Understanding the basic components of the Universe, its structure and evolution.

A Strategic Roadmap for the CSIC

September 23, 2020

Chapter 6

Understanding the cycle of matter in the Universe

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This challenge addresses the processes that form and transform nuclei, atoms, molecules, and dust into stars and planets across the history of Universe. This baryonic matter follows a life-cycle that is intimately related to that of stars (from birth to death). The enriched chemical products of stellar evolution replenish the surrounding interstellar medium through stellar winds and supernova explosions which, in turn trigger new star formation and maintain the cycle alive. This challenge requires to understand the formation, physical properties, chemical composition, and evolution of stars, protoplanetary systems, and planets, as well as the interplay with their natal interstellar medium. It involves the application of several techniques: from astronomical observations and development of new instrumentation, to powerful computational models and laboratory experiments.

6.1 Introduction

This fundamental science challenge aims at addressing the processes that form and transform nuclei, atoms, molecules and dust grains into stars and planets, and vice-versa, the enrichment and return of matter to the interstellar medium (ISM, the space between stars). This baryonic matter, the stuff we are made of, follows a life-cycle that is intimately related to that of stars, from their birth to death (Fig. 6.1). The formation and fate of a star basically depends on its mass and composition. Depending on its initial mass, the star will follow two well differentiated evolutionary paths: a slow track for low-mass stars (the vast majority of stars in the universe) and a faster track for high-mass stars (at least 8 times the Sun's mass). The latter are very scarce and their evolution is far less understood. Although massive stars "live fast, die young" , they have a profound impact on the interstellar environment and on the life-cycle of matter. Further, they also "leave beautiful corpses" in the form of neutron stars or black holes which, if formed in binary systems, may end up merging and sending us a final post-card through gravitational waves.

The first step of the cycle occurs inside stars, where nuclear fusion converts light nuclei into heavier elements at the stellar core. Some of the nuclear reactions taking place in stellar interiors, or at the stellar dead-throes and final explosions, are still not well characterized. This limits the predictability of nucleosynthesis models (see Fig. 6.2). In any case, observational evidence shows that the enriched chemical products of stellar evolution replenish the surrounding ISM through stellar winds and supernova explosions which, in turn agitate the ISM, trigger new star formation, and maintain the cycle alive. The ISM is the reservoir of baryonic matter and, as galaxies evolve, its constituents are gradually converted again into stars by processes that are not yet fully understood. Long thought to be a scaled up version of low-mass star-formation, our knowledge of how massive stars form is still very incomplete. A critical difference is that massive stars reach maturity (emitting mighty ionizing radiation and powerful winds) when they are still embedded in their natal cloud. Thus, their impact on the surroundings is more dramatic. At the other extreme of the stellar mass distribution, the lack of appropriate observations has rendered very difficult to assess the formation of very low-mass stars and brown dwarfs.

In many objects, molecules are the most usual form of baryonic matter. Molecules exist in a very large variety of environments: from interstellar clouds, to planet-forming disks, to the atmospheres of (exo)planets and cool stars. Around 200 species, including prebiotic molecules connected to the origin of life, have been detected in space, more than 20 % first discovered by CSIC researchers. Unfortunately, we still do not understand how these molecules form and lead to the observed diversity and complexity. Even though the dust-to-gas mass ratio in the ISM is only about 1 %, dust plays many fundamental roles. However, we do not know the processes that lead to the formation of dust in evolved stars. Yet we do see rocky planets. Thus, it is crucial to understand how dust grains grow and how they are ultimately incorporated into planet-forming disks, to bridge this enormous gap in size (microns to km). Indeed, the detection of proto-planets is a great observational challenge and a mandatory step to constrain the existing theories of (exo)planet formation.

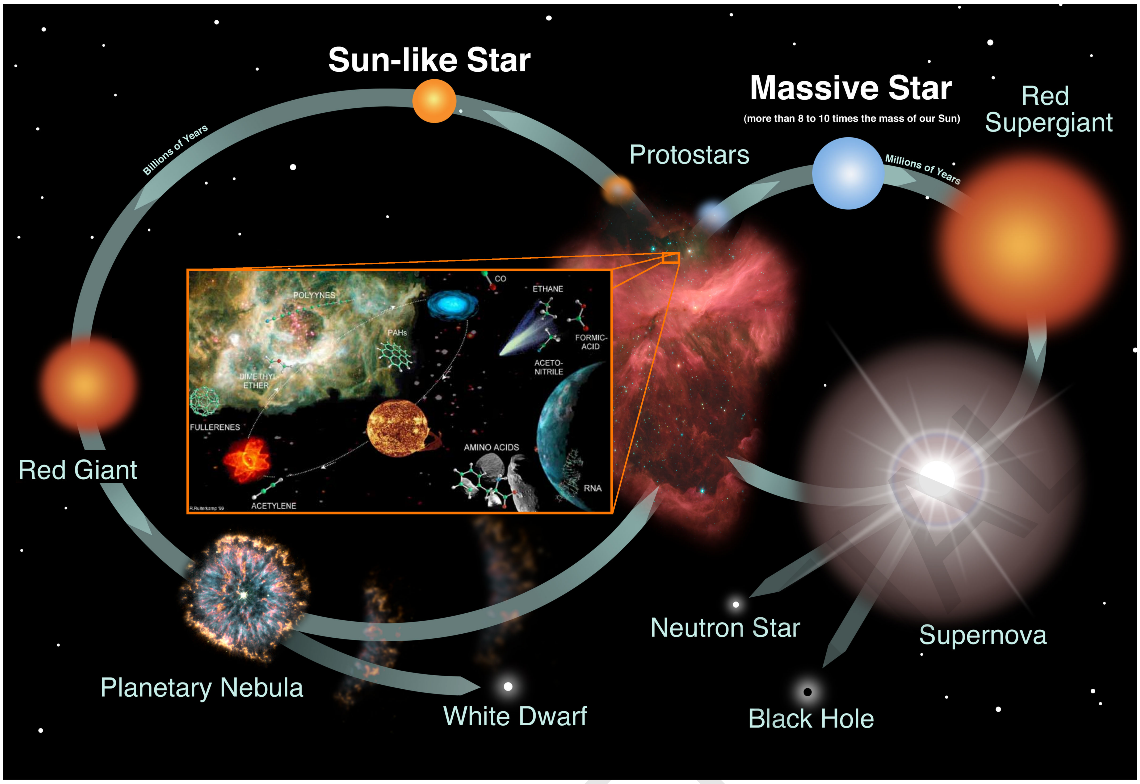


Figure 6.1: Simplified view of the life-cycle of matter in a galaxy

All in all, this challenge translates into understanding key aspects of the formation, physical properties, chemical composition and evolution of stars, protoplanetary disks and planets, as well as their interplay with the ISM. We advance here that this is a monumental task that includes the study of objects and processes with energy-, time-, and spatial-scales that vary by tens of orders of magnitude. Indeed, understanding the life-cycle of baryonic matter, in our Galaxy and beyond, requires a very multi-disciplinary approach, and involve the simultaneous participation of several disciplines distributed among different CSIC institutes: from stellar to interstellar physics, from nuclear to molecular processes; and the use of very diverse techniques: from observations at nearly all wavelengths, to powerful computational models and laboratory experiments (able to reproduce the relevant astrophysical processes), to developing new instrumentation for future telescopes.

The main questions that we would like to answer in the next years can be summarized in the following challenges (that we develop in more detail in Section 6.3):

1. **How do stars and planets form? What mechanisms transform molecular clouds into young stars surrounded by planetary systems?**
   6.3.1) Understanding high- and low-mass star formation. Studying the evolution from interstellar clouds to protoplanetary disks.
   6.3.2) Understanding planet formation: Protoplanetary disks and planet formation mechanisms. Bridging the gap between dust grains and already formed planets.
   6.3.3) Evolution of chemical complexity: from simple to prebiotic molecules.

2. **How do stars evolve from maturity to death across cosmic history?**
   6.3.4) Understanding massive stars and their evolution as cosmic agents. Enrichment and feedback with the galactic environment. Supernovae explosions and formation of black holes and neutron stars. Gravitational wave sources.
   6.3.5) The life cycle of low-mass stars. Asteroseismology. Evolved stars and their circumstellar envelopes as present-day dust and heavy elements factories. The end points of stellar evolution. Nucleosynthesis in cataclysmic events.

3. **Which are the nuclear, atomic, and molecular processes that drive and enrich the cycle of baryonic matter?**
   6.3.6) Understanding nuclear reactions and nucleosynthesis in stellar evolution.
   6.3.7) Characterizing the key physical and chemical processes that drive the evolution of the interstellar and circumstellar media.

Owing to the multi-disciplinary aspects of these challenges, tackling them will often imply a coordinated work between up to now relatively different communities at CSIC.

