Evolution of matter from the interstellar medium to exoplanets with the JWST

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1. Executive summary

The launch in late 2018 of the James Webb Space Telescope (JWST) will profoundly change our current understanding of the evolution of extraterrestrial material as it passes from the most diffuse regions of the interstellar medium of our Galaxy to star formation sites, protoplanetary disks and exoplanets. The largest ever launched space telescope (mirror diameter of 6.5 m), the JWST will observe in the infrared with a sensitivity and a spatial resolution better than one to two orders of magnitude than its predecessors. P2IO teams working on extraterrestrial matter have come together to propose a project combining observations with the JWST, numerical modeling and laboratory experiments in order to prepare for the interpretation of the JWST observations. This project brings together a unique set of complementary skills (at the IAS, SAp-AIM, CSNSM, IPNO) which, federated, will place the P2IO community in a leading international position for the scientific exploitation of the JWST. The leverage will be very strong, since the last year of the project will coincide with the first year of operations of the JWST that will then continue at least until 2024 and probably beyond. A budget of 743 k€ is required over the period mid 2016 - end 2019 to fund the training of PhD students and postdocs, complete laboratory equipment, provide animation and to present scientific results.

2. Context, position and objectives

2.1 Position of the project

2.1.1 Context: the James Webb Space Telescope

In Oct 2018, the James Webb Space Telescope (JWST) will be launched by an Ariane rocket. The JWST project is an international collaboration between NASA, the European Space Agency (ESA), and the Canadian Space Agency (CSA). The NASA Goddard Space Flight Center (GSFC) is managing the development effort. With a primary mirror diameter of 6.5 meters, the JWST will be the largest telescope in space. The telescope has been fully optimized to observe in the InfraRed (IR) wavelength range from 2 to 10 μm[1]. It will also offer the possibility to observe down to 0.6 μm and up to 28 μm, with unprecedented performances.

This flagship mission is expected to perform transformational science encompassing four scientific themes: First light and reionization of the Universe, Assembly of galaxies, Birth of stars and protoplanetary systems, Planets and origin of the life.

In the JWST IR wavelength range, the previous space telescope was the Spitzer telescope[2], with a 0.85 m mirror. Going from a 0.85 m to a 6.5 m mirror dramatically improves the performances in terms of sensitivity and angular resolution. The angular resolution, diffraction limited, will be almost an order of magnitude (factor 7) better than that of Spitzer, so that the JWST will concentrate the signal from a point source in a spot 50 times smaller than that provided by Spitzer. The sensitivity on point sources will also be increased by a factor of 50.

A suite of 4 instruments will be located at the focal plane of the telescope and will allow various instrument observation modes: imaging, spectroscopy and coronagraphy:

- A Near-IR Imager and Slitless Spectrograph (0.6-5 μm): NIRIS provided by the Canadian Space Agency,
- A Near-IR CAMera (0.6-5 μm): NIRCAM provided by the University of Arizona,
- A Near-IR SPECtrometer (1-5 μm): NIRSPEC provided by ESA, with components provided by NASA/GSFC,
- A Mid-IR Instrument (5-28 μm): MIRI, provided by a European Consortium of laboratories under the auspices of ESA, and by the NASA Jet Propulsion Laboratory (JPL).

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[1] The JWST will be diffraction limited from 2 μm and will no longer be zodiacal light limited beyond 10 μm.
[2] Spitzer is still in operation but with very limited capabilities: imaging at 3.6 and 4.5 μm.

All the instruments have been delivered to NASA/GSFC, where they have been integrated into the so-called Integrated Science Instrument Module (ISIM), which will be connected to the telescope. The third and final cryovacuum tests of the instruments at Goddard are currently being performed. The rest of the JWST hardware is completed. The primary mirror is made of 18 hexagonal segments from beryllium. The integration of the segments has started at Goddard and will be completed in 2016. Then the telescope and ISIM will be integrated and the end-to-end tests will be performed in 2017 at the Johnson Space Center in Florida. The JWST will be in orbit around the L2 point at 1.5 million km away from the Earth; it is therefore out of question to go there and make repairs, as was the case for the HST which was orbiting the Earth at an altitude of about 600 km. The JWST telescope and the near IR instruments will cool down passively to about 50 K. The MIRI instrument will be cooled down to 7 K by a dedicated cryocooler.

The JWST will be an observatory, so that astronomers have to apply for observing time. The Space Telescope Science Institute (STScI) at Baltimore will operate the JWST after launch. Calls for proposals will be issued on a yearly basis. The first call is scheduled for November 2017. The nominal lifetime of the JWST is 5 years; the consumables (for example fuel) will allow for a ten year mission. The submitted observing proposals will be reviewed by an expert committee and a ranking will be made. Given the broad thematic coverage, the large improvement in performance brought by the JWST, the uniqueness of such an observatory, we can expect that the requested observing time will be much higher than the available time. Getting JWST observing time will be highly competitive and it is important to be well prepared.

2.1.2 Implication in the JWST project

Two astrophysical laboratories members of the P2IO LabEx, Irfu-SAp and IAS embarked upon the JWST adventure at the end of the 90's. They are members of the consortium of laboratories which built the MIRI instrument (Rieke et al. 2015, Wright et al. 2015). MIRI provides a suite of versatile observing capabilities including imaging, low and moderate resolution spectroscopy and coronagraphy, all with unique performance. The instrument consists of two main subsystems:

- an imager which provides imaging over a 2.3 square arcminute field of view with 9 filters between 5 μm and 27 μm, coronagraphy in 4 wave-bands between 10 μm and 27 μm, and low spectral resolving power (R ~ 100) spectroscopy between 7 and 12 μm (Bouchet et al. 2015)
- an integral field spectrometer which provides the medium resolution spectroscopy capability (R ~ 3000, Wells et al. 2015).

The European project is organized around a European Principal Investigator (G. Wright from ATC Edimburgh, UK) and 9 Co-PI, one Co-PI for each of the European countries participating in the project (other than UK). The French Co-PI (P.-O. Lagage) is from a P2IO laboratory (Irfu-SAp). Each country has 3 Co-Investigators; A. Abergel (IAS) is one of these. The French laboratories involved in MIRI (Irfu-SAp, Irfu-SEDI, Irfu-SIS, IAS, LESIA at Paris Observatory and LAM at Marseille) have focused their participation on the imager, under the technical and scientific management of Irfu-SAp. The French participation is funded at the level of about 50% by CNES (full cost), which roughly means that the manpower is provided by the institutions and the hardware funded by CNES. CNES is responsible to ESA for the French contribution.

2.1.3 Timescale and acces to JWST observations

One important “reward” from building an instrument for a space mission is Guaranteed Time Observations (GTO). 900 hours of JWST observing time is granted to each team building an instrument for the JWST. The team has to define the scientific use of the observing time and has priority for the chosen observations. As MIRI is a 50/50 partnership between Europe and US, Europe has 450 hours GTO. Scientists from the European MIRI consortium have issued proposals to use this time. The final selection consists of three large programs of 105 hours each (characterization of exoplanets, study of protoplanetary disks, high red-shifted Universe), one medium size (55 hours) program (protostar), and three small (<20 hours) programs (submm Galaxies at z~4, Nearby Galaxies, SN1987A); 40 hours have not yet been attributed. A proposal to use part of this time to study the interstellar medium (ISM) in coordination with GTO from other instrumental teams will be discussed in March 2016.

At the moment, to have access to MIRI GTO, you have to be PI, Co-PI, Co-I or MIRI scientist. To become a MIRI scientist, you need to have worked the equivalent of 2 years for the project (tests, pipeline…). The GTO will also be opened to PhDs and postdocs, as well as a few experts which bring expertise not present in the consortium (for example in terms of modeling); the exact way the door will be opened is not defined yet, but we can expect that several postdocs, PhDs and a few experts will join. A large fraction of the French MIRI scientists are positioned in the program of exoplanet characterization (the Co-Pi coordinating the program being P.-O. Lagage) and to a lesser extend to the protoplanetary disk large program and also the smaller ISM program. When we are well on track in terms of defining the observations, reducing the data and will received good support from CNES for that, the modeling needed to interpret the data is lagging behind. One of the aims of the project presented here is to increase the modeling and laboratory experimental efforts in order to be ready to interpret the JWST data coming from the GTO observations. A large part of the GTO has to be done the first year of operation of the JWST (which will start 6 months after launch, so in April 2019); the proprietary time for GTO is one year; after that the data are public. Thus we have about 3 years to be ready. The P2IO flagship projects timescale (mid 2016- 2019) is perfectly timed with this need.

The GTO is only part of the “story”, since a large fraction of the time (~80%) will be Open Time (OT). Due to the unique performance of the JWST, the access to OT will be extremely competitive. At least five calls for OT proposals should be issued: the first one in November 2017 (deadline in February 2018), and the second one in September 2019 (deadline in December 2019). One goal of our projet is also to prepare open time proposals for these two first calls in collaboration with our national and international partners (e.g., IRAP Tououse; LESIA and LERMA/Paris Observatory; IRAM Grenoble; CSIC Madrid; …). The science with the JWST will be highly competitive and, if we plan to play an important role, we have to be well prepared.

Note also that, at the beginning of the JWST science operation (from April 2019), about 500 hours from the STScI director time pool will be devoted to an Early Release Science program (ERS). The program will be defined from proposals submitted by the community (call issued in March 2017; answers to the call due in July 2017). Informal discussions are just starting and we are part of them. The aim of this program is to provide, soon after the launch, JWST data to the community, so that the community can prepare for the second call for open time (end 2019), having already been confronted with real data. That is why the ERS data will be immediately public. This proposal will make us ready tu use these early data too.

2.2 Impact on the P2IO community and the training in the Paris-Saclay University

Our project will take full benefit of the expertise and the « excellence » recognised at an international level of the different P2IO laboratories concerning the physical and chemical evolution of the interstellar matter, the structure and the dynamical evolution of disks in relation with the planetary formation (IAS, SAp/AIM), the laboratory analyses of extraterrestrial matter and analogue materials (CSNSM, IAS, IPNO), the development, the operation and the exploitation of space instruments working at long wavelengths (IAS, SAp/AIM). This project represents a unique opportunity to build within the Paris-Saclay University a high level multi-disciplinary and multi-laboratory team (instruments, observations, data processing, modeling, simulations, laboratory experiments) by:

1. strengthening the interactions between all of the actors in the field of extraterrestrial matter already engaged within the four P2IO laboratories: IAS, Irfu-SAp, CSNSM, IPNO. The expertise covered by these teams is highly multidisciplinary, with expertise in instrumentation, observation, data reduction, astrophysics interpretation, modeling, simulations, laboratory experiments.

2. encouraging the development of studies at the interface between the different fields such as :
   - exoplanet atmosphere composition / planet formation in disks,
   - physics in disks / physics in interstellar photon-dominated regions (PDRs),
   - dust modeling / laboratory experiments,
   - dust in disks / extraterrestrial material analysis (presolar grains, interplanetary dust particles)

3. improving and extending the modeling, which will be the key to taking full advantage of the JWST observations

4. funding laboratory experiments which are also not easily funded by other means.

This P2IO team will be driven, to the highest international standards, for interpreting the JWST observations and requesting new observations. It will be a major actor in the scientific exploitation of the JWST during the next decade. The project is fully in line with the LabEx goals to build ambitious projects gathering teams from various laboratories to combine a wide range of expertise.

