, instead of foreseeing typical workshops for the duration of the network, as is done in COST actions. This would give more flexibility to react to recent outstanding questions. On the other hand, having a biennial or triennal all-hands conference inviting the network community to discuss the recent achievements and the short-term prospects is a powerful way to keep prospective alive.

Interface to already existing European structures or networks

It may seem natural to get the producers of astrophysical observations (ESO, ESA, ...) in a network dedicated to a laboratory astrophysics. However, it's unclear how such a network would select the providers. Indeed, modern astrophysical questions require a large complementarily of observing means (space-based and ground-based, multi-wavelength, different compromises between angular/spectroscopic resolution and field of view). Moreover, a given class of laboratory experiments may be useful to interpret very different kinds of observations. Finally, the European astrophysics community sometimes is part of worldwide consortia outside ESO or ESA. In these cases, specific laboratory experiments may be the key to interpret the data. We thus propose that the network be a natural interface to the astrophysical data providers by having in their science advisory committees astrophysicists members of these observatories.

Laboratory astrophysics also has natural interfaces with other European networks created 1) to model astronomical data through an interdisciplinary network (Molecular Universe), 2) to access easily to and to manipulate atomic and molecular data through data diffusion infrastructures (VAMDC), and 3) to provide astrophysical models that use the laboratory results (EMBRACE).

The challenges for the next decade first lie in the requirement to model complex systems at the frontier between molecular physics and solid-state physics, in order to explore the growth of matter complexity in space. Second, with the development of laboratory experiments more and more data will have to be published and the complexity of the data will increase (to handle surface processes or state-to-state chemical rates). Third, studies of the interstellar medium are inherently statistical. The turbulent nature of the ISM implies that models must have a statistical component to reveal the laws that underlie for instance the formation of stars. In addition, the advent of new generations of observatories (NOEMA, ALMA, SKA, GAIA, JWST, ...) will deliver huge amounts of data implying that science questions will have to be reformulated into statistical ways.
As a consequence, enforcing networking activities between producers of data, publishers, and astrophysicists should be a priority. All parties would benefit from it: astrophysicists would have access to new data more easily, and they would understand their domain of

validity, and the underlying processes. Modern electronic ways of distributing the data would give a better feedback to physicists and chemists on the data they produce. Astrophysicists would also help physicists and chemists to identify challenging issues with direct applications to astrophysics. This would also ensure that the money invested in laboratory astrophysics becomes public with a huge legacy value. Instead of trying to solve alone the challenges described above, the laboratory astrophysics network should thus also have a clearly defined interface with chemistry/physics modelers and publishers of data who organize themselves at the European level. The discussion should enable the evolution of the databases and models/simulations in consistence with the improved understanding of physical processes, e.g., concerning the processes at the surface whose understanding is currently exploding.

Delivering and upgrading a road-map to structure the community

An important action of a European network would be to deliver and regularly upgrade a road map for the community. Indeed, there are more needs in laboratory astrophysics to understand the observational data than experiments to deliver these. Providing a road map discussed between astrophysicists who understand their needs and physicists/chemists who understand their possibilities and interests is required to ensure that significant positive progress is made over a decade or so. Among the current questions of interest that this road-map could address are the definition of the steps needed to compare results from different experimental setups quantitatively and the definition of reference systems to be used in astrophysical models.

For instance, expert validation on a regular basis is required to keep the microphysics databases up to date. This is usual today for the gas phase (e.g., HITRAN or KIDA), but much work remains to be done for the solid phase. On a higher level, it would be useful to publish the network of reactions used in models, so that future groups can reproduce the results they read in publications. KIDA offers the possibility to publish networks, but it is unclear whether this is extensively used. Another useful step would be to provide guidelines on the ways to select reactions to build up a reaction network for a given purpose (e.g., study of deuteration, ...). In ice chemistry, we can ask whether one or several reference surfaces could be defined as typical analogues of interstellar grains. Even though this could turn out to be impossible, agreeing on some reference surfaces would help the community to compare the results from different laboratory experiments. Finally, we note that benchmarking astrochemical models happened only once more than 5 years ago for one type of model (photon dominated regions). This kind of work should be sustained over decades. All these themes could be the occasion to define a first road map for laboratory astrophysics focused on studies of the interstellar medium.