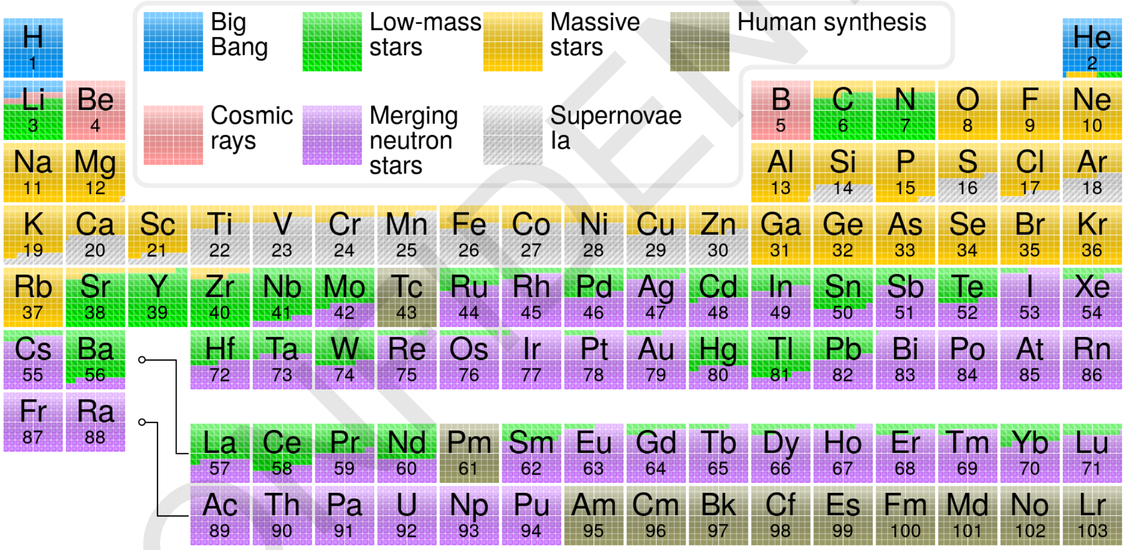


Figure 6.2: Proposed origin of different elements currently found in the Solar System and neighborhood, still a puzzle under debate in nucleosynthesis.

6.2 Impact

This challenge is at the crossroad of astrophysics, astrochemistry and nuclear physics, with relevant implications for particle physics, cosmology, planetology and theories of the origin of life. It deals with the immense task of understanding the formation of elements, molecules and dust, how they aggregate into the basic building blocks of the observable sky: stars and planets, and how this matter is returned back to the ISM. Planets are a *by-product* of the poorly known mechanisms that convert a fraction of the ISM into new stars. The detection and characterization of mature exoplanets is a very active field or research. Here we propose to go one step back and try to understand how these planets actually form. This includes studying planet-forming systems and detecting individual proto-planets. In at least one of these planets, ours, the type of complex molecules we currently detect in the ISM and around protostars conspire and lead to the emergence of life. Understanding how planets form and how molecular complexity evolves from interstellar clouds to planets will have a deep impact, both scientifically and for society.

The Milky Way is the best laboratory to study the many aspects of the life-cycle of baryonic matter in great detail (at high spatial resolution), providing useful templates to better understand the spatially unresolved emission from much distant galaxies. One example is the *feedback* of massive stars (the impact of their winds, ionizing radiation, and supernova explosions) at disrupting interstellar clouds and star formation. Recent studies of nearby regions by CSIC astronomers suggest that the relevant *feedback* processes act on much smaller spatial scales (0.2-2 parsec) than are resolved by current cosmological simulations that simulate the evolution of our universe (more than 50 parsec). Future observations of representative samples of massive star clusters using next-generation instrumentation will provide validation for these theoretical models used in broader contexts.

It will be impossible, however, to understand the cycle matter from the perspective of a single area of research. Instead, and this is a major change that will impact the way we do science, it will require the simultaneous participation of areas of expertise able to encompass the tremendous range of scales and processes we need to investigate. Understanding processes as “simple” as the agglomeration of a submillimeter-size dust grain in a protoplanetary cirumstellar disk or the photo-dissociation of a prebiotic molecule by an ultraviolet photon requires that astronomers, quantum chemists, surface scientists, and laboratory experts seat and discuss in the same table. These are just two examples. Developing networks or platforms that promote these collaborations will imply that CSIC researchers may be able to have a leading role in solving some of these challenges.

Finally, parallel societal and applied benefits often result from the development of our instrumentation, which finds application in medicine for nuclear astrophysics, or in communications, electronics, and cryogenics for other branches of the research described in this chapter. Recent examples of our groups are the development of a proton scanning device and a neutron dosimeter for proton therapy treatments and a gamma-ray imaging device for diagnosis in oncology, or the use of radio receivers in laboratory experiments.

6.3 Key challenges

6.3.1 Understanding high- and low-mass star formation.

The formation of stars is one of the fundamental processes in nature. It is an extremely complex process, which transforms the huge (tens of pc in size), diffuse (just a few hundred particles per cm^3) and cold (about 10 K) interstellar clouds of molecular gas, into hot and dense objects such as the stars. During this process the clouds of interstellar matter will shrink in size by about seven orders of magnitude, their density will increase by about 20 orders of magnitude and their temperature by six orders of magnitude. Therefore, a precise tracking of all the phases of this process, in which the physical conditions undergo such drastic changes, is a real challenge, which requires powerful observational facilities, computing tools and a deep knowledge of the physical (and chemical) properties of matter in conditions far beyond the usual ones in terrestrial laboratories.

Nowadays it is well established that individual stars form as a consequence of the gravitational collapse of dense cores of molecular gas and dust ($\sim$0.1 pc scale) resulting from the fragmentation of interstellar (pc-scale) molecular clouds (Fig. 6.3a-b), frequently after the development of filamentary structures. Because of the rotation of the core, matter does not fall directly onto the central (proto)star but through a circumstellar accretion disk that is developed at scales of $\sim$10-100 au. A fraction of the infalling matter is ejected in a direction perpendicular to the disk, in the form of a collimated jet that removes the excess of mass and angular momentum (Fig. 6.3c-d), thus allowing the formation of the star. In turn, a planetary system can be formed as a result of the evolution of the accretion disk (Fig. 6.3e-f). Thus, the investigation of the fragmentation and collapse of molecular clouds, and the development, evolution and properties of the protostar-disk-jet systems are essential steps to better understand the process of formation of stars and planets. Both gravity and magnetic fields are essential ingredients in the whole process. Radical progress has been made on these topics since the pioneering simulations of a collapsing cloud by Larson, fifty years ago, and we anticipate even more advances in the coming decades. Specifically, we identify the following key challenging points:

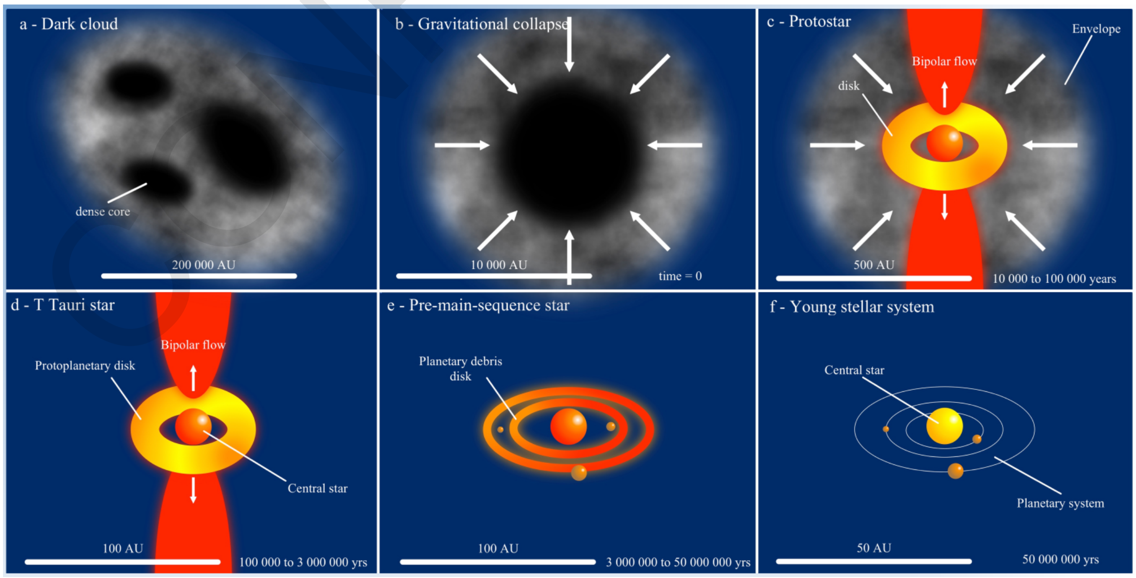


Figure 6.3: Sketch of the different stages in the overall process that transforms interstellar molecular clouds (a-b) into stars and planets (e-f). The development of a disk-jet system (c-d) plays a central role in the whole process [3].

How is star formation triggered in molecular clouds? The connection with small-scale cores. The role of interstellar filaments and the factors that determine the process of cloud fragmentation must be investigated. The relationship between the initial mass function of the cores and that of the resulting stars, as well as the whole process of clustered star formation must be better understood.

How do massive stars ($> 10\ M_\odot$) form? Because of their fast evolution and large distances, the early stages (prior to the HII phase) in the formation of massive stars are still poorly known. Can the process be a scaled-up version of low-mass star formation (e.g., monolithic collapse), or is a totally different process (e.g., coalescence of low-mass stars) required? Recent results (observation of disks and jets in massive stars) suggest a similar process, but there are no good examples for the most massive stars. What is the maximum mass that a star can reach?