Our goal is also to train young astrophysicists who will work on the scientific exploitation of the JWST data, and so more than half of the requested budget is dedicated to PhD and postdoc salaries. In addition, we will disseminate our expertises to larger audiences at different levels within the new and ambitious Master of Physics at the Paris-Saclay University: “General physics”, “Astrophysics”, “Astronomical and Space-based Systems Engineering”, “Large Instruments”, etc. We are already involved in core syllabus and laboratory work in numerous fields related to our project: exoplanets, ISM, MHD, radiative transfer, spectroscopy, numerical methods for astrophysics, modeling, signal processing, accelerators, irradiation with accelerator experiments, …

2.3 Scientifc objectives

Stars and planets are formed from interstellar matter in galaxies. The densest parts of dusty and gaseous interstellar clouds collapse to form protostars surrounded by disks. These « protoplanetary disks » are the nurseries for planetary systems. It is not possible to reach a complete understanding of planet formation processes without analysing the physical and chemical properties of interstellar dust and gas. The dynamics, density structure, temperature, chemical composition, dust-to-gas ratio in interstellar clouds and disks are key ingredients to determine the initial conditions of stars and planets, and the evolution of the new protostars and protoplanets in their native disk.

The sub-millimetric and millimetric space missions Herschel and Planck, together with the large ground facilities working in visible-IR (VLT) and radio (ALMA) spectral ranges, have recently shown the spectacular richness of structures in the ISM (e.g., network of filaments structures on every length scale intimately connected with star formation) and protoplanetary disks (multiple rings and gaps, spirals, candidate protoplanets, etc), which bring new insights to the physical processes leading to the formation of stars and planetary systems. These observations notably relaunched the debate on the formation of planets: contemporary rapid formation by gravitational instability contemporary with the formation of the star or later in the disk, slower formation by aggregation of dust grains, planetesimal formation combining to form rocky cores, and if the mass of the nuclei is sufficiently large, accretion of the material and formation of giant planets. With the JWST the gain in angular resolution and sensitivity will allow a quantitative jump in the observations from the ISM and to disks and exoplanets.

The goal of our project is to bring a complete understanding of the different physical processes, at micro and macro scales and in relation with the dynamics and the physical and chemical properties, which are acting in the evolutionary sequence from the ISM to the formation of planets. We will combine access to imaging and spectroscopic JWST observations of interstellar clouds, protoplanetry disks and exoplanets together with the development of modeling tools and laboratory experiments which are mandatory to interpret the data.

3. State of the art and key questions

3.1 Interstellar dust

Interstellar dust is a key player in the physics and chemistry of the ISM. It is responsible for the re-distribution of stellar radiation from the UV-visible into IR-mm photons via absorption and thermal emission. Additionally, photo-electron emission following UV photon absorption heats the interstellar gas. Further, grain surfaces provide the necessary and unique sites for the catalytic formation of simple (H_2) to complex (macro-) molecules, driving the interstellar chemistry.

In the ISM the dust is mainly composed of amorphous silicates, a-Sil, hydrogenated amorphous carbons, a-C:H, and polyaromatic molecular structures, with key spectroscopic signatures in the mid-IR. Understanding these materials and how they evolve in response to their immediate environment is an essential and developing area of ISM dust research. This is particularly so for a-C:H materials. A detailed knowledge of the evolution of the dust properties, through the effects of constructive and destructive processing (accretion, coagulation, fragmentation, erosion, etc.), is essential if we are to advance our understanding of the role of dust in star formation and the evolution of the ISM in galaxies.

The dust thermal emission at far-IR to mm wavelengths was recently well-explored with Herschel and Planck. For example, an interpretation of the Planck observations of the diffuse ISM dust emission with classical models show wide variations, indicating a discrepancy between the observed and modelled dust extinction and thermal emission arising from large interstellar grains with radii ~ 100-200 nm (Fanciullo et al. 2015). Only the Jones et al. (2013) dust model, developed at the IAS, appears to fare well and to be consistent with the observed variations in the diffuse ISM dust extinction and emission (Ysard et al. 2015). Further, analysis of dust emission from dense clouds, and in the transition between the most diffuse and the densest regions of the ISM (Juvela et al. 2011), seems to be consistent with the recent dust evolution optical property modeling due to accretion and coagulation processes developed at IAS (Köhler, Ysard & Jones 2015) that can also explain the observed cloudshine and coreshine (e.g. scattering in the near- and mid-IR) within the framework of a self-consistent dust model (Jones et al. 2015, Ysard et al. 2015).

Somewhat in contrast to the dust in cold cores, some of the most interesting and enigmatic observations of dust within and adjacent to excited regions of the ISM, i.e., photon-dominated regions (PDRs), show that dust within the sharp and highly-irradiated edges of molecular clouds undergoes significant evolution (e.g., Compiègne et al. 2008; Arab et al. 2012; Pilleri et al. 2012, 2015). In PDRs, the UV field varies as a function of depth within the cloud, providing an unique opportunity to study how the dust populations and the gas content evolve with the excitation and physical conditions, from diffuse regions to molecular clouds. It is here that abundant, small hydrocarbon radicals and molecules, such as CCH, c-C_3H_2 and C_4H are observed and it appears that the evolution of hydrocarbon nano-particles in PDRs may play a pivotal role in the formation of molecular hydrogen and the observed hydrocarbon species, which may in fact be the photo-dissociation products of carbonaceous nano-particles (e.g., Pety et al. 2005, 2012; Guzman et al. 2015; Jones & Habart 2015). The evolution and survival of nano-grains and the formation of H_2 and organic fragments is a delicate balance between the effects of photolysis, radiolysis and hydrogenation (e.g., Pety et al. 2005, 2012; Alata et al. 2014; Guzman et al. 2015; Jones & Habart 2015) and provides a real test for current ISM chemical models. This overall scenario is indeed supported by laboratory experiments on the thermal and UV photolysis of a-C:H materials (Smith 1984; Alata et al. 2014; Duley et al. 2015).

In PDRs the dust is « warm » (T ~ 50 K) compared to the diffuse ISM (T ~ 15-20 K) and the smallest carbon grains emit a large fraction of their energy in the mid-IR where JWST will observe. JWST will for the first time allow us to spatially resolve the thin transition of atomic to molecular gas at the cloud edges (~0.001 pc or ~1'' in nearby clouds at a distance of ~400 pc). One of the major results gleaned from previous work on dense PDRs is that the transition region corresponds to a sudden change in the density (10^2 to 10^6 cm^{-3}) and temperature (10 to 100 K) at scales less than 0.005 pc (or < 5'' at 400 pc). Thus, JWST observations of the dust emission and numerous key gas lines (atomic fine-structure, rotational and ro-vibrational lines of H_2 and simple organic molecules) from PDRs will be key in unlocking the secrets of interstellar dust in the nano-particle size regime and, thus, in allowing us to make perhaps the most significant advances ever in bringing forward our currently incomplete view of dust and its evolution in interstellar media. To enable us to carry this out, as a key part of this project, we are fully involved in the development of suitable modeling tools, the definition of guaranteed time observations of PDRs, and will prepare open time observations.

3.2 Protoplanetary disks

Protoplanetary disks are the cradles of planet formation. Dust is the primary reservoir of matter available to form terrestrial planets and the cores of giant planets. Dust evolution and its link with the gas content which represents over 90% of the total mass in young disks is thus crucial to understand the pathways to planet formation. With modern large ground instruments (VLT, ALMA), the wealth of the recently identified structures in disks (cavities, rings, spirals, dust traps, gas condensation, etc.) reveals a complex distribution of dust and gas such as the series of rings in the young HL Tau system (ALMA Partnership et al. 2015). In order to interpret these structures, dynamical and physico-chemical processes are currently investigated. The situation is complicated because dust physically and chemically interacts with the gas and the dust properties change drastically in disks over small spatial scale and on short timescales. Disks are highly active sites of the physico-chemical changes in gas and dust, however the dust properties are still poorly constrained because of the lack of spatially resolved observations in the IR. A better knowledge of the properties of dust which forms the basis of any viable disk model is needed.

The upper layers of proto-planetary disks are exposed in the inner regions to the stellar flux and in the outer regions to the ISM and are reminiscent of PDR interface regions (e.g., Kamp & Dullemond 2004). PDR physics and diagnostics are thus unavoidable in the interpretation of the infrared signatures coming from the upper layers of proto-planetary disks. These layers are warmer than the shielded disk midplane since the heating photons are absorbed there by the nano- and (sub-)micron dust particles. The nano-particles, which are very well coupled to the gas, heat the gas which then influences the disk vertical structure (Gorti & Hollenbach 2008) and can explain the detection of several excited gas lines (e.g., Meeus et al. 2012). Moreover, the smallest grains are excellent tracers of the physical conditions (UV flux, Av, geometry) and may play a key role in the formation of H_2 and organic fragments as in PDRs. The disk surface with rich gas-phase and gas-grain chemistry leads to the synthesis of numerous gaseous species. Several recently observed molecules (such as CCH) could result from efficient photo-destruction of nano-particles and/or photodesorption and photodissociation of hydrocarbons derived from grain ice mantles in the outer surface layers of the disk (Kastner et al. 2015). Finally, nano-particles that escape settling are observed with the gas in the inner holes of « transitional disks » with no dust IR or millimeter emission and where on-going planet formation may have started (Geers et al. 2007 ; Maaskant et al. 2013, 2014; Kraus et al. 2013).

In contrast to small grains, large dust grains formed by accretion and coagulation become dynamically decoupled from the gas since they gravitationally settle towards the disk mid-plane. With dust settling and coagulation, dust particles are expected to concentrate in the mid-plane, and grow up to the final stage of planetesimals. On the other hand, observations show large quantities of dust in « old » disks, meaning that dust should not rapidly disappear. The efficiency of the coagulation and settling processes critically depends on the structure (e.g. compact sphere vs. fluffy aggregates) and sizes of the dust particules (e.g., Gonzalez et al. 2015), and also on the gas turbulence, which contradicts the idea that the large particles sink towards the mid-plane. The precise quantification of these processes and the determination of the complex shape and composition of the grains in the first coagulation phases are thus important. In the context of numerical simulations of disks, their final outcome is strongly dependent on the dust evolution.

The proposed project aims to characterize the JWST observations of protoplanetary disks that will mainly probe the gas and dust content at the surface of the disks with a spatial resolution of 10-100 AU and for distances up to 500 AU. In particular, spatially- and spectrally-resolved IR emission data will allow us to study, with a accuracy never before attained, the dust composition as a function of the distance from the star. Around low-mass stars, we should be able to detect dusty material phase changes such as water or $CO/CO_2/NH_3/CH_4$ ice sublimation. Such phase changes will be a key to determine the final architecture of planetary systems. On the other hand, JWST will also observe the scattered light by dust providing key complementary information on the composition, size, and structure of the dust grains present in the upper disk layers. The respective contribution of the IR emission and scattered light from the star and inner disk in the spectra observed by JWST depends on the stellar spectrum, disk structure, and dust composition and structure. Finally, spatially resolved imaging will allow us to study the large-scale geometry of the disks. In particular, one of the most striking direct indications for a flared disk structure around HAe star actually comes from our VLT observations of spatially extended nano-grain emission (e.g., Lagage et al. 2006). A full understanding of the physical observables (dust emission/scattering) will allow us to constrain the disk structure in fine detail, which is essential for the study of the disk dynamics and the chemistry. The project will benefit from 100 hours of guaranteed time observations of disks.

3.3 Exoplanets

The study of exoplanets is one of the fastest growing fields in astrophysics. Since the first detection of an exoplanet (Mayor & Queloz 1995), more than 2000 exoplanets have been discovered (http://exoplanet.eu/). One of the key findings has been the large diversity of exoplanets, with the observation of exoplanets with no equivalent in the Solar system, such as “hot Jupiters” (Jupiter mass planets in close orbit of their host star), “inflated” Jupiters (Jupiter mass planets with radius larger than Jupiter radius), or superEarths (exoplanets with intermediate masses between Neptune and Earth masses which appear to be the most numerous exoplanets in our galaxy). We have been active in this field through our participation in the CNES lead COROT mission, which has led to the discovery of the first rocky exoplanet: Corot7b (Léger et al. 2009). The search for exoplanets, especially rocky exoplanets orbiting in the so-called "habitable" zone of their host star, will remain very active, especially through two space missions using the so-called transit search method: the NASA TESS mission (to be launched in 2017) and the ESA Plato mission (to be launched in 2024), and through many ground-based instruments using various detection methods (radial velocity, transit, lensing, direct imaging, …).