What the PCMI community could bring to a European network centered on laboratory astrophysics

The long PCMI experience is one first strong asset for a European Laboratory Astrophysics network. This implies that there exists a community that succeeded in overcoming the main barriers when setting up a network that brings together astronomers, physicists, and chemists. For instance, having researchers understanding the vocabulary and concepts used by other communities take some time. Beyond vocabulary and concepts, it is also difficult to understand the (instrumental, theoretical, observational) limitations of each community.

The PCMI community always took great care to help each community to share a common understanding and it is ready to share this expertise. The PCMI community is also used to regular prospective exercises and other networking activities.

French teams often play key roles in the development or the maintenance of databases and e-infrastructures for the publication of atomic and molecular data or high-level astrophysical data. For decades, CNRS/INSU and the French observatories have developed a strong policy in favor of sharing data. The most well known example in Astrophysics is the Centre de Données de Strasbourg (CDS) that was created in 1983. Since 2000, CDS promotes the diffusion of astronomical and other kinds of data in French observatories, and shares its expertise with them. These efforts led to the creation of many data centers in France, and hence, many French teams have a strong expertise in the publication of data. This asset is reinforced by the general CNRS/INSU policy concerning data publications. Recently, data centers have been formalized in most French observatories. Their role is to guarantee sustainability in the long term of the various databases / e-infrastructure publishing data related to astrophysics, including atomic and molecular databases. This scientific policy benefits from the special status of "fonctionnaires" (i.e. state workers) of French researchers and technical staff. Some permanent scientific staff in French observatories are responsible for publishing data and maintaining diffusion infrastructures in the long term. It is then not surprising to find French teams leading the data publication components in European projects (VAMDC, Sup@VAMDC, Euro-Planet, ..). First, they benefit from the data centers infrastructures of their observatories during the project, and at the end of the project, when no more funding is coming from Europe, they are still able to maintain the infrastructure.

Above all, PCMI provides a network of cutting edge teams in laboratory astrophysics. The next section provides a list that was gathered from a call to the PCMI teams that are willing to participate in a European Laboratory Astrophysics network with their expertise.

4 Statement of interest to participate to a European Network of Laboratory Astrophysics

By alphabetical order of the group or PI name.

Adam Walters, (awalters@irap.omp.eu)
Molecular spectroscopy for radioastronomy

Atoms, molecules, solid state in astrochemistry
François Dulieu (francois.dulieu@obspm.fr), Saoud Baouche, Henda Chaabouni, Emanuele Congiu, Stephan Diana.
Gas-surface processes; reactivity at the interface gas-solid and in the ices; synthesis of organic molecules, thermal desorption; mass spectrometry; infrared spectroscopy;

Electronic spectroscopy of small radicals
Patrick Crozet (patrick.crozet@univ-lyon1.fr), Heather Harker, Jerome Morville, Amanda Ross
Visible and near infra-red (Ti:sapphire) laser spectroscopy; cavity enhanced spectroscopy; molecular Zeeman effect in open-shell & metal-containing species.

Equipe Astro
Thierry Chiavassa (thierry.chiavassa@univ-amu.fr), Isabelle Couturier, Fabien Borget, Grégoire Danger, Louis d'Hendecourt, Fabrice Duvernay, Nathalie Piétri, Patrice Theulé
Astrochemistry, Spectroscopy, Low temperature chemistry, Ice chemistry; Solid state radical and thermal chemistry, Gas phase molecules identifications and quantifications; Refractory organic residue analysis, Analytical chemistry and Astrobiology.

Equipe Chimie Théorique
M. Hochlaf (majdi.hochlaf@u-pem.fr), R. Linguerri, H. Mouhib
ab initio calculations, electronic spectroscopy, potential energy surfaces; reactive and non-reactive collision rates. VUV spectroscopy; molecule-surface interactions, molecule-cluster interactions, photophysics and photochemistry.

