CHALLENGE 5

IN SEARCH OF LIFE

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1. INTRODUCTION AND STATE-OF-THE-ART

The search for life in the universe and its origin is one of the most fundamental questions of human knowledge and science. The question “When and where the chemical complexity existing on Earth appeared, especially that related to the origin of life” expands now far beyond the Earth and the solar system pushing the human kind for exploring the universe in an unprecedented inter- and multi-disciplinary approach as it will be shown in this chapter.

Solar system objects with many and diverse environments have and have had the possibility to host life nowadays or in their past history. The possible existence of large subsurface liquid water reservoirs in several icy satellites is one of the promising lines of future research in the search of life in the solar system. This search will require multidisciplinary approaches to detect and analyse organic and chemical features as well as morphologic and sedimentary structures that could be related to life. This study crosscuts different research disciplines and technologies.

While the origin of life on Earth is still based on a number of working hypotheses, the search for evidence of life in the solar system is related to the search of the presence of water either on the surface or at the subsurface of the planets, moons and asteroids. This has been the first approach based on our knowledge of life conditions on Earth. Discoveries based on research on Earth environments and life have proven the existence of life in so called "extreme environments". Potential habitable environments in other planets are under conditions similar to some extreme environments on Earth. Therefore, the study of extremophiles and Earth analogues is now and will be in the next decades crucial to assess the possibilities of life in the solar system. Earth's history and extinguished forms of life in the past are also a source of potential scenarios to be considered.

On the other hand, the search for life on exoplanets is mostly limited to finding planets where the conditions on their surface are not too hostile to the delicate equilibriums required to develop complex biochemistry. Still, the parameter space of all possible chemistries of all possible imaginable lives is vast, so for practical reasons the searches are limited to Earth-like life footprints that we can identify remotely. More in particular, the best prospects for remote detection of life on exoplanets are on the detection of combinations of atmospheric species that would not exist in a purely abiotic setup.

The search for extinct and extant life in universe is an ambitious and pluridisciplinary approach that involves expertise in different fields: astrobiology, astrophysics, biophysics, (astro)chemistry, geology, mineralogy, geobiology, paleontology, microbiology, lichenology, phycology, botany, and mycology, among others. Therefore, it happens in three broad areas, namely: Solar System exploration, Exoplanets and their host stars, and Interstellar medium and Astrochemistry. We make a review of the state-of-the-art in these three areas, and then proceed to identify key challenges to be addressed in the next decades.

1.1. Solar System exploration - Mars, Icy Moons and Titan

Chemistry and laboratory experiments have taught us that the basic "biochemical" building blocks of life can be obtained from simple molecules and gases. However, we still don't know how to make informative polymers from them, or how to obtain polymers with catalytic activities. This is one of the widest gaps in the steps for the origin of life. Experimentation, simulation and modelling in the "test tube" is essential. In building macromolecular and supra-macromolecular structures for life, the chirality of the basic elements as well as compartmentalization processes played critical roles. Understanding primitive metabolisms and primitive bio-catalysts will shed light to this still dark part of the origin of life.

The chemistry of meteorites (especially of carbonaceous chondrites) shows a rich composition in amino acids and precursors of nucleobases, and, as the sensitivity and resolution of astrochemical instruments (both in space and on Earth) is improving, newer and more complex molecules are being discovered in the interstellar space. Since the discovery of extremophiles several decades ago, we have learnt how diverse, robust, and versatile can be the biochemistry that allows microbes thriving at the limit, under extreme physicochemical parameters. Microbial life thrives on Earth in all places where there is a minimum water activity. Due to extreme physicochemical parameters (e.g., temperatures from -20 to 113º C, pH ranges from 0 to 12, high salt, high or low pressure) dominating in those places, they can be considered as analogues of current or ancient environments in other planetary bodies in the solar system.