How do young stars grow? Understanding star formation requires knowing how material from the surrounding circumstellar disk accretes onto the stellar surface. For low-mass young stellar objects (YSOs) there is consensus that accretion is magnetically driven, while for more massive stars without magnetic fields it is believed that accretion may proceed directly from the disk to the star through a “boundary layer”, but it is still necessary to understand how young stars of all masses grow through disk-to-star accretion. Intermediate mass Herbig Ae/Be stars represent a fundamental regime that bridges the gap between the accretion properties of low and high-mass young stars. Understanding stellar accretion has implications on the way that “macroscopic” parameters like the “star formation rate” are estimated, on the disk lifetime and dissipation processes, on modelling protoplanetary disks, and on outflows driving the angular momentum transfer.

How do protostellar jets are ejected and collimated? Young stars are associated with ionized jets characterized by thermal emission which provides a means of determining their physical properties, such as density, mass-loss rate, and temperature. It is believed that these jets are ejected through a magneto-centrifugal mechanism, but the magnetic field, which must play a fundamental role in this mechanism, is still a major unknown in YSOs. Our detection of non-thermal synchrotron radio emission in a protostellar jet may represent a major milestone to understand the ejection/collimation mechanisms in YSO jets, since synchrotron emission allows to measure and map the magnetic field. There are synchrotron jets in many other astrophysical scenarios (relativistic jets in X-ray binaries or active galactic nuclei), whose magnetic fields have been studied for decades, but lacking thermal emission to determine other physical parameters. A systematic study of thermal and non-thermal emission in YSO jets could decipher their ejection/collimation mechanism, making it possible to extrapolate it to all astrophysical jets (in synergy with Challenge 9.10). The strong shocks in the non-thermal lobes of the YSOs’ jets seem to be equally key to understanding the generation of cosmic rays in the Galaxy. On a broader scope, understanding how magnetic fields collimate the ionized astrophysical jets is of interest for the design of Tokamak fusion reactors, whose purpose is to confine by a powerful magnetic field a hot ionized plasma to produce energy in a controlled thermonuclear fusion (synergy with Theme 8).

6.3.2 Understanding planet formation.

It is well established that star and planet formation are intimately related processes that occur during the first $\sim$10 Myr of stellar evolution. Also, there is solid evidence that the formation of planets occurs in disk-like structures of gas and dust, called "protoplanetary disks", that surround the young stars. The first indications of such structures came from the analysis of the spectral energy distributions (SEDs) of young stars, which show infrared excess above the stellar emission due to the dust of the disk. Later-on, direct imaging confirmed that circumstellar disks are indeed common structures during all the stages of the star formation process. However, the exact planet formation mechanism is still unknown. Also, it is unknown at which stage in the star-forming process does planet embryos start to appear. Two main paradigms are considered. The "core-accretion" model is a bottom-up view where micron-sized dust particles in disks coagulate and grow until massive enough solid cores experience runaway accretion to finally form planets. The "disk-instability" scenario is a top-down perspective where planets are directly formed in collapsing regions within the disks that are cold and massive enough to experience gravitational instabilities. An important difference between these two views is the timescale of planet formation: 3-10 Myr according to core-accretion, and $\ll$1 Myr according to the disk instability model. Thus, a better understanding of how planets form requires to constrain when the very first steps of the planet formation process start to take place.

Most of the observational information supporting our planet formation theories is based on small (micron to submm sized) dust particles at early stages of the process, and on already formed planets ($>$1000 km) at the latest stages. Thus, it is of crucial importance to bridge this gap by directly detecting planets that are actually forming. Four decades ago, the quest for protostars was considered by Gareth Wynn-Williams the "Holy Grail" of infrared astronomy. In the present decade, the direct detection of a protoplanet has become an equivalent key challenge. The compilation of a large enough sample of protoplanetes in different evolutionary stages, the possible study of their environment and associated physical processes, the detection of circumplanetary material and accretion onto the planet (and possibly outflow) would clarify the whole process of planet formation. When planet formation is better understood, then even the quest for proto-moons can become a very active area of research in the coming decades.

The problem of understanding planet formation is identified by the major space and astrophysical agencies as one of the most important challenges for the next decades. Only by understanding the processes that lead to planet formation we could put our own solar system in perspective. This has an obvious, direct impact on society's self-perception in a universal context. Some key challenging points are described in what follows.

The quest for protoplanets. Our current knowledge about planet formation is fundamentally limited by the scarcity of detections of forming planets. Detecting a true planet embryo (i.e., a protoplanet) is a challenging task since the presence of circumstellar material and the activity of young stars make it difficult to apply the methods generally used for mature stars. Our current observational efforts rely on high-spatial resolution techniques, either aimed at the direct detection of accretion signatures of circumplanetary material falling onto the planets, through imaging and spectroscopy at optical and IR wavelengths, or the detection of the circumplanetary material itself, through imaging with large cm/mm interferometers. The future development of appropriate observational techniques, along with the use of forthcoming facilities promise a strong improvement on our detection rate of forming planets around young stars. This will allow us to obtain reliable statistics for many types of stars and different evolutionary stages, in order to get robust answers on the timescale of planet formation and, thus, on the planet formation mechanism itself.

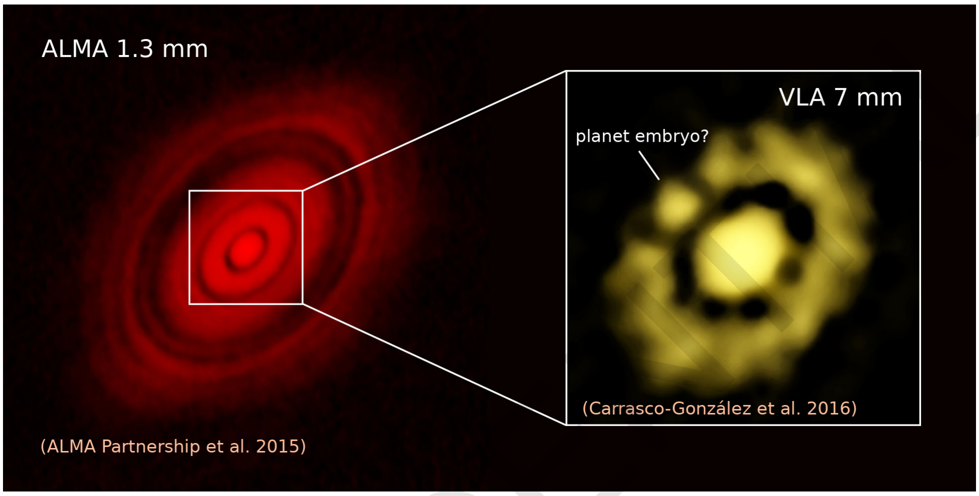


Figure 6.4: (Left) ALMA and VLA images of the HL Tau protoplanetary disk, revealing a sequence of bright and dark rings [4]. The VLA image, at a longer wavelength and lower opacity, shows details of the innermost ring substructure that remain hidden in the ALMA image, suggesting the fragmentation of the ring to form a planet embryo [5].

Protoplanetary disks. It is necessary to determine the physical/chemical properties of protoplanetary disks, their evolution and comparison with the properties of mature exoplanetary systems. Also, it is necessary to find ways to accurately measure disk masses, e.g. based on stellar accretion rates, different gas probes, and detailed disk modeling. It is not well understood how do microscopic dust grains can grow up to planetary scales since a number of mechanisms in the disk work as barriers to their growth. This study in hampered by the fact that some key processes occur in regions of the disk that are opaque even at mm wavelengths, and only can be explored at longer wavelengths (near 1 cm) where the emission is optically thinner and can penetrate these regions (Fig. 6.4). However, since dust emission decreases steeply with increasing wavelength, very sensitive observations are required. This kind of observations are currently a big challenge but they should be easier to perform with the forthcoming large facilities such as the ngVLA and the SKA. Protoplantary disks are made of gas and dust. However, gas is almost absent in the interplanetary medium. Thus, the last stages of disk evolution should be characterized by the dispersal of its gas. Photoionization and photoevaporation by high energy radiation (mainly extreme UV and/or X-ray radiation) are favored mechanisms for gas removal. However, it is still unclear how these processes work and which is the dominant one.

What determines the final mass and composition of a planet? A major question in the formation of a planetary system is to discern what determines the formation of a rocky planet, like our Earth, versus a giant gaseous planet, like Jupiter. The study of the so-called snowline (the frontier between the outer parts of the disk where molecules are frozen onto dust grain mantles and the inner parts where they are released to the gaseous phase) can provide the clue to solve this question, but the role of planet migration and the relationship with the metallicity of the host star must also be better understood. Other pending questions include: What is the minimum mass for a disk to form a planetary system? What is the maximum mass of a star to host a planetary system? Which is the role of magnetic field? How do planets form around binary stars?