Equipe Cosmochimie
François Robert, Romain Tartèse, Sylvie Derenne, Pierre Cartigny, Lambert Baraut, Christophe Lécuyer, Bernard Marti, Mathieu Roskosz (mathieu.roskosz@univ-lille1.fr), L. Remusat, Lisseth Gavilan, Nathalie Carrasco, Bernard Marty, Bernard Bourdon, Eric Quirico, Pierre Beck, Lydie Bonal, Hugues Leroux
Plasma, Isotopes, Organic Matter, silicates, radical chemistry, gas-grains reactions,
Electron and ion irradiation, UV and X-ray irradiation of silicates and organic matter

Equipe Interstellaire (théorie)
Alexandre Faure (alexandre.faure@univ-grenoble-alpes.fr), Caire Rist, Laurent Wiesenfeld
Inelastic and reactive collisions, electronic structure calculations, electron-impact excitation

Equipe Molecules, Clusters, Dynamics
Jérome Cuny, Florent Xavier Gadéa, Mathias Rapacioli, Aude Simon (aude.simon@irsamc.ups-tlse.fr), Fernand Spiegelman
Theory, molecular modeling, polycyclic aromatic hydrocarbons, molecular clusters, condensed phase, electronic structure, density functional based approaches (DFT and DFTB), ab initio molecular dynamics, spectroscopy

Equipes Planeto et interstellaire
Lydie Bonal, Pierre Beck, Bernard Schmit, Eric Quirico (eric.quirico@univ-grenoble-alpes.fr), Véronique Vuitton, François-Régis Orthous-Daunay, Alexandre Faure et Pierre Hily-Blant
Physics and chemistry of the interstellar medium and cometary environment; cometary grains. Surfaces of planets and small solar system bodies, cosmochemistry: origin of water and organic matter, meteorites and interplanetary dusts analysis, thermal and radiolytic synthesis of organic matter. Atmospheric chemistry of Titan, Mars and its cryospheres, volatile cycles. Spectroscopy and reactivity of ices, ice thermodynamics. Spectro-gonio-radiometry of icy surfaces.

Equipe PCMT
Stéphane Briquez, Denis Duflot, Maurice Monnerville (maurice.monnerville@univ-lille1.fr), Daniel Peláez-Ruiz, Céline Toubin
Molecular Mechanics, Molecular Dynamics ,Developement of Force Fields, Electronic structure calculations (Ground and excited states, including Rydberg),Calculation of Potential Energy Surfaces, Calculation of surface crossings, Quasi Classical Trajectories, Nuclear Quantum Dynamics , Reduced dimensionality, Time dependent Wave packet
MultiConfiguration Time Dependent Hartree, Representation of the PES in MCTDH, Gas phase scattering and reactivity, Rate constants, Cross Sections, Reactivity , State to state reactivity , Theoretical IR and UV Spectra,Theoretical Photoelectron Spectra, Non Born-Oppenheimer dynamics, Photoreactivity and photophysics, molecule-surface interactions
Grain chemistry ,Adsorption, Tunneling, Thermal desorption, Photodesorption, Diffusion
PAH, Astrophysical ices

Equipes PhAS (Julien Montillaud) et SPACE (Sylvain Picaud)
Aurélie Guilbert-Lepoutre, Ludovic Martin-Gondre, Julien Montillaud , Sylvain Picaud (sylvain.picaud@univ-fcomte.fr).
Theoretical properties of carbonaceous nanograins; structure calculations of soot-like nanoparticles; photoevaporation dynamics and statistics of PAHs and carbonaceous nanograins; use of PAHs and carbonaceous nanograins properties in Galaxy scale models; gas/surface interactions; adsorption properties on ice surfaces; models of thermal evolution for TNOs (trans Neptunian objects) and comets.

Equipe THEOMOL
Olivier Dulieu (olivier.dulieu@u-psud.fr), Maurice Raoult
Expertise: formation of negative molecular ions; quantum chemistry of small molecules; quantum dynamics at low energy; electron-molecule collisions

Fabien Gatti (fabien.gatti@u-psud.fr)
Molecular quantum dynamics, MCTDH, wavepackets.