A second phase in exoplanet studies has started: the characterization of their atmospheres via spectroscopic observations. Numerous atomic and molecular features are present in the visible and IR spectral range. The determination of the elementary composition of an atmosphere can bring key hints for various questions about exoplanets, such as their internal structure (Valencia et al. 2013), their formation (Öberg et al. 2011; Helling et al. 2014; Ali-Dib et al. 2014, Kreidberg et al. 2014). The study of the atmosphere by itself (temperature-pressure vertical profile with possible thermal inversion, 2D maps from phase curve, ingress and egress transit observations, possible presence of clouds, etc) is interesting as it allows testing atmospheric models, circulation models, climate models, in completely different regimes from those found in the solar system. So far the results concerning atmospheric composition are few and have been somewhat controversial. The observations, data reduction and analysis are challenging in terms of removing systematics and due to the limited spectral coverage of the present facilities such as HST or Spitzer. Moreover the impact of clouds remains poorly constrained. The JWST will allow us to make a big step forward in the field of exoplanet atmosphere characterization. Indeed, thanks to its four instruments and its large collecting area, the complete spectra from the visible to the mid IR will be obtained for a large range of exoplanet masses and temperatures[3].

[3] The instruments cannot observed simultaneously the same field; for exoplanets observed via transit, from 2 (faint targets) to 4 transits are needed to have a 0.6-12 μm spectrum.

The project proposed here is based on exoplanet characterization with the JWST, with the emphasis on determining the elementary composition of their atmospheres in order to constrain planet formation and to investigate cloud models and arrive at robust constraints on this composition. Indeed finding C/O ratios greater than the solar value (0.5) would be an excellent hint in favor of the core-accretion model of exoplanet formation. A claim for a high C/O value (>1) in the WASP-12b exoplanet (Madhusudhan et al. 2011) has triggered the development of several models, from simple (Oberg et al. 2011; Helling et al. 2014) to more sophisticated (Ali-Dib et al. 2014 and references here-in), in order to explain the large C/O ratio in the framework of core accretion planet formation in a protoplanetary disk. The claim of a high C/O ratio in Wasp-12B and other giant exoplanets has recently been questioned by Benneke (2015). The JWST will settle the question. We will benefit from the 105 hours of MIRI GTO of exoplanets we are coordinating and of the synergy with disk specialists.

Note that the work on exoplanet characterization we plan to conduct in the framework of the JWST might have a leverage on a longer time scale that the JWST lifetime. Indeed the ARIEL mission dedicated to the characterization of a statistical sample of 500 exoplanets has been selected for a competitive phase A study in the framework of the M4 slot of the ESA 2015-2025 cosmic vision program. If selected mid 2017, the mission will be launched in 2026, just after the nominal lifetime of the JWST. We (SAp, IAS) are strongly participating in the ARIEL mission, which is led by G. Tinetti (UCL).

3.4 Laboratory experiments

Understanding the nature and evolution of dust and their influence on the gas phase from the ISM to protoplanetary disks and into planetary systems are fundamental questions that will be addressed by coupling the observations with the JWST with the analyses of interstellar dust laboratory analogues and cosmic dust. The spectral range observed with the JWST (0.6-28 µm) contains in addition to molecule in gas phase numerous features and bands due to carbonaceous and silicate dust. The interpretation of the spectroscopic data in this spectral range is currently limited by a lack of suitable wide wavelength coverage laboratory data for analogues of amorphous/crystalline silicates and amorphous carbonaceous analogues, a-C(:H), and a deeper understanding of the consequences (spectral changes and material released into the gas phase) of irradiation processes (photons, electrons, ions). This research field is currently actively explored in the laboratory at the national and international levels (e.g., IRAP Toulouse, IPR Rennes, PIIM Marseille, LISA Créteil in France; CAB Spain; NASA-AMES & NASA-GSF USA; Sterrewacht The Netherlands; INAF Italy; Jena, Germany…). Together the IAS, CSNSM and IPNO are gathering a unique set of expertise in laboratory experiments that represents a major strength for the Paris-Saclay University teams. A key aspect of the present project is to study in the laboratory the links between both the ISM gaseous phase and its carbonaceous and mineral dust to relate it to primitive samples originating from solar system small bodies, i.e asteroids and comets.

A few million years after the collapse of the molecular cloud core, the parent of the solar system, dust first accreted in planetesimals, then in planetary embryos and finally in planets. In the current solar system architecture, asteroids and comets are small bodies that escaped planetary accretion. While some asteroids are fragments of differentiated planetary embryos after disruptive collisions, others never experienced differentiation. Traces of the physical and chemical conditions at the epoch of solar system formation have thus been preserved in those objects that escaped significant modifications by parent body processes. Comets being stored since their formation, in the outer regions of the solar system at very cold temperatures, are expected to have best preserved the composition of the protosolar cloud. Extraterrestrial matter collected on Earth or brought back by space missions is studied in the laboratory to unravel the formation mechanisms of the planets, and of their individual compositions (including the origin of water and organic matter). For this purpose, laboratory analyses as well as experimental work simulating the physical evolution of dust in the disk have to be combined with astronomical observations of objects in our solar system or of protoplanetary disks expected to be similar to the young solar system.

The most primitive of solar system matter is found in cosmic dust (in interplanetary dust particles – IDPs – and micrometeorites – MMs) and primitive meteorites (chondrites), which have undergone little, if any, parent body alteration (e.g. Ishii et al. 2008, Dobrică et al. 2009, Scott & Krot 2005). These samples contain high-temperature dust from the innermost part of the disk (Ca-Al-rich inclusions – CAIs), diverse minerals formed within a range of temperatures, and organic matter formed at low temperature. Pristine organic and mineral cometary matter originating from the outer regions of the protoplanetary disk of our solar system is best preserved in ultracarbonaceous Antarctic Micrometeorites (UCAMMs) from the CONCORDIA collection (CSNSM) (Duprat et al. 2010). The presence of high temperature minerals (formed near the young Sun) in samples of comet 81P/Wild 2 collected by the Stardust mission shows that large scale radial mixing was at work in the solar protoplanetary disk (Brownlee et al. 2006). The IR spectra of minerals analogous to those found in CAIs and a very few IR spectra of some CAIs were reported in the literature (Morlok et al. 2008). Using these spectra, tentative CAI detections in disks have been reported before but are only marginally significant. At Paris-Saclay, thanks to a privileged access to the IR SMIS beamline of the SOLEIL synchrotron, the IR analyses of different extraterrestrial materials (particles from comet Wild 2 and from asteroid Itokawa, meteorites, IDPs, UCAMMs, etc.) or of ISM carbonaceous analogues (a-C:H, etc.) have been conducted in the last decade (e.g. Brunetto et al. 2011, Dartois et al. 2013 and references therein). Because of the difficulties of having both the capabilities of producing adequate analogues, of sample handling of micrometer-sized samples and privileged synchrotron access, only a few teams in the world are working on the IR signatures of such unique samples. Recent technological developments should allow us, in the near future, to achieve an increase in the spatial resolution of the IR microscope at the SMIS beamline (IR micro-tomography).

In primitive extraterrestrial matter, a small proportion (<1%) of presolar grains inherited from the protosolar cloud are mixed with matter formed in the protoplanetary disk (Zinner et al. 2005). These presolar grains are mostly minerals and are identified based on their highly non-solar isotopic compositions. Both the (presolar) ISM and protoplanetary dust have been strongly modified by physical processes (heating, photon and ion irradiation, etc.) in the disk. The proportion of presolar carbonaceous and mineral grains that were initially incorporated in the solar system and to what extent they have survived or were modified are still unknown. The evolution of both these organic and mineral components in astrophysical radiative environments can be studied through irradiation of these materials by particle accelerator facilities using a wide range of energies simulating the diffuse ISM or interplanetary medium context. Irradiation experiment protocols were developed at ALTO-Tandem (IPNO) and CSNSM for this purpose. They will be used together with other facilities (GANIL, GSI and CAB) in order to access the full range (particle/energy) needed to simulate various radiative environments. Irradiations of solid phases in the ISM also release molecules and radicals affecting the chemical complexity of the surrounding gas phase. The AGAT system at IPNO has no equivalent for the determination of the actual reactions rates and branching ratios that must be implemented in chemical networks used in astrophysical models.

4) Scientific programme

The scientific program is organized into 3 work packages (WP) dedicated to the preparation of JWST observations (WP2), the modeling and the simulation (WP3) and laboratory experiments (WP4). The coordination between these 3 scientific WPs is assured in the WP1 (see Sect. 6.1). For each WP, we detail the different tasks and provide a a table with details for each task the dates, the people in charge, and the deliveries : publications in peer review journals, database, software, simulators, etc. For publications, the author lists and orders will be defined according to the work done. The PhD students and postdocs will be first authors for a significant fraction of the publications. The results will be publisehd in journals such as A&A, ApJ, Icarus, GCA, and Science or Nature for some results of interest to a large scientific public (exoplanets, disks, etc). All results will also be systematically presented in international conferences, and this is only for clarity that the oral presentations are not mentioned in the tables.

4.1 Preparation of JWST observations (WP2)

This work package is organized in 3 tasks:

Task 1: Improving the MIRI instrument simulator.

The instrument simulator is a key tool to prepare observing proposals. We aim to perform thorough simulations for our programs,

- starting with the modeling of expected images and spectra from the telescope for data from ISM regions, protostellar disks and exoplanets using state to the art astrophysical models,
- then using the telescope-instrument simulator we will simulate observed images or spectra along with their associated uncertainties,
- we will then use the data reduction pipeline and
- retrieval methods to extract physical properties from the data (for example molecular composition for the exoplanet atmosphere spectra) and assess the uncertainties on these quantities.

In the framework of MIRI, we have participated in the development of the MIRI instrument simulator. The first version should be made available to the community in spring 2016, with only a few functionalities missing. We propose to implement one of them: a precise simulation of disks observed in the coronagraphic mode of MIRI, which is of great interest for our disk program, but also for our program of exoplanets observed with the direct imaging techniques (exoplanet are often embedded in a disk).

Task 2: Data reduction pipeline.

The data reduction pipeline is under development at STScI with inputs from the instrumental teams on the different instruments (data reduction algorithms, calibration files, …). As part of the MIRI instrumental team we are working with STScI and are members or leaders of several working groups for the MIRI imager pipeline. In a first step, the STScI data reduction pipeline will be limited to the standard level (what we call level 2: L2). The L2 pipeline will not use all the instrument properties, such as the complex shape of the Point Spread Function. Therefore we will also develop and implement high level data reduction tools (e.g., deconvolution, …) for our observing programs.

Task 3: Exoplanets.

Exoplanets observations are among the most difficult to be done with the JWST. Two observing techniques will be used: the so-called transit techniques and the direct imaging techniques. For a transit, the star luminosity can decrease by a factor 10^{-5} during typically a few hours. Therefore to reach the photon noise limit, a lot of systematic effects have to be understood and corrected. One cause of systematics is detector instabilities. We have already devoted a lot of effort to characterizing these instabilities in collaboration with JPL (Dan Dicken, postdoc funded by the LabEx Focus, is in charge of this activity at SAp). The detector behavior can now be corrected at the % level, which is enough for most of the programs, but insufficient for the exoplanet program. Additional detector tests, mostly dedicated to the preparation of exoplanet observations, will be conducted in the next few years. We will continue to be the privileged JPL partner for these studies which are driven by the needs of exoplanet observations but could also improve the quality of all data products. Another item concerning exoplanets is the development of a specific data reduction pipeline and the organization of data challenges to test and improve the pipeline.