Debris disks as a tool to study exoplanetary systems. The outer part of our solar system is populated by a large number of rocky bodies and dust distributed in a ring called the Kuiper Belt. This belt constitutes a relic of the accretion disk that surrounded the young Sun. Imaging similar dust belts around close-to-Earth stars with known exoplanets can inform us on the architecture and dynamical history of their exoplanetary systems, as we have done in an exploratory work with ALMA of Proxima Centauri, the star closest to the Sun. This kind of observations inform us on the dust content of the interplanetary medium in these systems, which is related with meteorite impacts and possible mass extinctions, and therefore with planet habitability. Also, it is of great interest for trajectory planning and optimization of projects like the Breakthrough Starshot mission, which aims to send ultra-light spaceprobes to Proxima Centauri at a fraction of the speed of light, since collisions with dust particles could pose a fatal threat to any of these high-speed probes.

6.3.3 Evolution of the chemical complexity: from simple to prebiotic molecules

The number of molecular species discovered in space gives an idea of its high level of chemical complexity. Understanding how this degree of complexity is attained in different environments (from interstellar clouds and planet-forming disks to the surface/atmospheres of comets, moons or planets) represents a great challenge that involves different disciplines (astrochemistry, laboratory astrophysics, planetary geology, and astrobiology).

Among these molecules, there is a sub-set termed “complex organic molecules” (or COMs) defined as carbon-bearing compounds with more than 5 atoms. Some of these COMs are of prebiotic interest since they represent key ingredients in theories of the origin of life. Examples are formamide (NH_2CHO), glycolaldehyde ($CH_2(OH)COOH$) or urea (NH_2CONH_2), which could have been precursors of amino acids, sugars and nucleobases in a young Earth and perhaps in other planets. Despite the increasing number of detected prebiotic molecules in the ISM, we still do not understand when and how they form.

We currently know that chemical complexity starts in dense and cold (about 10 K) starless/pre-stellar cores, the precursors of Solar-type systems. Several COMs have been detected in these objects, revealing an unexpectedly rich chemistry. Once a protostar is formed and heats its environment, chemical organic complexity reaches its maximum during the stage called "hot core" (around massive protostars) and "hot corino" (around low-mass protostars). The first detections of the prebiotic molecules urea or glycolonitrile ($HOCH_2CN$) have been reported, respectively, toward these two environments. At a later stage, a few COMs such as methanol (CH_3OH) have been recently detected in proto-planetary gas disks. The organic reservoir in disks, however, is likely locked as ice mantles around grains. JWST will probe this solid material. CSIC researchers are frequent users of ALMA and VLA (detecting gas-phase COMs) and have guaranteed time in JWST (to image the ice emission in protostars and protoplanetary disks).

A major question to answer in the next years is whether all this organic material can be transferred to, and retained by, small Solar-system bodies. And also whether the prebiotic content can be delivered to young Earth-like planets, triggering the biochemical processes involved in the origin of life. In this context, the main goals are: i) to understand how complex the chemistry can be along the process of star formation (i.e., whether even larger prebiotic COMs such as amino acids, complex sugars or nucleobases can be found in space); and ii) to determine whether COMs can be delivered to young planets that present similar conditions to those of an early Earth. CSIC is very well positioned to reach these goals because several groups are very active in this field. Both observationally (using ALMA, VLA, IRAM, and JWST and SKA in the future) and developing dedicated astrochemical models (IFF and CAB). These groups should strengthen their collaborations with theorists and experimentalists (at IEM, CAB, and other institutions) who are experts in the synthesis and spectroscopy of COMs (see Sect. 6.3.7).

6.3.4 From the First Stars to the present-day Universe: Massive stars as cosmic agents

Cosmic History has witnessed the lives and deaths of multiple generations of massive stars. In life they are extreme sources of UV-radiation that create ionized bubbles and inject kinetic energy into the interstellar medium (ISM). Their extremely disruptive death as supernovae (SNe) and/or γ-ray bursts (GRBs) is also a source of energy and life: it releases fresh atoms produced by the fusion nuclear reactions that fueled the star along its evolution. This is the origin of most of Oxygen and other elements crucial for life (P, Si, S, Na, K, Ca, Mg) that were inherited by planetary systems like our own later on.

All this interaction with the environment, referred to as *feedback*, enters small and large-scale processes spanning the age of the Universe, including triggering or inhibiting subsequent generations of stars and planets, dust creation and destruction, and galactic-scale gas flows in star-forming galaxies. Many astrophysics fields ingest models of the formation and evolution of massive stars as a function of chemical composition, which is a proxy for the varying environment from the Big Bang to the present day.

Massive stars have been extensively studied in the Milky Way (MW) and the nearby Large and Small Magellanic Clouds (LMC, SMC). Their chemical metallicity (Z), ranges from Solar-like ($Z_\odot$) to 1/5 $Z_\odot$. In terms of cosmic history, 1/5 $Z_\odot$ means that we are not looking back enough in time to cover the characteristic metallicity during the the period of maximum star formation in the Universe ($\sim$10.000 million years ago). *We also lack information at the extremes:* the first stars of the Universe (Z$\sim$0), crucial to model the first 200.000 years after the Big Bang, and the massive stars currently forming in the nuclei of massive spiral galaxies, such as the Center of the Milky Way ($2\,Z_\odot$).

What is the impact of metallicity in massive stars winds? The momentum of the stellar UV photons will be transferred to the metal ions in the stellar atmosphere, launching strong stellar winds which will peel off the outer layers, reducing the amount of available stellar fuel. Thus, mass-loss will modulate evolution, feedback, and the final fate of the star. Recipes for the winds and their metallicity dependence are implemented in all codes of massive stellar evolution. However, theory has been shown to fail at both luminosity and metallicity extremes, including the effect of wind inhomogeneities. Therefore, *quantifying the true mass loss of massive stars during their evolution is a fundamental challenge in the field. CSIC researchers are leading joined international efforts.*

What is the impact of metallicity in massive stars evolution? Observations provide important constraints to the evolutionary models. At low metallicity and high rotation regimes, massive stars are expected to follow chemically homogeneous evolution (CHE) leading to a completely different evolutionary path. Very hot and luminous CHE stars could responsible for extreme HeII emission in star-forming galaxies and also provide a channel to form $\sim$30 $M_\odot$ double black holes, progenitors of gravitational wave events. However, no CHE star has been observed to date, reflecting the *ill-constrained evolutionary sequence of massive stars beyond the MW-SMC metallicity range. CSIC researchers are leading the exploration of this domain.*

What is the role of binaries? A major but necessary challenge is to convolve the evolution of massive stars with their belonging to a binary system. Interaction with a nearby companion can induce mass loss/gain, even stellar mergers, with a deep impact on the evolution of the star. Massive binaries can explain long-standing problems such as the UV-excess detected in star-forming galaxies and the origin of short-GRBs, but new questions arise. Already the first gravitational wave detected, GW150914, evinced the existence of $\sim$30 $M_\odot$ double BHs larger than any model could form. *Much work is left to do both on the observational and the theoretical side to understand the real impact of binarity on the evolution of massive stars.*

Strategy: a metallicity ladder to study massive stars at all cosmic epochs

The MW and nearby galaxies make a sequence of metallicity that emulates the chemical evolution of the Universe (see Fig. 6.5). By studying local analogs in multiple metallicity-points we can construct a paradigm that holds at all cosmic epochs. The challenge requires exceptional-quality, multi-epoch ultraviolet, optical, and infrared spectroscopy of larges samples in different galaxies. *On-going and near-future massive spectroscopic surveys with formidable collecting power and multiplexing capabilities will enable, for the first time, multi-epoch access to of entire massive stars populations in the Local Group.* Further, exquisite spatial resolution will break down nearby multiple-systems providing new insight into the hierarchical spatial arrangement of massive stars.

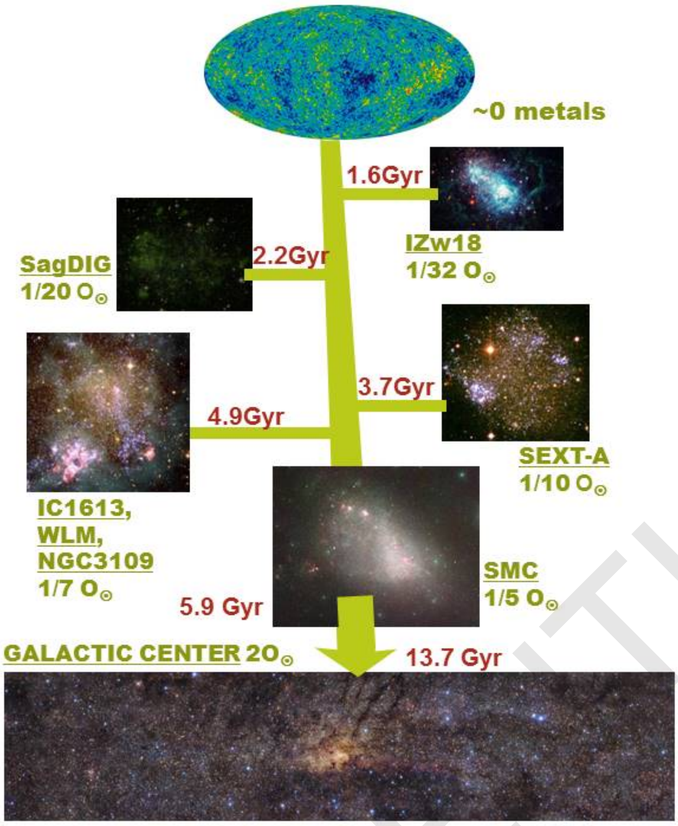


Figure 6.5: Nearby star-forming dwarf galaxies and the Milky Way provide a sequence of increasing metallicity that simulates the Universe's growth in chemical complexity with time. We study massive stars in these environments emulating analogs from the early Universe to the present-day.