Florin Lucian Constantin (FL.Constantin@univ-lille1.fr)
Constrains on the variability of fundamental constants using molecular spectroscopy, hydrides, acetylene, model and analysis of high resolution molecular spectra. Fourier-transform spectroscopy (IR, mm) and Fourier-transform- microwave spectroscopy, laser spectroscopy THz optoelectronic detection.

Groupe COMEX
Astrid Bergeat (astrid.bergeat@u-bordeaux.fr), Kevin Hickson, Jean-Christophe Loison, Sébastien Morales, Christian Naulin
Kinetics, Dynamics, low temperature, reactive and inelastic bimolecular collisions, chemical models, CRESU, CMB (Crossed Molecular Beams).

Groupe théorie
Thierry Stoecklin (Thierry.stoecklin@u-bordeaux.fr) & Philippe Halvick
Ab inito calculation,PES fiiting ,inelastic and reactive quantum and QCT calculations
Calculation of infra red spectrum, radiative association cross section, electron molecule collisions

Ices and carbon dust
Philippe Parent (parent@cinam.univ-mrs.fr), Carine Laffon, Daniel Ferry
Interstellar ices and carbonaceous nanoparticles : physical chemistry, X-ray and UV photochemistry, heterogeneous chemistry.
Synchrotron soft X-ray absorption spectroscopy (NEXAFS)and photochemistry, X-ray and UV photoemission (XPS, UPS), infrared spectroscopy, high-resolution electron microscopy (HR-TEM).

KIDA
Valentine Wakelam (valentine.wakelam@u-bordeaux.fr), Pierre Gratier, Jean-Christophe Loison, Dahbia Talbi.
Gas-phase reactions, Gas-grain interactions and grain surface reactions. Kinetic data, Database, Experiments and Theory.

LOMC - Reactive processes group
Ioan Schneider, Fabien Dumouchel, François Lique (francois.lique@univ-lehvare.fr)
Electronic collisions, dissociative recombination, gas-phase reactions, inelastic collisions, electronic structure calculations, spectroscopy

Nanograin platform & Nanocosmos
Christine Joblin (christine.joblin@irap.omp.eu), Karine Demyk, Hassan Sabbah, Anthony Bonnamy, Claude Meny, Patrick Moretto-Cappelle, Jean-Philippe Champeaux, Loïc Nogues
cosmic dust analogues: nanograins and PAHs, NIR to FIR/submm Fourrier Transform spectroscopy at very low temperature temperature (cryostat) and at high temperature/pressure (environmental cell), Fourier-Transform ion cyclotron resonance and time-of-flight mass spectrometry, laser desorption laser ionization (L2MS), molecular analysis, cryogenic ion traps, photodissociation, laser spectroscopy, reactivity involving isolated nanograins/PAHs.

Quantum Astrochemistry : from solid to gas
Alexis Markovits (alexis.markovits@upmc.fr), Françoise Pauzat, Yves Ellinger, Isabelle Fourré, Olivier Parisel, Ozge Ozgurel (PhD)
ab-initio post Hartree-Fock methods, First principle solid state periodic methods, Molecular processes: gas phase; interface gas/solid; inside solid. Astrophysical media: Interstellar medium; planetary composition; comets

Reaction kinetics and infrared spectroscopy
Abdessamad Bénidar, Ludovic Biennier, André Canosa, Sophie Carles, Robert Georges, Ian Sims, Sébastien Le Picard (sebastien.le-picard@univ-rennes1.fr)
Gas-phase reaction kinetics and dynamics ; Gas-phase high resolution/high sensitivity infrared spectroscopy; Physical chemistry / chemical physics ; Low temperature chemistry ; Low and high temperature infrared spectroscopy ; Use of uniform supersonic flows (CRESU), supersonic and hypersonic expansions ; Cavity ringdown spectroscopy ; Infrared Fourrier Transform spectroscopy ;

Laser photochemical techniques ; Ionisation/mass spectrometry techniques ; Chirped pulse in uniform supersonic flows (CPUF).