Note also that we have developed solid links with STScI and several of us plan to spend a few months at STScI after the launch during the commissioning phase. Given the large expertise acquired when building, testing and developing the data reduction pipeline of MIRI, we have decided with the CNES to develop at Paris-Saclay (SAp, IAS) an expertise center in order to help the community to prepare and analyse the observations with the MIRI imager. This center will use the technical infrastructure Virtual data of P2IO for the data production and dissemination. This will be made in collaboration with our French partners in the MIRI consortium (LAM Marseille, LESIA/Paris Observatory) and in coordination with our European MIRI partners and with ESA.

	WP2 : Preparation of JWST observations	Date	People in charge	Deliveries
1	Improvement of the MIRI observation simulator: - add simulated disk observations with the coronagraph - other improvements necessary for our programs	2016	<u>R. Gastaud</u>, P. Bouchet, A. Coulais, P.-O. Lagage, E. Pantin	Software + upgrade of the user manual
2	Data reduction pipeline (imager): - Providing data reduction algorithms to the STScI - Implement/test the STScI standard pipeline at Paris-Saclay - High level pipelines not implemented by STScI	2016 2017-2019 2016-2017	<u>P. Bouchet, K. Dassas</u> A. Abergel, A. Coulais, D. Dicken, R. Gastaud, P.-O. Lagage, E. Pantin, PhD	Software, Documentation, Test reports Software & documentation
3	Exoplanet specifics: 1) MIRI Detector test campaings at JPL (one per year); Definition, participation, data reduction and interpretation. 2) Specific data pipeline • Member of the STScI WG to specify data pipeline for long observations (mainly exoplanet transit observations) 3) Data challenges: • data reduction, retrieval techniques benchmarking • pipeline Improvement following the data challenge results	2016-2018 2016-2017 2017-2018	<u>D. Dicken,</u> P. Bouchet, A. Coulais, R. Gastaud, P.-O. Lagage +collaboration with JPL and MPIA <u>D. Dicken,</u> P. Bouchet, A. Coulais, R. Gastaud, P.-O. Lagage. M. Ollivier +collab. (STScI and MPIA, SRON…) <u>P.-O. Lagage</u> P. Bouchet, A. Coulais, R. Gastaud, P. Tremblin, E. Pantin, PhD + STScI, MPIA, SRON, …	Test report Technical note Document with results 1 paper probably in PASP Software and associated documentation

Requested funding : Half of the salary of a PhD.

4.2 Preparation of the data analysis

4.2.1 Modeling & simulations (WP3)

a) Dust in ISM, PDRs & disks

In the last few years, the laboratory and modeling/observing studies at the IAS have led us to the same conclusion: that the solid (hydro)carbon (a-C:H) phases of interstellar dust seem to be more vulnerable to processing/destruction than their silicate counterparts. The inherently complex structure and composition of a-C(:H) materials provides a modeling challenge because they undergo complex, size-dependent evolution due to photon absorption, leading to photo- or thermal-processing, and also by ion and electron collisions in shock waves and a hot gas. As a key part of this project, the specific aims of **Task 1** are to advance our understanding of the underlying micro-physical evolution of the properties of these grains in the transition zones of the ISM concerning :

a) the charge distribution as a function of the radiation field and gas density, taking into account the 3D structure of the small carbonaceous nano-particles,
b) the size distribution, the minimum size for the survival of carbonaceous nano-particles as a function of the local conditions: photo- and thermal-processing, Coulomb explosion, ion and electron collisions in shock waves and hot gas,
c) the modeling of the equilibrium composition of a-C(:H) materials as a function of the radiation field, and gas density/composition, taking into account the effects of CH bond photodissociation, a-C:H photofragmentation, accretion, hydrogenation.
d) the computation of grain optical properties (analytical approach using Mie, EMT, DDA) for (i) a grid of a-C(:H) materials (with various size and H content) and (ii) big aggregates of various size and composition (for instance mantle composition a-C/a-C:H, ice).
e) the inclusion of the results in the numerical tool DustEM (http://www.ias.u-psud.fr/DUSTEM/) which compute the emission and the extinction of a given population of dust grains heated by photons, with facility to update the grain size and composition dynamically and to provide an easy interface with radiative transfer codes.

In the ISM it is now evident that the equilibrium composition of a-C(:H) grains depends upon the local conditions. For instance, their hydrogen content, which is directly related to their band gap (i.e., their optical properties), is sensitive to thermal and UV processing. In the ISM it also likely that a-C:H grains might re-hydrogenate through H atom collisions. Hence, we will need to determine how their properties depend upon the local interstellar radiation field and gas density.

JWST observations will allow us to study the nature of a-C(:H) grains in detail because their characteristic mid-IR spectral signatures depend upon their hydrogen content. Thus, JWST will allow us to gain a deeper understanding of the balance between a-C(:H) grain UV-driven de-hydrogenation and H atom re-hydrogenation as a function of environment. The JWST will also allow the detection of dust scattered light due to large interstellar grains, whose emission has been extensively observed with Herschel and Planck but with angular resolutions lower by factors 100-1000. Further, combining JWST's spectroscopic and imaging capabilities we will track the effects of photo-fragmentation, accretion and coagulation on the dust composition, structure and size distribution and follow the spatio-temporal evolution of the dust. This work will thus focus a large part of our team's activities over the next few years.

Task 2 is a analysing and training phase using existing pre-JWST data. Indeed, our group has in hands a large database of mid-IR data (imaging and angularly resolved spectroscopy) obtained with VLT/VISIR and Spitzer for disk and PDRs, respectively, together with the access to numerous ancillary data (Herschel, IRAM, ALMA, …). We plan to select a few nearby sources with well understood geometry, based also on criteria of quality of the data and completeness. These sources will be typical targets for JWST observations. The PDRs and disks data will be analysed using our dust models (updated in Task 1) coupled to 3D Monte-Carlo radiative transfer codes in order to derive for PDRs and the upper layers of disks the spatial distribution of grain charge, size, temperature, and composition, subsequently of dust emission, scattering, and extinction. The task will be performed in close collaboration with the laboratory experiment team (WP4).

Task 3 is focused on the preparation of the JWST observations. The models developed either at the IAS or the SAp in tasks 1 and 2 will allow us to compute spectra and maps of PDRs and disks at various wavelengths for grids of input parameters describing the dust properties, the stellar spectra, and the geometries. These synthetic data will be introduced in JWST data simulators, providing state-of-the-art numerical simulations of JWST data. These simulations will be used to refine and validate for the JWST the analysis tools developped in Task 2. They will also be used to design and optimise the JWST observations in agreement with the scientific goals.

Task 4 concerns the analysis of the first JWST observations of PDRs and disks, using the models developped in the priovious two tasks, the laboratory results of WP4, and the expertise on MIRI of the WP2 team (instrument simulator, data processing).

	WP3 / ISM, PDRs & Disks	Date	People in charge	Deliveries
1	**Dust properties modeling** a) Charge distribution b) Size distribution c) aC(:H) equilibrium composition d) Grain optical properties e) DustEM service	 2016-2017 2016 2017-2019 2016-2019 2016-2019	 Verstraete Bocchio, Jones Dartois, Godard, Jones, Ysard Jones, Ysard + collab (Köhler, UK) Verstraete, Ysard	 1 paper for a) & b) 1 paper (A&A) 2 papers (A&A) Updated DustEM tool for the community
2	**Analysing/ training with pre-JWST data** - PDRs - Disks	 2016-2019	 PDRs PhD, Abergel, Wagle Disk postdoc, Pantin, Habart, Ysard, Miville-Deschênes Collab. with the lab. experiment team (WP4)	 1 paper (A&A) 2 papers (A&A) + Models to be used for task 4
3	**Simulation of JWST observations** - PDRs - Disks	 2017-2019 2017-2019	 ISM PhD, Abergel Disk PhD, Disk postdoc, Habart, Ysard, Pantin	 Simulated JWST data
4	**Analysis of JWST observations** - PDRs - Disks	2019-2020	 ISM PhD, student Abergel Disk postdoc, Pantin, Habart, Ysard Collab. with the lab. experiment team (WP4)	 2 papers (A&A) 2 papers (A&A)

Requested funding : Half the salary of 2 PhD students and 1 postdoc.

b) Exoplanets

Modeling the spectra of the exoplanets that will be observed by the JWST (in emission or in transmission) requires the development of a range of models going from 1D models with very detailed physics to 3D models with simplified physics. The direct imaging and transit observing technics will be used. To interpret emission spectra from exoplanets observed with the JWST via direct imaging, we have at our disposal the 1-D ATMO code first developed to study brown dwarfs (Tremblin et al. 2015), then used to study exoplanets detected in direct imaging (Tremblin et al. 2016 submitted) and recently to study irradiated exoplanet observed in transmission (Drummond et al., in prep.). This code uses the most up-to-date molecular opacities (Exomol for CH_4, H_2O, etc) and features two major improvements compared to state-of-the-art codes (Phoenix: Allard et al. 2013 or Saumon & Marley 2008):

1) The use of a complete network of out of equilibrium chemistry (from Venot et al. 2012), which is key to predict the effect of turbulent mixing in the atmosphere on the species abundances. The use of this network permits to take into account out of equilibrium chemistry of any composition, whereas the simplified models (such as those of Zahnle & Marley 2014) are limited to composition near the solar composition. This code feature is key for our program which aims at finding exoplanets which are likely to have non-solar composition because of the formation processes in the proto-planetary disk.

2) An effective model that takes into account the chemical instabilities in the atmosphere. The state-of-the art models interpret the redshift of brown dwarf and exoplanet spectra as due to the presence of clouds in the atmosphere. Tremblin et al. (2015) have developed an alternative explanation based on internal layers that could be cooler due to turbulence generated by chemical instabilities. Tremblin et al. (2016) have shown that this alternative scenario explains naturally the resurgence of the FeH molecules and the increase of the J-band flux at the L/T spectral transition, two effects not explained with models based on clouds. Thus turbulence induced by chemical instabilities is a phenomenon prevailing in these atmospheres.

The work in organized in four tasks:

Task 1: Benchmarking of atmospheric exoplanet models.

A benchmarking of the ATMO code with the two other codes available in the European laboratories part of the MIRI consortium (the LESIA code, the MPIA code) has started and will continue in 2016.

Task 2: Simulate the expected effects of composition variations for different scenarii of planet formation in disks.

The ATMO code will be used to generate a grid of spectra for an atmosphere with various C/O ratios, metallicities, according to the various scenarii of planet formation in protoplanetary disks. Then we will generate simulated data through the MIRI simulator, for exoplanets detected by direct imaging and for the exoplanets transiting their host star, and reduce the data (we will use the deliveries of WP2). Finally we will apply various retrieval methods in collaboration with the University College of London, where has been developed state of the art methods (Waldmann et al. 2015), to determine how precisely can the C/O ratio and metallicity be retrieved

Task 3: Implementation of clouds in the ATMO model.

The new interpretation of the brown dwarf sequence without clouds does not exclude the presence of clouds, but suggest that the vertical condensation/transport cycles are of a different type than those used so far. New models of clouds have to be developed in the framework of this new model. They may permit to reproduce the absorption feature observed at 10 μm in warm brown dwarfs, probably due to the presence of silicates, which is poorly reproduced by the present models of clouds (Stephens et al. 2009). This task will benefit from our works on dust conducted in WP3 and WP4 (IAS, CSNSM, IPNO). The effect due to the presence of clouds is also expected in exoplanets observed via the direct imaging technics; JWST observations, especially with MIRI, will be able to test the new models.

Task 4 : Development of 3 D models from the DYNAMICO code.