Spectroscopic analysis techniques, perfected for decades now, will yield accurate stellar parameters. However, such an exceptionally large database will need an automatic approach and in the next few years we will embrace *machine learning*. The results of these studies will enable defining the evolutionary sequence of single and binary massive stars.

Establishing true mass loss rates requires parallel theoretical developments. Increasing computing power will enable implementing wind models computed from first principles, and relaxing the simplifications historically adopted to save computing time. Nonetheless these advances must be verified by observations. *A multi-wavelength approach, combining data from present and future facilities such as LUVOIR, GTC, VLT, ELT, JWST, SPICA and ALMA, will finally constrain the true mass loss rates of massive stars. CSIC researchers are leading science and observational programs for the current and future (next ∼10-15 years) facilities and are, therefore, placed in a privileged position.*

6.3.5 The life cycle of low-mass stars

Asteroseismology of low mass stars

In the last decade, asteroseismology has opened a window into stellar interiors and we can, for the first time, poke into their detailed internal structure. Results from the Kepler mission have made ever more evident the inadequacy of state-of-the-art stellar models for providing an accurate description of the dynamical evolution of stellar interiors. What is the size of convective cores during H-core and He-core burning, that determine the lifetime of stars? What are the mechanisms driving transport of angular momentum and chemical species? Dynamical processes are fundamental in the evolution of stars because they determine their chemical structure, the transport of nucleosynthesis products to the surface, and the underlying structure of stars in thermonuclear explosions. Yet, the physical descriptions used in stellar evolution theory today are toy models at best.

It is not computationally possible to model simultaneously the long-term evolution of stars and the dynamical processes in stellar interiors. Instead, the fundamental challenge is to: 1) identify most critical phases of stellar evolution and stellar domains in which multi-dimensional effects play a major role, and most relevant dynamical processes, 2) develop (magneto-)hydrodynamic multidimensional simulations that capture in detail these processes, 3) use those simulations to construct phenomenological models to be used in stellar evolution codes to model their long-term impact in stellar evolution.

Some test cases of this paradigm have been done in the past, and results have had a large impact in stellar physics. Current computational power allows for a much wider range of possibilities. Asteroseismic data from Kepler offers a large constraining and testing power of models and this will only improve in the next decade with PLATO.

Evolved stars and their circumstellar envelopes as present-day dust and heavy elements factories; enrichment of the ISM

During the asymptotic giant branch (AGB) phase, late in their evolution, low-mass stars inject enriched elements into the ISM and are the primary production factories of cosmic dust in the Milky Way. Understanding what cosmic dust is made of, and its cycle since its formation until it is incorporated into planets is an ambitious goal. AGB photospheres gradually expel huge circumstellar envelopes of molecular gas and dust. Grains are thought to form in the innermost layers of these envelopes. Which are the gas-phase precursors, how do condensation nuclei grow, and how these particles evolve toward the grain compositions and size distribution observed in the ISM is not known.

Observations that spatially resolve the dust formation layers of AGB stars are very challenging. ALMA observations of the dust formation zone in CW Leonis, the closest and richest (more than 60 molecules have been detected, many of them by CSIC researchers) carbon-rich AGB star reveal hundreds of unidentified molecular lines. The spectrum of many molecules containing C, Si, Mg, Fe, Al, Ti, and Ca is not known. Assigning these lines may take years, but they hide the inventory of the molecular seeds of grain formation. A related problem is the formation of polycyclic aromatic hydrocarbons (PAHs). Recent laboratory experiments carried by CSIC groups suggest that their formation in AGB stars, as believed before, may not be efficient. It is still a mystery how these widespread aromatic species are formed. Shedding light on the dust formation processes and on the life-cycle requires input from chemistry, mineralogy, plasma and surface physics. Multi-wavelength observations, models, and lab experiments resembling the conditions in AGB envelopes are needed to investigate the many processes involved.

Planetary Nebulae

Low mass stars will undergo the planetary nebula (PN) phase, before becoming naked white dwarfs. PNe are glowing shells of gas and dust around stars that have just left the AGB phase, and show a spectacular variety of morphologies. During the post-AGB phase, the central star shrinks and raises its temperature until it is hot enough (about 25000 K) to photoionize the circumstellar envelope formed earlier by the slow wind during the AGB phase. There is broad consensus that non-spherical PNe are created by binary (or multiple) stellar systems, but there is a plethora of models to explain how the PN is shaped. In the case of close binaries, this could happen through the formation of toroidal structures in a common envelope phase during the AGB phase. In wider binaries, jets could break the spherical symmetry of the circumstellar envelope, opening cavities over which the ionization front will proceed when the PN is created. During the PN phase, also, the heating of the central star and the shocks produced by interaction of the fast post-AGB and slow AGB winds lead to the alteration of the chemical composition of the nebula, and the molecular yields to the ISM. Moreover, PNe show spectral lines of elements such as neon and helium, which are otherwise not observable in cooler phases of stellar evolution, and are therefore unique tracers of late phases of AGB evolution and chemical evolution of the Milky Way and galaxies of the Local Group.

Some of the open questions are: (a) When does jet launching start and which is the exact mechanism of jet launching and collimation? (b) Where are the binary central stars? (c) What is the chemical elements and molecular inventory of matter in PNe?

Multifrequency observations with high angular and spectral resolution can determine the morphology, kinematics, energetics of the ejected material. In conjunction with state-of-the-art hydrodynamical simulations and an active search for binary companions and magnetic fields in the central stars of PNe, this is mandatory to assess the shaping mechanism of PNe, and their contribution to the chemical enrichment of the ISM.

Understanding thermonuclear supernovae

Low mass stars end up their lives as white dwarfs and host spectacular thermonuclear explosions if they accrete matter from or even merge with a companion. Explosions can involve only the outer layers of the white dwarf (novae), or can completely obliterate the star producing a thermonuclear supernovae (SNe), or Type Ia SNe. Ashes of these explosions return to the ISM and are major components of galactic chemical evolution.

The apparent homogeneity of Type Ia SNe explosions initially paved the way for the discovery of the accelerated expansion of the Universe. Observations have later on revealed a large degree of heterogeneity, and the most fundamental question remains unanswered. Which is the dominant channel leading to Type Ia explosions? The so-called single degenerate (SD) channel in which a white dwarf accretes matter from a normal companion until reaching the critical mass for explosion, or the double degenerate (DD) in which two white dwarfs merge, or even collide, and then explode?

The characterization of the environment surrounding the star before the explosion can yield very valuable information regarding the SD or DD channel. Radio interferometric observations of Type Ia limited to 25 Mpc from us have been used to constrain stellar mass loss before the explosion, which should be absent in the DD channel, but not in the SD channel. On the other hand, Type Ia produce several radioactive isotopes. ^{56}Ni in particular drives the evolution of the lightcurve, and emits γ-rays when it decays. Observations in γ-rays have been obtained only for one Type Ia by INTEGRAL, and have allowed a direct determination for the first time of the amount of ^{56}Ni produced in a Type Ia explosion. While thousands of Type Ia lightcurves have been observed, very little is known with certainty about the inner workings of the explosion mechanisms.

In the future, with the Squared Kilometer Array (SKA) in radio, Athena in X-rays, and a possible γ-rays mission (similar to eASTROGAM, previously proposed to ESA), it will be possible to make qualitative progress in our understanding of Type Ia explosions.

6.3.6 Understanding the role of nuclear reactions and nucleosynthesis in stellar evolution

Nuclear fusion in stars converts light elements into heavier nuclei up to the iron region, where nucleons are maximally bound. Nuclei beyond iron are basically produced by a variety of neutron-capture processes. The particular sequence of nuclear reactions and their rates depend on the mass of the star. The end-products of star evolution are typically compact objects, white-dwarfs in the case of low-mass stars, black-holes or neutron stars in the case of massive stars. Additional contributions to the chemical evolution arise from nuclear processes taking place at explosive events on compact stars (Supernovae Ia, Novae) or neutron stars mergers. Nuclear physics is a crucial ingredient for understanding of the evolution and explosion of stars and of the chemical evolution of the Universe.

The aim is to understand the origin of the chemical elements and to answer the fundamental question of where and how the rich variety of present nuclear species has been created from the original composition of hydrogen and helium after the Big Bang. The broad picture exists but our current knowledge of the underlying nuclear physics involved is still incomplete in many basic respects and the unambiguous identification of the astrophysical sites for all of the nucleosynthesis processes is still an open question. Two outstanding examples are 1) understanding the puzzle of element formation from iron to uranium through neutron reactions and 2) determining the oxygen/carbon ratio at the end of He burning phase in stars that determines later stages of stellar evolution and involves the carbon producing triple alpha process ("the reaction of life") and other light-nuclei reactions [53, 54]. CSIC researchers are well positioned to contribute to both.