Mars is the first priority in the way of searching for life outside the Earth. The advances on the metabolism of extremophiles together with the somewhat controversial, potential martian microbial fossil in the ALH84001, boosted the planetary science community to retake the exploration of Mars. Several NASA orbiters, landers and rovers together with ESA's orbiters have provided valuable information in the last 20 years. Mars was warmer and wetter than it is today and had liquid oceans, an active magnetic field and a thicker atmosphere by the time (3.5-3.8 billion years ago) life arose on Earth. Given the similarity between the two planets, it seems reasonable to think that whatever steps led to life on Earth could also have occurred on Mars. We assume that life originated on Earth, however, this might not be true or it might have occurred in other planetary environments too. The solar system has offered since its origins a variety of scenarios where, at least a complex prebiotic chemistry might have taken place.

The geophysical study of Mars subsurface (and of any other body of the solar system with a solid surface) where life could be harboured is achieved by indirect geophysical methods from the distance. Subsequent approaches include the installation of geophysical instrumentation on the surface, as has been done already on the Moon and Mars. This surface geological experiments combined with surface seismometers (NASA's Insight mission, in operation) and surface *georadar* techniques, are revealing the internal structure of the planet, and will provide a first exploration of the soil composition at relatively shallow depths (<100m).

Mars is a good example to illustrate how exploration helped to understand the main constraints and conditions for the possibility of life. The first photographs provided by the cameras on Viking landers and orbiters showed that geological features formed on Mars resulted from combinations of internal and external processes. Orbital sensors and robotic analyses of Martian minerals subsequently have identified a variety of water-containing clays, sulfate minerals precipitated from briny solutions, ice in the regolith, and subsurface hydrogen that is presumably water-ice. In rocks and surface materials, extensive hematite (Fe_2O_3) deposits have been identified more recently by the Mars Exploration Rover Opportunity.

The story of Mars exploration illustrates how the process of finding evidence for live in other Solar System sites will also develop. The first surface photographs provided by the cameras on Viking landers and orbiters, showed that geological features formed resulted from combinations of internal and external processes. Orbital sensors and robotic analyses of Martian minerals subsequently identified a variety of water-containing clays, sulphate minerals precipitated from briny solutions, ice in the regolith, and subsurface hydrogen that is presumably stored in abundant water-ice. Very recently, evidence of water in liquid state has been reported using radar observations from orbit using data from ESA's Mars Express.

Icy moons: Several decades of space missions to the outer solar system have proven that there are many moons beyond planet Mars with large volumes of liquid water in their interiors (Prieto-Ballesteros et al., 2019). Europa and Enceladus moons achieve the main requisites of planetary habitability in addition to liquid water: chemical elements essential for life, and available energy to maintain metabolisms. These two ocean worlds have a rocky seafloor, which is probably geologically active, in contact with the liquid water. The interaction between them may provide energy and chemical species to the aqueous solvent. In both there are evidences of endogenous features that connect the ocean and the surface, i.e., the plumes that expose materials on the surface that come from the interior, including the biosignatures of subsurface life, if any. In addition to the rise of materials by this mechanism or other types of cryovolcanism, subduction processes are thought to be occurring on Jupiter's moon Europa, supporting the hypothesis of endogenous dynamics able to recycle chemical elements such as carbon or sulfur. Considering the terrestrial life case, chemolitotrophic metabolisms, and a very low biomass of cells affected by extreme physico-chemical parameters like the acidity or the redox state are expected in this deep environment. So far, the best terrestrial analogues considered to better understand the geochemistry and the habitability of these dark hypothetical niches are: aphotic systems where serpentinization or other type of aqueous-rock interaction occur, deep cold brines, and subglacial liquid-water environments.

The Saturn moon Titan, on the other hand, possesses a large inventory of organic molecules at different physical state on the surface but not evidence of a link between the surface and its deep ocean. Titan is a target to studying the prebiotic chemistry and the origin of life, offering an organic alternative to the liquid water to act as the solvent that supports life. Indeed, it is predicted that if life emerges in Titan, it would be different than the one we know on Earth.

1.2. Exoplanets and their host stars

The search, characterization and study of exoplanets is a prominent branch of the search for life beyond Earth in nowadays science. Among them, those with bulk properties like our own world are the ones with higher astrobiology interest. Currently, we have the capabilities to detect planets sharing some properties with Earth —especially around stars smaller than the Sun, or red dwarfs—, but no true Earth analogue has been identified yet. Also, the information that we can learn from exoplanets is much more limited than the one we can obtain from Solar System bodies. Essentially, and in the most favourable scenarios, we can measure the masses and sizes of these planets, and we will be able to infer whether they have atmospheres and identify the presence of key molecules in some of them.