The strongly irradiated exoplanets show an atmospheric circulation that breaks down the spherical symmetry and imposes the use of Global Circulation Models (GCM) to calculate the spatial variations of the temperature-pressure vertical profiles with latitudes and longitudes. A new GCM model, the so-called DYNAMICO model, is currently under development (partly at CEA) in the framework of Earth studies. This new code is adapted to the architectures of massively parallel computers and will allow us to reach high spatial resolution. This code is available to us and we have started to use it to study the global circulation in exoplanet atmospheres, focusing in particular on the impact of small scale instabilities induced by the dynamics (Fromang et al. 2016) or by the chemistry (Tremblin et al. 2016). Such 3D models will help predict the robustness and variability of spectral signatures of transmission spectra observed with the JWST (e.g. post-treatment with 1D codes).

	Description	Date	People in charge	Deliveries
1	Benchmarking of atmospheric exoplanet models	2016	P. Tremblin . P-O. Lagage + MIRI consortium exoplanet modeling group	1 paper (ApJ)
2	Simulate the expected effects of composition variations (e.g., C/O ratio) for different scenarii of planet formation in disks, for direct imaging and for the exoplanets transiting	2016-2017	P. Tremblin, P.-O. Lagage + student at UCL	At least 2 papers (ApJ or A&A)
3	Implement of clouds in the ATMO model	2017-2018	P. Tremblin, postdoc	1 paper (ApJ or A&A)
4	Development of 3 D models from the dynamico code: Post-processing of 3D models with ATMO to produce 2D maps of the atmosphere transmission spectra, study of simple clouds prescriptions.	2016-2018	S. Fromang, P. Tremblin + postdoc	1 paper (ApJ or A&A)
5	Analysis of the first JWST exoplanet observations in ERS and in GTO	2019	P.O. Lagage, PhD (of WP2), S. Fromang, M. Ollivier, P. Tremblin and international collaborators	At least 1 paper (Nature or Science)

Requested funding : 1 postdoc for tasks 3 and 4 and a participation (63 K€) to a meso-machine

4.2.2 Laboratory experiments (WP4)

Our understanding of ISM dust is currently limited by a lack of suitable, wide wavelength coverage laboratory data for analogues of amorphous silicates and carbonaceous materials, and by poorly-quantified radiative processes (photons, electrons, ions). For an optimal preparation of the JWST data analysis, we focus in this package on laboratory experiments to constrain the formation and evolution of carbonaceous and silicate dust from the ISM to the protoplanetary disks. These experiments comprise the synthesis of interstellar dust analogues, the analysis of natural extraterrestrial samples and experimental simulations of their evolution in interstellar and interplanetary space. They will be supported by technical staffs at CSNSM, IAS and IPNO (see Sect. 6.5).

<u>a) Organic matter</u>

Task 1: Production of analogues for carbonaceous interstellar dust linked to cometary samples

Analogues of carbonaceous dust particles observed in the ISM can be synthesised and studied at IAS and at the SOLEIL-SMIS synchrotron beam line in order to characterize their spectroscopic properties and optical constants. Such data are crucial in the energy balance of astrophysical models. Moreover, the fate of these materials as they enter the dense phases of the ISM is a key issue in determining the links between the materials found in protoplanetary disks and their interstellar precursors. Such a study will provide new constraints on their interaction with the gas phase that are currently the subject of numerous modeling and discussions at the international level.

Achieving such goals crucially depends on the production of laboratory analogues relevant to the astrophysical context. The SICAL experiment at IAS provides a unique facility to produce carbonaceous interstellar dust analogues that are well characterized in both the IR and visible ranges. The characteristics of a-C:H produced by SICAL adequately reproduce the observed spectroscopic signatures of interstellar grains. We will devote a dedicated work on carbon dust analogues with varying content in heteroatoms, that a-C:H doped in N and O produced using SICAL and SIDONIE (CSNSM) facilities. This panel of analogues will be further extended to polyaromatic hydrocarbons in the frame of external collaborations (ISMO). Studying carbonaceous dust containing heteroatoms is crucial as the solar system most primitive organic matter (as measured in cometary dust like UCAMMs) contains variable proportions of heteroatoms.

Task 2: Investigation the origin of cometary organic matter from the CONCORDIA micrometeorite collection

For about a decade, the CSNSM team has been collecting cometary dust particles originating from the outer regions of the Solar System (ultracarbonaceous Antarctic micrometeorites or UCAMMs, 30-200 μm in size). These particles are recovered from snow in the central regions of Antarctica, in the vicinity of the French-Italian CONCORDIA station. UCAMMs are dominated by organic matter and show a minor component of mineral aggregates that most probably formed in the inner regions of the protoplanetary disk and were ejected into the comet forming regions by radial mixing in the early history of the disk. UCAMMs are characterized by microanalysis techniques, in house or through collaborations to elucidate their chemical composition, structure and evolution across submicron individual grains (scanning and transmission electron microscopies coupled with X-ray and electron energy loss spectroscopy - EDX and EELS (CSNSM), micro-IR, Raman, SIMS, NanoSIMS, STXM, XANES). The organic matter of UCAMMs shows a nitrogen-rich polyaromatic component, that exhibits extreme anomalies (deuterium enrichments) of its hydrogen isotopic composition. Such characteristics are reminiscent of cold chemistry in the outer regions of protoplanetary disks.

To understand the formation mechanisms of the cometary organic matter, and assess a potential interstellar heritage, we will carry out a comparison of the characteristics of interstellar carbon dust analogues with that of cometary UCAMMs and of cometary dust particles from the comet 67P/Churyumov-Gerasimenko (COSIMA analyser on the Rosetta mission for which we have a CoI and thus a direct access to the data). UCAMMs are the most relevant extraterrestrial particles available in the laboratory for a direct comparison with future JWST data of the composition of dust in the ISM or the external regions of protoplanetary disks.

Task 3: Evolution of physico-chemistry in the ISM

Throughout the incorporation of matter in a protoplanetary disk, the grains and gas are immersed in a radiative environment including UV, cosmic rays, stellar winds. It is therefore primordial to study the composition of the solid matter precursors and their evolution under irradiation. Exposure to this harsh radiative environment results in both a partial (or complete) destruction of the dust grains and/or their chemical modification. It also induces the release of many species into the gas phase. In turn, the gas phase may have a feedback effect on the dust by accretion and/or low velocity implantation. The observed dust properties result from these gas-grain interactions.

Our motivation is to pursue laboratory experiments on interstellar analogues, aiming at constraining the impact of energetic processes, in particular cosmic rays, influencing the fate and composition of dust grains, as well as the species released in the gas phase. The evolution of organic matter in the outer regions of the disk will be studied through the irradiation of solid interstellar carbon dust analogues (IPNO ALTO, CSNSM ARAMIS/SIDONIE, GANIL, GSI UNILAC,...). In particular, the interstellar dust analogues will be irradiated with fast ions simulating the interaction with cosmic rays at temperatures representative of dense clouds and cold disks (20-40 K), and at room temperature. The irradiated samples will be characterized by mass spectrometry to understand the impact of irradiation of carbonaceous solids on the gas phase and derive stopping power dependent cross-sections and production yields.

The release into the gas phase of species that originate from the evolution of solid phases has drastic consequences on the molecular budget and isotopic composition of the gas phase itself. Astrochemical models including only gas phase reactions fail to reproduce the observed molecules abundances, whereas observations strongly support the evidence of the dust grain modifications in molecular clouds and disk interfaces. It is therefore important to understand the species' production yields and to constrain the reactions rates and branching ratios that must be implemented in astrophysical chemical networks models. Dedicated experiments must be conducted to obtain these branching ratios. Branching ratios of chemical reactions involving such molecular species ($C_nN_yH_z$) will be measured with the AGAT experiment at ALTO-IPNO. These data will be implemented in the international KIDA database (Kinetic Database for Astrochemistry), which is crucial for gas phase chemistry models of the ISM.

Task 4: Synthesis and preparation of the interpretation of JWST data.

The results of these laboratory measurements will be inserted in models of interstellar dust in the ISM, PDRs and disks and compared to radio to IR observations (collaboration with the WP3 team). In situ IR spectroscopy will simultaneously provide the experimental characterization of the evolution of the solid phase and spectra that can be directly compared to JWST observations. We will quantify the impact of heteroatoms (N and O) on the evolution of organic matter from the ISM to the protoplanetary disks. The JWST spectra will be compared to the spectroscopic changes in the solid phase and the radiolytic generation of new molecular species, and also to chemical and structural characterization of cometary organic matter.

	Description	Date	People in charge	Deliveries
1	Production of doped analogues - N then O-doped a-C:H by plasma (IAS) - N, then O, S-doped by ion implantation (SIDONIE, CSNSM)	2016-2017	Dartois, Godard, Duprat, Postdoc	3 papers (A&A, Icarus or ApJ)
2	Analysis of cometary organic matter from the CONCORDIA micrometeorite collection (Raman, EDX, SIMS, etc), Comparison with Rosetta/COSIMA data	2016-2018	Engrand, Duprat, Godard, Dartois, PostDoc	2 papers (A&A, Icarus or ApJ)
3	Evolution of physico-chemistry in the ISM - Branching ratios & reaction rates (CnNyHz) with AGAT (ALTO/IPNO). - High- (GANIL, GSI, …) and low- (SIDONIE, ARAMIS) energy ion irradiation	2016-2018 2016-2017	Chabot, PostDoc Dartois, Godard, Duprat, Engrand	4 papers (A&A, Icarus or ApJ) Delivery to the KIDA database
4	Synthesis and preparation of the interpretation of JWST data	2018-2019	Engrand, Dartois, Duprat, Godard, Chabot, PostDoc Collab. with the modeling team (WP3)	3 papers (A&A, Icarus or ApJ)

Requested funding (the postdoc is already funded by P2IO): 150 k€ for equipment (see Sect. 8 for details)

b) Mineral matter

Our goal is to provide valuable information on the IR signatures of the primitive silicate dust in order to prepare the analysis of the JWST data. The laboratory IR spectra of IDPs and primitive meteorites will be associated with complementary analyses (Raman micro-spectroscopy, field-emission scanning and transmission electron microscopy and energy dispersive X-ray analyses) providing information on grain morphologies, structures, textures, size distributions, and quantitative compositions. IDPs derive from a broad range of dust-producing bodies extending from the inner main asteroid belt to the Kuiper belt. Two classes are generally considered: anhydrous porous IDPs with pyroxene and olivine rich sub-classes (CP IDPs) and hydrated phyllosilicate–rich IDPs (CS IDPs).

The CP IDPs[4] are almost unique among other known classes of extraterrestrial materials as their non-equilibrated mineralogy, low density, high porosity (up to 70%) and fragile structure consistent with matter being aggregated in the disk and never thermally processed. Primitive meteorites, with morphological and mineralogical characteristics close to those of IDPs mainly consist of (1) a very porous matrix of agglomerated olivine/pyroxene/amorphous silicates, (2) chondrules, and (3) Ca-Al-rich inclusions (CAIs). CAIs are the oldest objects of our solar system (4.567 ± 0.001 Ga) and they formed at high temperature (T>1300 K) from precursors directly condensed from a gas of solar composition. CAIs can be divided into (1) large coarse-grained once-melted CAIs, and (2) fine-grained CAIs[5] that escaped significant melting.

Task 1: Sample preparation

The micron-sized samples will be prepared in our dedicated clean room. We need a new high-resolution microscope to optimize sample handling. We plan to perform the IR measurements on (a) whole 3D particles, (b) particles flattened using diamond compression cells (e.g. Brunetto et al., 2011, Merouane et al. 2014), (c) on slices of particles prepared by focused ion beam in the framework of an existing collaboration with IEMN at Lille.