Many properties of the nuclei involved in nucleosynthesis processes (s, r, p, rp, and other less common processes, see Fig. 6.6), such as masses, weak-interaction rates (beta-decay, electron capture and neutrino interactions), and nuclear reaction rates (capture of neutrons, protons and alpha particles on a variety of targets), have not yet been determined with enough precision (up to two-orders-of magnitude uncertainty in some cases). These properties also determine to a large extent the different stages of the stellar evolution. These uncertainties are mainly due to the extremely small reaction rates involved in some processes, as well as the difficulty of measuring the properties of very unstable

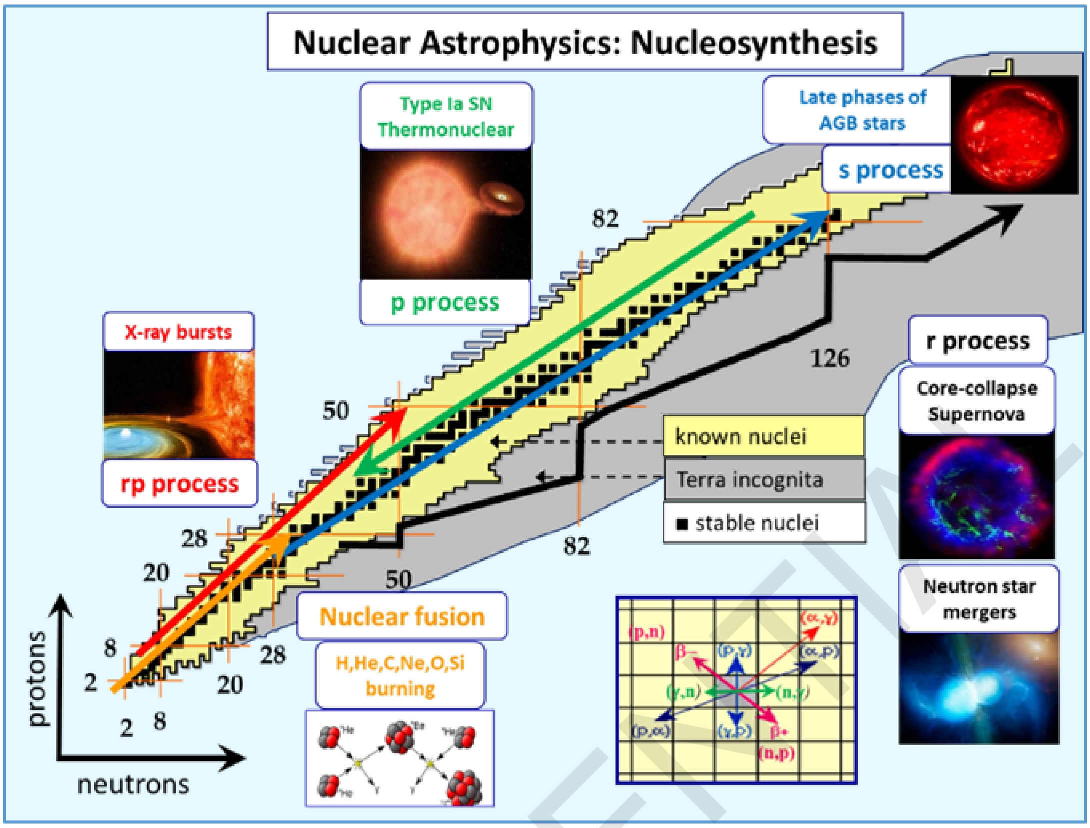


Figure 6.6: Schematic chart of nuclides showing the various astrophysical processes of relevance for nucleosynthesis, as well as the most likely astrophysical sites where they occur.

nuclei of relevance in others. A significant push in this direction is expected in the coming years with a new generation of accelerator facilities, generating a wealth of new data from high intensity radioactive-beam and neutron-beam facilities, but also from underground laboratories, stable-beam, and neutrino facilities [55]. Nuclear theory complements the experimental information providing predictions of the properties of key nuclei that have not yet been produced in the lab and connecting experimental measurements under terrestrial conditions with relevant astrophysical quantities at stellar densities and temperatures.

The specific challenges that we will address in the coming 10-20 years, based on their involvement at new/future facilities (like n_TOF/CERN, ISOLDE/CERN and FAIR), are:

Nucleosynthesis in massive stars (see also 6.3.4)
-Understand the rapid neutron-capture process (r process) in core-collapse supernovae and neutron-star mergers and the weak-s process during the core He-burning phase to assess their relative contribution to heavy element formation throughout the history of the Universe. This will require better knowledge of masses, beta-decay half-lives, beta-delayed neutron emission and neutron-capture rates of very neutron-rich unstable nuclei, which are expected to be accessible at the new experimental facilities.

Nucleosynthesis in low-mass stars (see also 6.3.5).
-Understand light ion fusion reactions at the low energies typical of stars contributing to

light element formation. This involves extremely low cross-sections and unstable targets that will require radioactive beams and very low background underground measurements.
- Improve our knowledge on neutron-producing and neutron-capture reactions of nuclei close to stability in particular on some key unstable isotopes, acting on the slow neutron-capture process (s-process) that occur in AGB stars and contribute to the heavy element formation. Both powerful neutron beams and underground labs are required.

Thermonuclear explosions. Novae, supernovae Ia, and X-ray bursts.
- SNe Ia account for 2/3 of cosmic iron and are dominant for many iron-peak elements.
- SNe Ia are the current dominant sources of iron-peak elements (see Fig. 6.2). Novae and X-ray bursts contribute to the synthesis of rare isotopes. Nuclear masses, weak-decay, proton/neutron capture rates of both unstable proton- and neutron-rich nuclei are needed.

6.3.7 Characterizing the key physical and chemical processes that drive the evolution of the interstellar and circumstellar media

The multi-wavelength emission from the interstellar and circumstellar media results from a plethora of subtle physical and chemical processes that occur at microscopic level, mostly molecular. The molecular content of many objects of the sky is indeed surprisingly rich and changes with time. Hence, molecular abundances serve as proxies for their evolution. Molecular emission (infrared to radio) probes many dust-obscured environments in which UV to visible light is heavily attenuated (star-formation, galactic nuclei, etc.). Molecules are not only *exotic* species, chemically interesting by their own, they are also powerful diagnostic tools in astrophysics: of physical conditions, magnetic fields, gas kinematics, or ionization rates. They also play a critical role in protostellar gas cooling.

High-precision understanding of the Molecular Universe. The unprecedented detailed information, both spectroscopic and spatial, that the next generation telescopes will provide of so many environments will only be usefully interpreted through implementing new astrophysical models combining magnetohydrodynamics, thermodynamics, chemical evolution and radiative transfer. These models in turn critically require as input accurate spectroscopic information, cross-sections, and rates for all micro-processes that form, destroy, and excite molecules and atoms in space (chemical reactions and collisions).

Physical conditions change drastically in the evolution from clouds to stars and planets. Ultraviolet photons from massive stars penetrate inside molecular clouds (Fig. 6.7) heating the gas to about 1,000 K, photo-dissociating molecules, exciting polycyclic aromatic hydrocarbons (PAH), and processing dust grains. The details of these microscopic processes are not well understood. This affects our ability to quantify many astrophysical parameters; for example the lifetime of star-forming clouds exposed to ultraviolet radiation or the origin of the strong PAH emission from very distant starburst galaxies. In the coldest objects inside molecular clouds (10 K in prestellar cores) chemical reactions on the icy surfaces of dust grains drive the formation of complex molecules. Surface reactions at such cold temperatures and low pressures, however, are very hard to study.

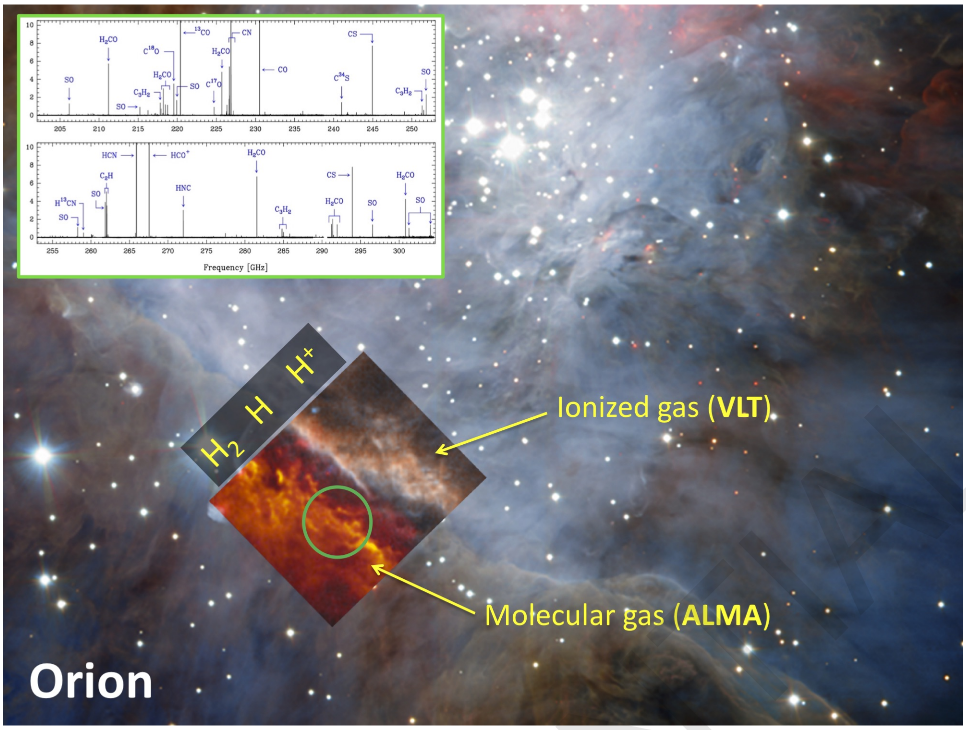


Figure 6.7: Central parsec of the Orion Nebula, illuminated by UV radiation from massive stars in the Trapezium cluster [6]. The inset shows the millimeter-wave spectrum of the molecular cloud edge (taken with the ICTS IRAM 30 m telescope at Pico Veleta, Spain).