Rotational spectroscopy of molecules of astrophysics relevance
Laurent Margules (laurent.margules@univ-lille1.fr), Stéphane Bailleux; Pascal Dréan; Manuel Goubet; Thèrése Huet; Roman Motiyenko; Georges Wlodarczak
High resolution spectroscopy, Fourrier Transform MicroWave spectroscopy, Terahertz, Large amplitude Motion, Radicals, ions

Molecular Spectroscopy, Collisional Processes and Applications
Tony Gabard, Grégoire Guillon, Pascal Honvault, Claude Leroy,
Vincent Boudon (Vincent.Boudon@u-bourgogne.fr)
Theory: Molecular spectroscopy, Gas-phase reaction dynamics, Quantum reactive scattering, Astrochemistry

Reactivity in Cryogenic Solids
Joëlle Mascetti (joelle.mascetti@u-bordeaux.fr), Christian Aupetit
Matrix Isolation Spectroscopy, FTIR and UV-visible spectroscopies, photochemistry, rare gas matrices, water ices, PAHs, organometallics of astrophysical interest, astrochemistry.

Spectroscopy of Molecules of Astrophysical Interest
Martin Schwell (martin.schwell@lisa.u-pec.fr), Isabelle Kleiner, Lam Nguyen, Yves Bénilan, Marie-Claire Gazeau, Nicolas Fray, Antoine Jolly
MicroWave Spectroscopy: experimental and theoretical, large amplitude motions , effective Hamiltonians, spectral analysis; Vacuum Ultraviolet spectroscopy (experimental): Quantitiative absorption spectroscopy at high and low temperatures, photoionization spectroscopy.

Spin, Photons and Ices
Xavier MICHAUT (xavier.michaut@upmc.fr) , Mathieu BERTIN , Géraldine FERAUD , Laurent PHILIPPE, Jean-Hugues FILLION
Ices ; Gas-Surface interactions ; Photon-induced processes ; Nuclear spin conversion ; Temperature-induced processes.

Theoretical Astrochemistry.
Dahbia Talbi (dahbia.talbi@umontpelier.fr); Yohann Scribano
Electronic structure calculations, Gas-phase reaction dynamics, Molecular spectroscopy.

State-selected ion-molecule reactivity and VUV photoionization
Christian Alcaraz (christian.alcaraz@u-psud.fr), Claire Romanzin, Roland Thissen
State-to-State ion reactivity; Photoionisation (non-dissociative and dissociative); Photodetachment; Photodissociation; Synchrotron and Laser VUV radiation (production and spectroscopy); Cation spectroscopy; Threshold PhotoElectron-PhotoIon (TPEPICO); Pulsed-Field Ionization - Zero Electron Kinetic Energy (PFI-ZEKE); RF Guided Ion Beam; Molecular Beam; Radicals; Clusters; Facility open to external users.

Structure, Reactivity, Dynamics : astrophysical interest
François Aguillon, Sabine Morisset (sabine.morisset@u-psud.fr), Nathalie Rougeau, Dominique Teillet-Billy
Hydrogenation of interstellar dust grains, dynamics, formation of molecules, binding energies, adsorption and desorption energies of atoms and molecules.

Systèmes Moléculaires, Astrophysique et Environnement

Séverine Boyé-Péronne, Bérenger Gans, Olivier Pirali, Marie-Aline Martin, Stéphane Douin, Pascal Parneix, Cyril Falvo, Laurent Coudert, Philippe Bréchignac, Karine Béroff, Thomas Pino.

Molecules, nanograins, soots, carbon chains, PAHs, molecular spectroscopy (from microwave to VUV), molecular dynamics of complex systems, molecular relaxation, photodissociation, isomerisation, ionisation, electronic and et vibrational fluorescence, high energetic atomic collision, ionic irradiation, statistical thermodynamic, laser spectroscopy, mass spectrometry, CRDS

VUV spectroscopy and photodynamics

Laurent Nahon (laurent.nahon@synchrotron-soleil.fr, Nelson de Oliveira; Gustavo Garcia

Very high resolution VUV absorption spectroscopy on small molecular systems (including radicals and transients); spectroscopy and fragmentation dynamics of state-selected cations by double imaging electron/ion coincidences on cold molecules; radials; clusters and complexes; Photostability on trapped ions (cations and anions); Asymmetric photon-induced processes on ices, thin films and in the gas phase in relation to the origin of life's homochirality.