Task 2 IR spectroscopy

1. Acquisition of IR signatures of bulk IDPs, meteorite matrix (microscope installed on the SMIS beam line (SOLEIL).
2. Acquisition of IR signatures of micron-sized subunits of IDPs, primitive matrix and CAIs, using our new focal plane array detector installed on a new IR microscope (currently being installed on SMIS-SOLEIL), and the IR synchrotron source allowing IR spectral imaging at a sub-micron resolution. Because the observed dust in disks is not aggregated in compact objects, these subunits best correspond to the dust of the disk. We will focus on the GEMS found in IDPs, the amorphous matter found both in IDPs and in the matrix of primitive meteorites, and on fine-grained CAIs found in primitive meteorites matrix. We will obtain sub-micron spatial resolution images allowing the extraction the IR signatures of each sub-unit. Other micro-spectrometers are available in our laboratories in the 0.4-1.1 µm range.

Task 3: 3D IR micro-tomography measurements of the porosity of IDPs and meteorite matrix.

These measurements will be performed using the IR tomographic equipment (Martin et al. 2013; Quaroni et al. 2015) that is currently being installed on SMIS-SOLEIL, allowing an IR spectral imaging in 3D of particles with a sub-micron spatial resolution. Tests are currently being performed using individual (~20 µm) particles extracted from the Paris meteorite mounted on a metallic needle using Focused Ion Beam preparation protocols. The 3D spatial distribution of different phases (minerals, carbons, etc.) and an estimation of the porosity will be obtained. Such data on IDPs and meteorite matrix will be key data in the models of grains either in the ISM or in the disks.

Task 4: Experimental study of the evolution of the primitive extraterrestrial dust under irradiation.

The evolution of primitive materials from ISM to protoplanetary disks will be studied thanks to ion irradiation of selected primitive extraterrestrial materials, similarly to what was performed on terrestrial analogues to interpret ISO observations. The ion irradiations will be performed on the same platforms mentioned above, and in particular on the INGMAR facility at the SIDONIE beamline (CSNSM), and the evolution of the irradiated samples will be monitored in-situ using VIS-IR spectroscopy. Submicronic analyses described in tasks 1 and 3 will then allow us to study the evolution of the structure and composition of the dust. In particular, the evolution of specific components such as GEMS and CAIs will be investigated ex-situ. Irradiation conditions will be chosen to simulate the expected irradiations conditions in disks.

Task 5: Comparison between laboratory and Spitzer/JWST data.

The IR signatures of cosmic dust materials will be analyzed and compared (in close coordination with the dust modeling team of WP3) to available data of T-Tauri disks, then to JWST data. Crystallinity and mineralogical gradients with a higher crystalline/amorphous ratio and a higher olivine/pyroxene ratio toward the stars have been observed in disks (e.g., Sargent et al. 2009), and in icy asteroids and comets by Vernazza et al. (2015) in collaboration with us. Using our database we will look for these gradients in chosen T-Tauri disks with the

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4 Major components of CP IDPs are (1) monocrystalline silicates (size from 0.1 to a few µm), of almost pure enstatite or forsterite (2) sulfides, (3) amorphous silicates such as GEMS (0.1 to 0.5 microns, Glass with Embedded Metals and Sulfides, Bradley, 1994b) and (4) organic matter.

5 Fine-grained CAIs are considered as high-temperature condensates and consist of aggregates of nodules of micron-sized high-temperature minerals (spinel, melilite, anorthite, pyroxene).

enhanced resolution of the JWST. The JWST has also the capabilities to detect GEMs, for which an interstellar origin is debated. In addition, being the first rocky materials formed in our solar system, the presence of CAIs in other protoplanetary disks would be diagnostic of comparable planet formation processes. Finally, recent observations reveal warm water vapor in disks near the protostars, while meteoritic observations favor silicate-liquid water interactions within planetesimals. In order to solve this contradiction and to shed light on the role of water in planetary formation, we will search for the dual presence of warm water vapor and hydrated silicate dust.

	Description	Date	People in charge	Deliveries
1	Sample preparation	Sep 2016-mid 2017	Aléon-Toppani, Djouadi, PhD	Samples ready for analyses
2	IR spectroscopy - bulk IDPs, meteorite matrix, CAIs - extraterrestrial objects at micron scales	Jan 2017-mid 2018	Aléon-Toppani, PhD, Brunetto, Djouadi	Database of IR signatures (0.4-60 µm) of extraterrestrial materials 2 papers (A&A, GCA or Icarus)
3	Measurements of the porosity of IDPs, and meteorite matrix	June-Dec 2018	Brunetto, Aléon-Toppani	Database of dust porosity 1 Paper (A&A, GCA or Icarus)
4	Evolution of the primitive extraterrestrial dust under irradiation	mid 2018-mid 2019	Djouadi, Brunetto	1 paper (A&A, GCA or Icarus)
5	Comparison between laboratory and Spitzer/JWST data	mid 2017- 2020	PhD, Aléon-Toppani, Djouadi, Brunetto Collab. with the WP3 team	4 papers (A&A or Icarus) : GEMS, Olivine/Pyroxene, Irradiation/Evolution, CAIs

Requested funding: half of the salary of 1 PhD student and 40 k€ for equipment (see Sect. 8 for details).

5) List of 10 papers related to our project

1. Baillié, K., Charnoz, S., Pantin, E., 2015, A&A, 577, 65. Time evolution of snow regions and planet traps in an evolving protoplanetary disk
   Modeling of the viscous evolution of a protoplanetary disk using state-of-the-art opacities. Idenfication of regions showing surface density features, linked to dust components sublimation, where planet migration traps can develop.

2. Bouchet, P., García-Marín, M. Lagage, P.-O. et al. 2015, PASP 127, 953, 612, The Mid-Infrared Instrument for the James Webb Space Telescope, III: MIRIM, The MIRI Imager
   We are deeply involved in the imager of MIRI. A special issue of the PASP journal has been devoted to MIRI: we have been co-authors of 8 out of the 10 papers and first author of the one about the imager.

3. Brunetto, R., Borg, J., Dartois, E., et al., 2011, Icarus 212 (2): 896, Mid-IR, Far-IR, Raman micro-spectroscopy, and FESEM-EDX study of IDP L2021C5: Clues to its origin
   Study of a chondritic porous aggregate IDP using mid 2-60 µm micro-spectroscopy, Raman micro-spectroscopy, field-emission scanning electron microscopy and energy dispersive X-ray (EDX) analyses.

4. Chabot M., Béroff K., Gratier P., Jallat A. and Wakelam V., 2013, ApJ, 771, 90, Reactions forming Cn=2,10(0,+), Cn= 2,4H(0,+), and C3H2(0,+) in the gas Phase: semiempirical branching ratios,.
   This article presents the branching ratios of chemical reactions relevant to gas phase chemistry in the ISM, suggesting the need for gas-grain interactions in order to reproduce the observed chemical abundances.

5. Compiègne, M., Abergel, A., Verstraete, L., Habart, E., 2008 A&A, 491, 797, Dust processing in photodissociation regions. Mid-IR emission modeling
   Modeling of the dust emission of nano-particles ins PDRs using ISO and Spitzer data. Strong abundance variations are detected, but not angularly resolved.

6. Duprat, J., Dobrica E., Engrand, C., Aléon, J., et al., 2010, Science 328 742. Extreme deuterium excesses in ultracarbonaceous micrometeorites from central Antarctic snow
   This publication demonstrates the origin of ultracarbonaceous Antarctic micrometeorites from cold regions of the protoplanetary disk (comets).

7. Habart, E., Testi, L., Natta, A., Carbillet, M., 2006, A&A, 449, 1067. Spatially resolved PAH emission in the inner disks of Herbig Ae/Be stars
   Adaptive-optics resolution VLT/NACO spectroscopy at 3 µm: for the first time the disk emission in the aromatic (3.3 µm), aliphatic (3.4 and 3.46 µm) and nano-diamond (3.43 and 3.53 µm) features is resolved.

8. Jones, A. P., Fanciullo, L., Koehler, M., Verstraete, L., Guillet, V., Bocchio, M., Ysard, N. 2013, A&A, 558, A62, The evolution of amorphous hydrocarbons in the ISM: dust modeling from a new vantage point
New dust model anchored by laboratory-data and with built-in capacity to follow dust evolution. Mantle accretion in molecular clouds and UV photo-processing in PDRs are likely the major drivers of dust evolution.

9. Lagage, P-O., Doucet, C., Pantin, E., Habart, E., et al. , 2006, Science, 314, 621L, Anatomy of a Flaring Proto-Planetary Disk Around a Young Intermediate-Mass Star
VLT/VISIR angularly resolved images of nano-particle emission characterizing large-scale disk geometry : one of the most striking direct indications for a flared disk structure around HAe star.

10. Tremblin et al. 2015 ApJ 804, L17, Fingering Convection and Cloudless Models for Cool Brown Dwarf Atmospheres
The *ATMO is one of the most advanced 1D- models of brown-dwarf and exoplanets atmospheres including equilibrium/not equilibrium chemistry and taking into account the chemical instabilities in the atmosphere. It will be one of the key tools to prepare the exoplanet JWST observations and then to interpret the data.*

6) Project organisation and Management

The project is built over a period of 3.5 years from mid 2016 to late 2019. One PhD will be initiated in September 2016 and three in September 2017 (these theses being co-financed, they will end in 2020).

6.1 General organization

Our project is divided in four work-packages :

WP1	Scientific coordination:	A. Abergel
WP2	Preparation of JWST observations:	P.-O. Lagage
WP3	Modeling and simulations :	E. Habart
WP4	Laboratory experiments :	C. Engrand (Organic matter), A. Aléon-Toppani (Mineral matter)

Each of the coordinators will spend over 30% of their time to this project, and will :

- coordinate the research activities within the WP;
- coordinate the dissemination activities (publications, reports , ...);
- make schedules and project deadlines respected.

6.2 Scientific coordination (WP1)

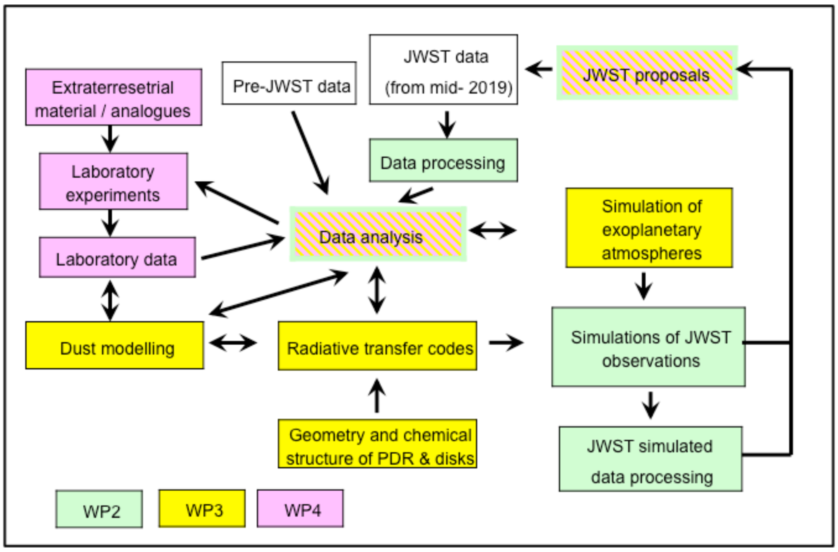
The overall project is coordinated by Alain Abergel who will spend at least half of his time and will be in charge of the work package “scientific coordination” (WP1). The coordinator will also be the rapporteur of the project responsible to the Labex and ensure the administrative management as well as the interface with the coordinators of the other WPs.

Internal face-to-face meetings will be organized on a regular basis (every two weeks) in order to discuss the results and to coordinate the next steps, and also to strengthen the interface between the different scientific work packages and tasks in our project. We will also be active in the coordination within the French community for the scientific preparation of the JWST and will participate in the organization of national meetings. We also propose to organize at Paris-Saclay an international conference on the perspective of the JWST for the study of extraterrestrial matter. Schools dedicated to the analysis tools developed by our project will also be organized. All these actions will be conducted in coordination with CNES, the National Program on Physics and Chemistry of the ISM (PCMI) and our national and international collaborators.