This challenge aims at articulating a platform between different communities working in low-energy (astro)physics, capable of dealing with the many open problems in molecular astrophysics from an *integral* point of view. It will be mandatory to combine state-of-the-art astronomical observations with *coordinated* computational simulations of molecular processes and laboratory experiments, both able to determine the cross-sections and precise rates of as many as possible gas-phase and surface processes of astrophysical relevance. From the laboratory point of view, the use of synchrotrons and ultra-vacuum chambers for realist experiments will be needed. However, the tremendous range of conditions probed make these rates hard, sometimes impossible, to measure them in the lab. In these cases, they can only be computed theoretically (by quantum simulations for simple molecules, by quasi-classical methods for complex organic molecules). Such simulations will have to make use of the most advanced high-performance computational methods, simulation techniques, increased CPU time, and big-data analysis tools.

Experimentalists should also improve their spectroscopic techniques to characterize the spectrum of new molecules that could potentially be detected in space. There is still an embarrassing number of unidentified features that populate the spectra of many astronomical objects (hundreds of unassigned “diffuse” interstellar bands in the visible, solid-state bands in the infrared, and many unidentified rotational lines in the radio). These features hide the secret of how carbon chemistry evolves from small hydrocarbon molecules to PAHs and fullerenes, and likely hide the signature of many more prebiotic molecules.

Assigning these features is a great challenge because it involves computing the structure of increasingly complex molecules, minerals, and ice mixtures. The detection of a new molecule in space requires such a line frequency accuracy that only spectroscopy laboratories able to synthesize the species and record its spectrum using the latest technologies (from radio to laser) can provide such precision. Spectroscopists will develop machine-learning tools to assign carriers in very crowed laboratory and astronomical spectra.

Following this roadmap, CSIC researchers in molecular astrophysics will be able to maintain their leading role in the detection of new molecules in space, and also in exploiting their diagnostic power in different environments of the life-cycle of matter. Succeeding in this challenge will allow us to accurately understand, not only how galaxies transform interstellar matter into stars and planets, but how they acquire their physical conditions, abundances, and degree of chemical complexity.

6.4 CSIC leadership and multi-/inter-disciplinarity

The present challenge has a major multi- and inter-disciplinary aspect as it connects several fields within physics, chemistry, biology and data science. Specifically, tackling this challenge from an *integral* perspective requires the simultaneous participation of the following disciplines, all of them with strong involvement of several CSIC ICUs:

- Astrophysics and Cosmology.
- High energy, nuclear and particle physics.
- Astrobiology and Astromineralogy.
- Astrochemistry and laboratory astrophysics.
- Computing modelling, data-driven science, and data analysis.

The strong inter-disciplinarity of our challenges is *also* reflected in the close synergies with other themes of this book, Theme 2 ("Origin and evolution of life" for the studies of the building of blocks of life in space), Theme 11 ("Artificial Intelligence, Data Science and Robotics" for the development of techniques to deal with vast ammounts of observational and computational data) and Theme 12 (Space exploration and colonization" for Solar System and exoplanet studies).

This challenge also presents very close synergies with the following topics within the current theme “Understanding the basic components of the Universe”:

- "Origin and fate of the Universe".
- "Formation and evolution of large structures and galaxies".
- "New instrumentation and techniques for understanding the Universe.
- "Understanding matter in extreme conditions".

CSIC researchers have demonstrated world-renowned expertise to face these challenges, both as users and developers of past, present, and future large national (ICTS) and international infrastructures and facilities:

- Optical and infrared telescopes (ESO, ENO, CAHA, GEMINI, NOAO, OSN, OAJ).

- ESA's, NASA's, and JAXA's space telescopes (GAIA, HST, HERSCHEL, SOFIA, JWST, INTEGRAL, TESS, KEPLER, XMM-NEWTON, CHANDRA, CHEOPS, PLATO, ARIEL, EUCLID, ATHENA, LUVOIR, eXTP, SPICA).
- Radio telescopes and interferometers (ALMA, IRAM, SKA, VLA, YEBES, EVLBI).
- Gamma-ray telescopes (CTA, MAGIC).
- Accelerators (CNA, CMAM, NUSTAR/FAIR, RIBF/RIKEN, NTOF-ISOLDE/CERN).
- Underground facilities (e.g., LSC-Canfranc).
- Laboratories for Molecular Astrophysics (e.g., IEM and IFF chambers, CAB-ISAC).
- Supercomputer facilities (e.g., CESGA, MARE NOSTRUM).

The strength of CSIC researchers and their excellent potential to exploit the synergetic and multi-disciplinary aspects of this research challenge are clearly depicted in the following list, which encompasses common areas in expertise and leadership by the involved ICUs (written in alphabetical order):

- Theoretical and observational research in the field of formation and evolution of stars, planets and planetary systems and, their interplay with the interstellar medium (CAB, IAA, ICE, IFF).
- Stellar physics, models of high-mass stars across cosmic time and asteroseismology (CAB, IAA, ICE).
- Spectroscopic characterization and detection of new molecules and building blocks of life in space. Development and maintenance of molecular data bases (CAB, IEM, IFF).
- Long-term synergetic collaborations between astrochemists, quantum theorists, and laboratory experiments in Molecular Astrophysics (CAB, ICMM, IEM, IFF).
- High-performance computing, quantum technologies, and machine-learning techniques (CAB, IAA, IEM, IFF)
- High spatial resolution techniques: multiwavelength interferometric observations using ALMA, VLBI, VLTI, VLA, IRAM-NOEMA, SKA (CAB, IAA, ICE, IFF).
- Development of instrumentation and involvement in the scientific and technological definition of future space- and ground-based facilities: ELT, SKA, PLATO, ARIEL, SPICA, eXTP, ESA's 2050 program, NASA's Decadal Survey (CAB, IAA, ICE, IFF).
- Nuclear physics: world-wide recognized theoretical activity. Experiments: ISOLDE/CERN, NTOF/CERN, GSI, RIBF/RIKEN. Key lead position in the development of the coming major European NUSTAR/FAIR facility and participation in Eurisol (IEM, IFIC).

6.5 Strategic plan and resources

The strategic plan is based on three fundamental pillars:

1) Scientific strategy to carry out the activities to solve the proposed challenge. This includes the development of specific theoretical and experimental roadmaps taking advance of CSIC leadership. Potential multi-disciplinary roadmaps/platforms and virtual/regional centers for: "Large international facilities (SKA, JWST, ELT)", "Nuclear Astrophysics", and "Molecular Astrophysics" (e.g., including astrochemists, astrobiologists, quantum theorists and laboratory experimentalists disseminated in various ICUs). Additionally, participation and development of large ground- and space-telescopes such as SKA or SPICA should be promoted, including the upgrade and maintenance of existing infrastructures for laboratory astrophysics. Finally, complementary expertise should be acquired on those research areas relevant to this challenge such as large-scale simulations of hydrodynamics for stellar interiors, multi dimensional radiative transfer, quantum simulations, radio interferometry, big-data analysis, etc.