The dissemination of our scientific results will be one of our top priorities, especially for the PhDs and postdocs. We also plan to participate in all outreach actions in the Paris-Saclay University (visits to our facilties, general public conferences, etc). We will also participate in the development of the French JWST website (under the CNES supervison).

A budget of 60 k€ is requested for this workpackage.

6.3 Organization chart



6.4 Work plan for each PhD and postdoc

6.4.1 WP2

PhD : "Exoplanet atmosphere characterization with the JWST" (2017-2020)

- 18 months: preparation to the exploitation of the observations of exoplanets with MIRI. During this first part, he/she will get familiar with the targets to be observed with MIRI (GTO and ERS), with the scientific objectives of the MIRI exoplanets observations, with the MIRI instrument itself (running the instrument simulator), with the data reduction. He/she will participate in exoplanet data challenges conducted prior to the JWST launch. He will participate in the 2018 detector test campaign and will reduce the data concerning exoplanets. Then, beginning of 2019, he/she will participate in the analysis of commissioning data. He/she will go to at least one conference a year and participate in summer schools.
- 18 months: scientific exploitation of JWST: data reduction and interpretation (retrieval) of observations of the exoplanet atmospheres available from the Early Release Science program and for the MIRI Guaranteed time Observations. He/she will especially be in charge of the measurement of the C/O ratio in relation with the planet formation in disk (making the link between exoplanets and disks). He will write papers and show the results in conferences. He/she will also participate in the preparation of open time proposals.

The PhD student, supervised by P.-O. Lagage (SAp) and M. Ollivier (IAS), will be based at SAp but will frequently go to IAS. He/she will benefit from an excellent environment with, next door, MIRI instrument specialists, MIRI data reduction specialists, next building, exoplanet modeling specialists and at IAS, specialists in dust and disk modeling, in exoplanet and data reduction. He/she will be member of the exoplanet working group of the MIRI European consortium, where he/she will find complementary expertise to that present at Paris-Saclay, especially for the use of the medium resolution spectrometer (SRON, MPIA Heidelberg, ATC UK). He/she will also be integrated in the network of collaborators with who we are coordinating the exoplanet GTO observations (T. Green (NASA Ames); C. Beichman (IPAC, US); R. Doyon (Canada); R. Soummer (STSCI, Baltimore), …).

6.4.2 WP3

PhD : Dust micro-physical modeling in disks; preparation of the analysis of JWST data (2016-2019)

- 2016-2017 : Analysis of the carbonaceous nano-particle spectra in the near- and mid-IR (VLT, Spitzer) around Herbig Ae/Be stars using the dust models available at IAS. Determination of the composition (aromatic/aliphatic rich) and the size distribution (a_{min}) as a function of UV field strenght and spectral distribution.
- 2017-2018 : Dust model + radiative transfer code. Prediction of the spatial distribution of the various emission features to be observed with the JWST for different disk density structures, inclinations.
- 2018-2019 : Comparison with ground-based spatially resolved data (VISIR/VLT) and JWST data simulations in collaboration with SAp. Participation to the preparation of open time observing proposals.

PhD : Dust emission in PDRs with the JWST (2017-2020)

- 2017-2018 : Modeling of the dust emission in nearby PDRs using Spitzer, Herschel and ground-based data (dust model + radiative transfert code). Evolution of the composition, the relative abundances, the size of the dust particles.
- 2018-2019 : Simulation of JWST data. Preparation of the analysis of first JWST data.
- 2019-2020 : Analysis of first JWST data. Modeling of the dust emission in nearby PDRs observed with the JWST (emission of small carbonaceous dust, scattered emission of large grains). Participation to the preparation of open time observing proposals.

The Disk PhD, supervised by E. Habart, N. Ysard (IAS), and E. Pantin (SAp), is expected to start in September 2016. A second PhD supervised by A. Abergel and L. Verstraete (IAS) is necessary for PDRs, starting in September 2017. Even if several micro-physical effects on dust and gas are comparable in disks and PDRs, the physical conditions are different by orders of magnitude in terms of local density and excitation. Morevover, the analysis of the JWST data will need a deep understanding of the objects and the use of ancillary observations spanning broad spectral ranges (UV, visible, IR, radio). The same student cannot work on the two kinds of objects during her/his PhD.

The two PhD students will be based at IAS and will benefit from the local expertises on the micro-physics of interstellar dust, dust modeling (including the DustEM tool), radiative transfer codes, ancillary observations of ISM and PDRs (Herschel, Planck, VLT, IRAM, etc), laboratory experiments (also at CSNSM and IPNO) and data reduction. The Disk PhD student will find at SAp the expertise on the MIRI instrument and simulator, and on ancillary observations of disks.

Postdoc: Protoplanetary disks; preparation of the analysis of JWST data (2017-2019)

- 2017-2018: Training phase on existing data. Comparison of the dust models with ancillary data (VLT). The postdoc will have access to a large database of mid-IR data (imaging and angularly resolved spectra) of protoplanetary disks using the VLT/VISIR instrument. The data will be confronted to the dust models developped at IAS (Task 1 of WP3) and applied to disks.
- 2018-2019: Numerical simulations and preparation of JWST observations. The postdoc, in collaboration with the Disk PhD student based at IAS, will perform state-of-the-art numerical simulations of JWST futures observations. They will use a combination of numerical tools we have developed either at the IAS or the SAp : dust modeling, radiative transfer in protoplanetary disks, JWST data simulators (task 1 of WP2). The analysis tools will be also tested on simulated data.

The postdoc, supervised by E. Pantin (SAp) and E. Habart (IAS), will be based at SAp and will benefit from the local expertise on disk simulations and observations (VLT/VISIR and JWST) and on MIRI instrument, the MIRI simulator and the data reduction. He will work closely with the IAS team in order to find exertise on modeling (dust, radiative transfer). The goal is to have a complementarity between the SAp postdoc and the disk PhD student to develop the numerical modeling for the disks. The Disk PhD will bring the deep knowledge about dust properties and modeling, including radiative transfer; the Disk postdoc will implement this knowledge into the radiative transfer model specific to the disks, to then use the outputs as inputs for the JWST data simulations.

Postdoc: Exoplanet modeling for the JWST (2016-2018)

- 2016-2017: Familiarization with the code 1D ATMO (3 months) and exploration of the variation of spectral signatures of exoplanetary atmosphere when varying the atmospheric composition (C/O ratio, metallicity) (9 months) :
  - Effects of varying the exoplanet atmospheric elementary composition (C/O ratio, metallicity)
  - Grids of 1D models will be produced
  - Systematic exploration of 3D effects
  - Quantify the impact of small scale instabilities induced by the dynamics or the chemistry
- 2017-2018: Implementation of clouds in the ATMO code in close collaboration with WP3 and WP4 concerning dust evolution. The elaboration of this new model of cloud will be guided by the spectral signatures observable with MIRI at 10 μm.

Based at SAp and supervised by P. Tremblin, the postdoc will benefit from the ATMO code, from the DYNAMICO code, and from the expertise in numerical simulation of the COAST Irfu team. He/she will also go to IAS and CSNSM for the dust expertise. He/she will have access to about 1 million CPU hours/year on a meso-machine to run the coded numerical simulations.

6.4.3 WP4

Postdoc: Formation and evolution of organic matter from the ISM to the protoplanetary disk (2016-2018)

- 2016-2017
    - Identification and analyses of UCAMMs by scanning electron microscopy (CSNSM)
    - Characterization of organic matter of UCAMMs by Raman and IR (IAS - SMIS-SOLEIL)
    - Data reduction of Rosetta/COSIMA analyses of cometary particles from 67P/Churyumov-Gerasimenko
    - Participation to implantation experiment to produce N-doped a-C:H analogues (IAS/CSNSM)
    - Participation to irradiation experiments to study gas phase chemistry in the ISM (reaction rates and branching ratios - IPNO (ALTO, AGAT))

- 2017-2018
    - Identification and analyses of cometary micrometeorites in the 2016 and 2018 collect.
    - Measurements of the isotopic compositions of light elements ((H, C, N, O) by secondary ion mass spectrometry (NanoSIMS) on analogues and UCAMMs.
    - Synthesis of the results and comparison with JWST results. Redaction of one or several article(s).

This postdoc was recently funded by P2IO, supervised by C. Engrand (CSNSM) and E. Dartois (IAS). In any case, it is included in our projet. To prepare the data analysis of JWST observations, the postdoctoral fellow will work at CSNSM on the link between interstellar carbonaceous dust and primitive organic matter stored in the cometary reservoir, in close collaboration with partners in the LabEx. CSNSM has a clean room facility (MYRTHO) to handle and store micrometeorites in clean conditions. Analytical scanning electron microscopy (SEM-EDX) is required for identification and characterization of extraterrestrial matter. Electrostatic accelerators at CSNSM cover energy ranges from keV to MeV to study the evolution of organic matter in interplanetary space (ARAMIS, IRMA, Astro line on Sidonie). Higher energies irradiation will be achieved through experiments at TANDEM (AGAT) to study gas phase chemistry. IR and Raman spectroscopy of organic matter is granted through access to the SOLEIL synchrotron by IAS. NanoSIMS analyses will be achieved through external collaborations (Orsay & USA).

PhD: IR signatures of primitive extraterrestrial material at the micron scale: application to the mineralogy of protoplanetary disks (2017-2020)

- 2017-2018
    - Sample Preparation of several IDPs.
    - Mineralogical and structural characterisation using both basic methods such as scanning electron microscopy (performed by the student) and more advanced methods such as transmission electron microscopy (performed by A Aléon-Toppani).
    - Acquisition of the IR signature of bulk IDPs: first results to be presented at a conference
    - Acquisition of the IR signature of the sub-units of the IDPs and in particular of GEMS

- 2018-2019
    - Acquisition of the IR signature of the sub-units of the IDPs and in particular of GEMS and data reduction
    - Comparison with the IR spectra of bulk IDPs and with existing astronomical observation
    - Experimental irradiation of selected IDPs
    - Writing of the papers in peer reviewed journals.

- 2019-2020
    - Acquisition of the IR signatures of the irradiated bulk IDPs and of its sub-units and data reduction
    - Adjustments between JWST data and IDPs/irradiated IDPs acquired by the PhD student.

Based at IAS, and supervised by A. Aleon-Toppani and Z. Djouadi (IAS), the PhD student will conduct experiments at the SMIS beam line, using IAS dedicated time on the IR microscopes, and at P2IO laboratories using the available setups (clean room, microscopes). The student will interact with different scientists within this P2IO proposal and will be supported by two IAS technicians.

6.5 Contribution of each proposer

42 permanent staff will contribute to the project; an average of 12.4 FTE per year will be spent, which means a total of 43 FTE for the 3.5 years. The contribution of each participant is given below:

Name	Position	Role in the project	FTE 2016	FTE 2017	FTE 2018	FTE 2019
Scientists						
IAS						
A.Abergel	PR	Scientific coordination, JWST observations : MIS, PDRs, disks	0,25	0,5	0,5	0,5
A. Aleon	MCF	Lab experiments on mineral Matter	0,15	0,3	0,3	0,3
R. Brunetto	CR	Lab experiments on mineral Matter	0,15	0,3	0,3	0,3
M. Bocchio	postdoc	Dust properties modeling: charge distribution	0,2	0	0	0
E. Dartois	DR	Lab experiments : production of a-C:H, IR and Raman spectroscopy, irradiation experiments	0,15	0,3	0,3	0,3
E. Habart	MC	PDRs and Disk : microphysic modeling	0,15	0,3	0,3	0,3
A. Jones	DR	Dust models	0,15	0,3	0,3	0,3
M.-A. Miville-Deschênes	DR	Structure of the ISM, Dust emission	0,1	0,2	0,2	0,2
M. Olivier	Astronome	JWST exoplanet observations	0,1	0,2	0,2	0,2
L. Verstraete	PR	Dust Models, DUSTEM tool, ISM, PDRs	0,2	0,4	0,4	0,4
N. Ysard	CR	Dust models, Radiative transfer codes, PDRs, Disks	0,15	0,3	0,3	0,3
G. Wagle	postdoc	Analysis pre-JWST data: PDRs	0,2	0,4	0	0
Z. Djouadi	MCF	Lab experiments on mineral Matter	0,15	0,3	0,3	0,3
Total IAS			**2,1**	**3,8**	**3,4**	**3,4**
IRFU/SAP						
P. Bouchet	DR-CEA	Dust, Data reduction, Expertise center Project Manager	0,25	0,7	0,7	0,8
D. Dicken	postdoc	Detector features impact, observation simulations	0,3	0,6	0,6	0,9
S. Fromang	DR-CEA	3D modeling of exoplanets	0,1	0,2	0,2	0,2
P.-O. Lagage	DR-CEA	Coordinator WP 2; JWST exoplanet observations	0,25	0,6	0,7	0,8
E. Pantin	DR-CEA	Disks: ground-based and JWST observations	0,1	0,2	0,3	0,4
P. Tremblin	DR-CEA	1D modeling of exoplanets, post-doc supervisor	0,1	0,2	0,2	0,4
Total SAP/AIM			**1,1**	**2,5**	**2,7**	**3,5**
CSNSM						
C. Engrand	DR	Lab experiments : analyses of UCAMMs	0,15	0,3	0,3	0,3
J. Duprat	DR	Lab experiments : analyses of UCAMMs, irradiation	0,15	0,3	0,3	0,3
M. Godard	MCF	Lab experiments : irradiation, analyses of UCAMMs	0,1	0,2	0,2	0,2
Total CSNSM			**0,25**	**0,5**	**0,5**	**0,8**
IPNO						
M. Chabot	DR	Detector design - Lab experiment : AGAT, irradiation experiments - gas phase model	0,5	0,5	0,5	0,5
G. Martinet	CR	Detecteur tests - Lab experiment : AGAT	0,1	0,15	0,15	0,15
S.Bouneau	MCF	Lab experiment : AGAT	0,05	0,05	0,05	0,05
N. De Sereville	CR	Lab experiment : AGAT	0,05	0,05	0,05	0,05
F. Hamache	CR	Lab experiment : AGAT	0,05	0,05	0,05	0,05
Total IPN			**0,75**	**0,8**	**0,8**	**0,8**
Total scientists			**4,2**	**7,6**	**7,4**	**8,5**
Technical support						
IAS						
O. Mivumbi	AI	Technical support for laboratory experiments	0,15	0,3	0,3	0,3
P. Duret	AI	Technical support for laboratory experiments	0,15	0,3	0,3	0,3
K. Dassas	IR	Center of expertise MIRI (technical coordinator, IDOC)	0,025	0,05	0,05	0,05
C. Cassou	CDD CNES	Center of expertise MIRI (IDOC)	0,25	0,5	0,75	0,75
Total IAS			**0,575**	**1,15**	**1,4**	**1,4**
SAP/AIM						
A. Coulais	IR-CNRS	Instrument simulator, Data reduction, software	0,2	0,8	0,8	0,8
R. Gastaud	Ingénieur CEA	Instrument simulator, Data reduction, software	0,25	0,5	0,5	0,8
Total SAP/AIM			**0,45**	**1,3**	**1,3**	**1,6**
CSNSM						
L. Delauche	T	Preparation and preliminary analyses of Antarctic samples	0,3	0,6	0,6	0,6
L. Delbecq	IE	Technical support for MEB analyses	0,075	0,15	0,15	0,15
D. Le Du	IE	Technical support for irradiation experiments	0,075	0,15	0,15	0,15
J. Bourcois	AI	Technical support for irradiation experiments	0,075	0,15	0,15	0,15
C. Baumier	IR	Technical support for irradiation and MET experiments	0,075	0,15	0,15	0,15
C. Bachelet	IR	Technical support for irradiation experiments	0,075	0,15	0,15	0,15
F. Fortuna	IR	Support for irradiation and MET experiments	0,05	0,1	0,1	0,1
Total CSNSM			**0,725**	**1,45**	**1,45**	**1,45**
IPN						
Service electronique	IR	Printed Circuit Board (PCB) design	0,1	0,1	0,05	0
Service electronique	AI-T	reception and tests	0	0	0,2	0,1
Service mecanique	IR	mechanical conception	0	0,05	0	0
Service mecanique	AI	drawings	0	0,2	0	0
Service Aquisition	IR	Incorporation of digitizer in AGAT DAQ	0	0,1	0,1	0,1
ALTO Staff	AI-T	Support for AGAT experiments	0,1	0,1	0,1	0,1
Total IPN			**0,2**	**0,55**	**0,45**	**0,3**
Total Technical support			**1,95**	**4,45**	**4,6**	**4,75**

7) Platforms used for the project

- WP2:
  - Characterization of detectors (to better understand the behavior of sensors and increase photometric accuracy) using the "Intrapix" platform developed with the support of P2IO.

- WP4:
  - Spectroscopy at the IR SMIS beamline of the SOLEIL synchrotron
  - Irradiation experiments ALTO-Tandem (IPNO) and Aramis/Sidonie (CSNSM). The INGMAR irradiation chamber mounted on Sidonie accelerator (CSNSM) has been supported by a P2IO R&D project). Other national/international facilities (GANIL, GSI and CAB) also used in order to access the full range (particle/energy) needed to simulate various radiative environments.

- WP2 and WP3:
  - JWST data management (processing and dissemination) at Integrated Data and Operation Center at IAS (IDOC, https://idoc.ias.u-psud.fr).
  - Data processing and part of numerical simulations using the "Virtual Data" platform.

8) Requested resources

The total funding request amounts to 743 k€ for the duration of the project (mid 2016 - late 2019). It covers the following needs:

	Laboratory	Actions/equiments	Total coast	Requested	Other fundings
WP1	All	Scientific animation	**60**	**60**	
Manpower					
WP2	SAP/IRFU	PhD 2017-2020	100	50	CEA or CNES
WP3	IAS	PhD 2016-2019 + PhD 2017-2020	200	100	CNES, University Paris-Sud
WP3	SAP/IRFU	2 postdoc 2016-2018	200	200	
WP4	IAS	PhD 2017-2020	100	50	CNES or University Paris-Sud
WP4	CSNSM/IAS	1 postdoc	100	0	P2IO (CSPD)
Total Manpower			**700**	**400**	
Equipments					
WP2	SAP/IRFU	Meso-machine	504	63	DIM-ACAV (Ile-de-France), grants (ANR, ERC, prize)
WP4	CSNSM	EDX for scanning electron microscopy	72	50	CNRS, ANR
WP4	IAS	Optical microscope	40	40	
WP4	IAS	Low temperature cryohead interfaced to a UHV chamber	50	50	CNRS, ANR
WP4	IPNO	Single Side strip silicon Detector (SSD)+ mounting, cooling system and vacuum flange, power supplies, PC	50	50	
Total Equipment			**716**	**253**	
WP4		Participation to the analysis costs at IAS, CSNSM, IPNO	**30**	**30**	
Total			**1506**	**743**	

Justification of the meso-machine cost for WP3:

3D atmospheric models of hot Jupiters require significant computational resources to be performed; about 50,000 CPU hours of single-core computer time is necessary for each simulation; we will run a few tens of models per year so that we estimate that 1 000,000 CPU hours will be used each year for the project. This is why the computation is parallelized over several processors. The so-called Tier-II machines (of intermediate size, as opposed to Tier-I supercomputers only available at the national level) represent the ideal compromise for this type of project which will require large grid of models to be produced. AIM is currently in the process of buying such a Tier-II machine with up to 1516 cores. The cost of the machine, 504 kEeuros, tax free, (quotation by Clustervision available but not enclosed as it is confidential; can be made available on request) will be covered by 220 k€, already secured from the Ile-de-France region (though funding by DimAcav), and from grants ANR, ERC, Prize) obtained by the various users of the machine. The least expensive solution to feed our need for the P2IO project is to join the pull (still possible) and just buy 2 cards with 96 cores each for a total price of 48 k€, and to participate in the master node and auxiliary equipment cost in proportion with the number of cores (192/1516), which gives an additional 15 k€. The total cost is thus of 63 K€.

The requested equipment (150 k€) for WP4 will be split as follows:

- Organic matter:

- CSNSM (50 k€): The identification of cometary particles in the CONCORDIA micrometeorite collection relies on scanning electron microscopy (SEM) equipped with X-ray energy dispersive spectroscopy. We are currently using the SEM-FIB at CSNSM for these applications, but the planning does not allow us enough analysis time. We are now owning a second-hand SEM (LEO440) that needs to be equipped with EDX (49.9 k€ hardware + 10k€ software) and backscattered electron detector (12 k€).

- IAS (50 k€): Acquisition of a fully equipped low temperature cryohead (46.5 k€) that will be interfaced to a UHV chamber (5 k k€ of mechanical adaptation). This vibration-isolated system must be conceived to be safely baked out. The CCS-XG-UHV/204 cryohead will be adapted to the existing chamber. It requires the externalisation of mechanical subsystems, including OFHC copper extension, precise low temperature silicon diode and heating UHV cartridge and high purity cold screen. A compressor is needed to operate the head, as well as a temperature lakeshore regulation and UHV electrical feedthrough connections.

- IPNO (50 k€): Acquisition of a Single Side strip silicon Detector (SSD) (10 k€) made with Neutron Transmutation Doped (NTD) silicon (10k€). This detector will be mounted on a printed-circuit board (PCB, 15k€ including design) that mechanically fits inside the AGAT setup detection chamber under vacuum (5k€ of mechanical adaptation). Cooling system and vacuum flange will be added to the chamber (5k€). The charge-current preamplifier (PACI) on the PCB has been co-funded by the previous P2IO R&D effort HIGHSPID. Power supplies for detector bias and preamplifier, and an acquisition PC will be needed (5k€).

- Mineral matter:

- IAS (40 k€): Acquisition of a optical microscope for the sample preparation of the micron-sized samples. The micron-sized samples preparation is critical for the project described in WP4 (silicate part) and requires a high-resolution optical stereo-microscope (~40 k€). Such instrument will be placed in our dedicated clean room. A relatively large working distance (60 mm) is needed to optimize sample handling. In addition, a moderate magnification (~375x) is adequate to assure both a safe sample manipulation and to distinguish different sub-units within the selected area (e.g. CAIs in meteorite matrix). A dedicated camera will also allow a first 3D characterization of the selected grains.

In addition to these equipments, we are also requesting a participation of 30 k€ to the analysing costs for experimental laboratory works.

In case of a cut in the funding by 15%, the least worst solution would be to remove 2 of the 4 PhD fellowships. Note that one postdoc has been already funded by P2IO and the requested participation to the meso-machine has been reduced, so our total request is lower than in the preliminary project submitted to P2IO late September (870 k€).

9) Risk Analysis

An obvious risk is a delay in the JWST launch. All instruments are fully operational, have been delivered to NASA and have been integrated into the instrument module which will be connected to the telescope. The JWST therefore is well on track for a launch in October 2018. The goal of our project is to be ready for the scientific exploitation of the JWST which should start 6 months after launch, and a lot of experimental and modeling works have to be conducted in the next four years, including the analysis of the numerous pre-JWST data we have in hand. We expect to work on the first JWST data with our PhD students and postdocs after the end of this project. Obviously the sooner the better, but in any case the P2IO multi-disciplinary and multi-laboratory team built in Paris-Saclay will continue the scientific exploitation of the JWST during the next decade.

The different platforms used in the analyses of extraterrestrial matter and the production and analysis of interstellar analogues could suffer some minor delays. However this is a minor risk, since the working plan can be flexibly rescheduled to spend more time on the working facilities.

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