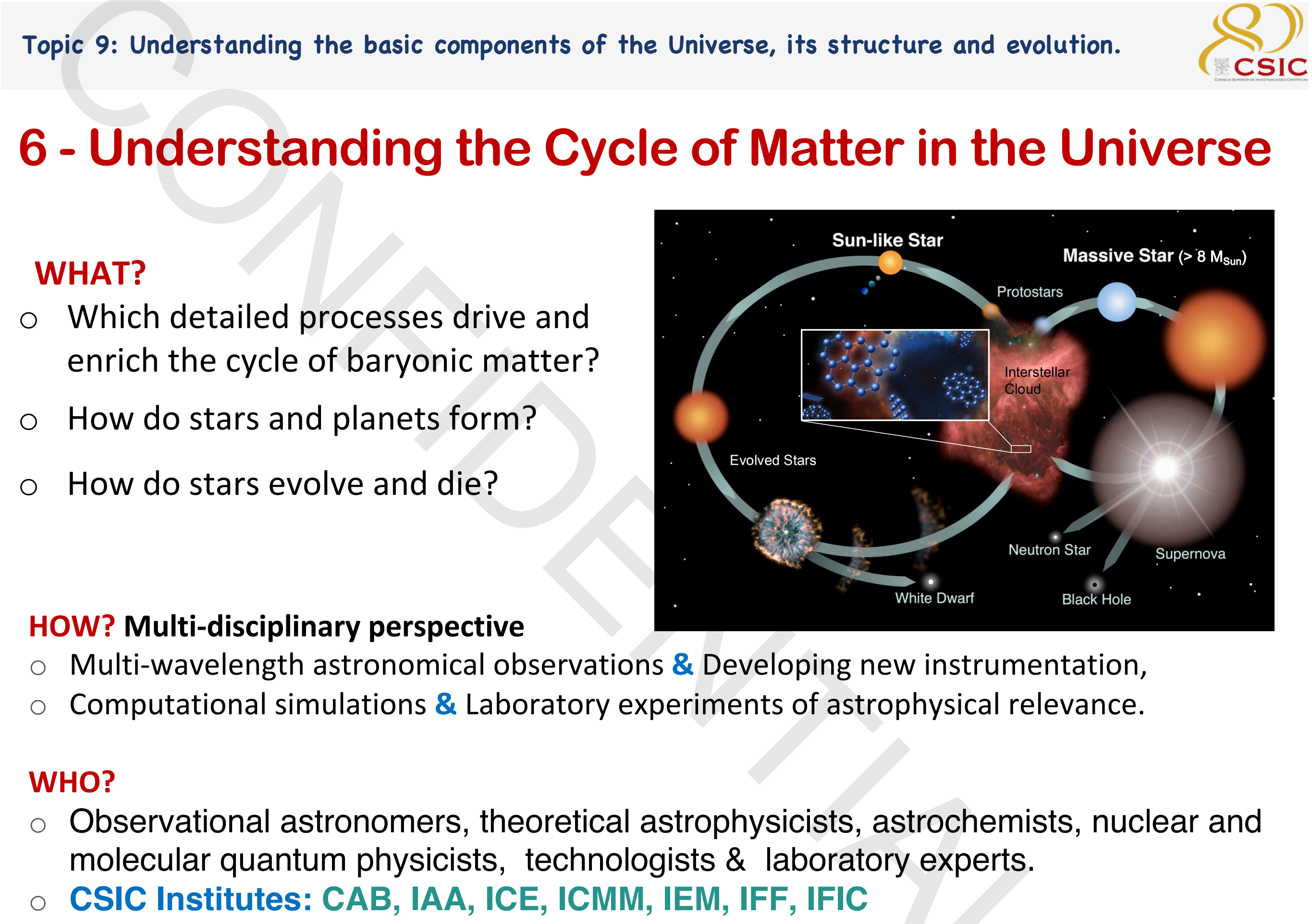
2) Foster and strengthen multi-disciplinary collaborations among the involved CSIC ICUs as well as with national and international research institutions. On the CSIC side, a collaboration among theoretical astrophysicists, observational astronomers, and nuclear, atomic and molecular physics research groups is mandatory. This can be achieved by supporting the formation of *virtual* centers/platforms (see previous point). In addition, interaction with computer and data sciences would be fundamental. Finally, apart from a vast number of international institutions (not listed here), we would like to stress some of our main national collaborations outside CSIC:

- Universities: UCM, UAM, UPM, ULL, UV, UAB, UB, UPC, UC, UGR.
- OPIS: IAC, INTA, CIEMAT.
- Other: OAN/IGN, IMDEA, IRAM-Granada, ING-La Palma.

3) Secure human and funding resources and outreach activities, which requires:

- Continuous training of scientific and technological personnel. Increase the currently poor number of pre- and postdoctoral researchers working in the different teams and supporting multi-disciplinarity.
- Stabilize scientific and technological personnel at a reasonable rate in the ICUs.
- Promote return of researchers consolidated abroad.
- Improve computational power to confidently address our main goals.
- Provide funds, technical manpower and institutional support to contribute to instrumentation development in large international participated facilities.
- Enhance outreach activities.

Annex: One slide summary for experts



Topic 9: Understanding the basic components of the Universe, its structure and evolution.

6 - Understanding the Cycle of Matter in the Universe

WHAT?

- ○ Which detailed processes drive and enrich the cycle of baryonic matter?
- ○ How do stars and planets form?
- ○ How do stars evolve and die?

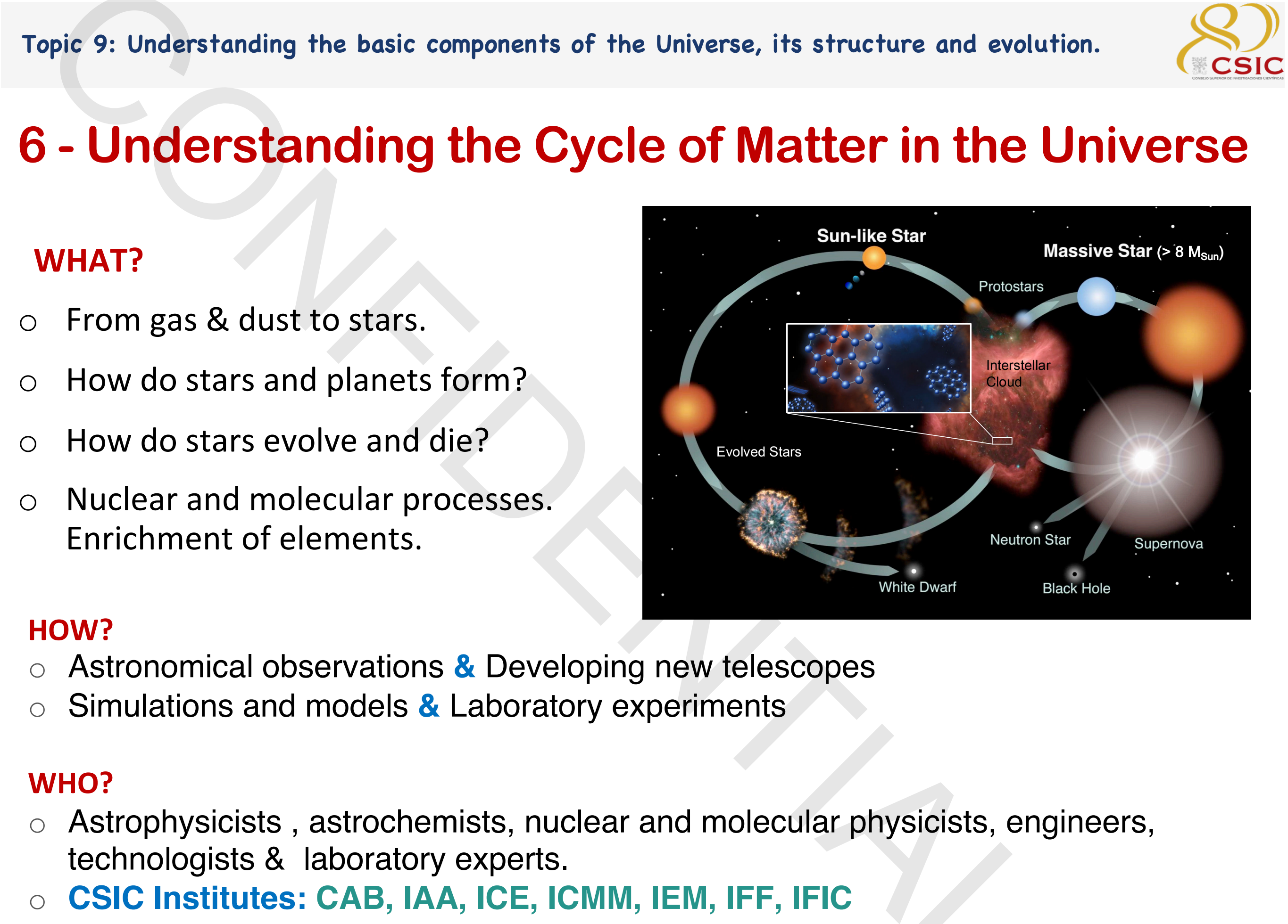
HOW? Multi-disciplinary perspective

- ○ Multi-wavelength astronomical observations & Developing new instrumentation,
- ○ Computational simulations & Laboratory experiments of astrophysical relevance.

WHO?

- ○ Observational astronomers, theoretical astrophysicists, astrochemists, nuclear and molecular quantum physicists, technologists & laboratory experts.
- ○ **CSIC Institutes: CAB, IAA, ICE, ICMM, IEM, IFF, IFIC**

Annex: One slide summary for the general public



Topic 9: Understanding the basic components of the Universe, its structure and evolution.

6 - Understanding the Cycle of Matter in the Universe

WHAT?

- ○ From gas & dust to stars.
- ○ How do stars and planets form?
- ○ How do stars evolve and die?
- ○ Nuclear and molecular processes. Enrichment of elements.

HOW?

- ○ Astronomical observations & Developing new telescopes
- ○ Simulations and models & Laboratory experiments

WHO?

- ○ Astrophysicists , astrochemists, nuclear and molecular physicists, engineers, technologists & laboratory experts.
- ○ **CSIC Institutes: CAB, IAA, ICE, ICMM, IEM, IFF, IFIC**