The discovery of the hot Jupiter 51 Peg b by Mayor and Queloz (1995) (Nobel prize in Physics in 2019) is considered the kick-off of *modern* exoplanet science. At the current time today, there are about 4000+ exoplanet candidates listed (http://exoplanets.eu). About 1000 of them have been found using the radial velocity technique, and about 3000 by using the transit method using ground-based surveys (such as super-WASP) and space-based surveys (like NASA's Kepler mission, Borucki et al. 2010).

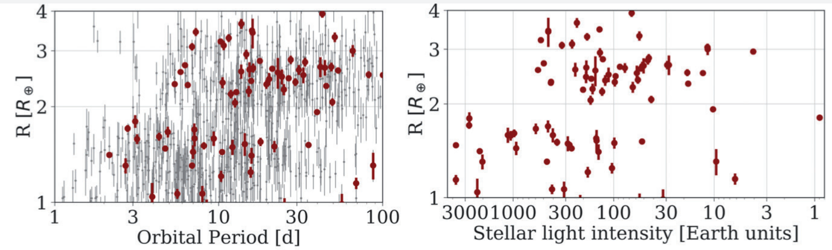
In the meantime, the direct imaging method has also been developing but remains mostly usable to self-luminous giant planets around young stars (ages below 30 Myr) as it entails major technological challenges. Other methods such as microlensing and astrometry have yielded smaller numbers (few tens) but they probe different areas of the parameter space. The niche case of long period gas giants is likely to dramatically change with the final data release of the Gaia/ESA astrometry mission by >2022 when thousands of new giant exoplanet detections are likely to be reported using astrometry. Concerning the detection of planets more like Earth, the two leading techniques (photometry and radial velocities) remain as the most likely ones to lead the discoveries in the next decade. These two methods are also yielding the detections of exoplanets that are likely to be characterized more in detail.

Planetary interiors and geological composition are also important for habitability. Not only the surface, atmosphere, and interactions between both play an important role to define an exoplanet as habitable. Firstly, there are aspects of planetary interiors such as the need for plate tectonics which continuously recirculate material thus maintaining a rich dynamic chemistry, and aspects related to the presence of a liquid mantle resulting in a powerful quasi dipolar magnetic field protecting the atmosphere and surface from harmful high energy radiation and particles (stellar and galactic). Secondly, there must be a strong dependence of the atmosphere to the initial planetary composition. The range of water content on exoplanets is expected to cover the range between less than a thousandth as on Earth to the several percent found in the icy moons of the Solar System. For example, in planetary systems that are more carbon rich, most of the oxides will be in the form of CO_2 gas forming thick atmospheres, while in others like in the Solar System most of the oxygen is likely to be bound to Silicon (SiO_2) and other metals, which is a solid (quartz). This kind of considerations make important differences that need to be addressed from an interdisciplinary approach.

In summary, there is substantial landscape to be explored on theoretical grounds that will mostly be needed to interpret near future exoplanet observations. This is needed to both help interpretation of atmospheric chemistries that shall be obtained soon and anticipate possible non-Earth like habitable conditions to guide searches with new planned facilities.

Our knowledge of the host stars, i.e the physical parameters as mass and radius, is fundamental for determining the exoplanet characteristics. An obvious example is that the stellar radius is needed to good precision (better than few %) to produce reliable size estimates for transiting exoplanets. Also, dating the star is the only way to determine the age of exoplanets and its potential life harbouring capabilities. Several methods can be used, depending on the available data. But in the last decade, particularly with the Kepler mission

FIGURE 1—Planet radii vs orbital period (left panel). Red symbols show exoplanets with radii determined from asteroseismically measured stellar radii. Grey symbols are based on spectroscopic and astrometric (Gaia) data. Right panel shows radii as a function of stellar irradiation received by planets. The radius valley around 2 Earth radii is apparent in the data.



(NASA), asteroseismology has emerged as the tool best suited to accomplish this task. In combination with astrometric data from Gaia, it has now become possible to determine stellar masses and radii for exoplanet host stars with precisions of just 2 or 3% (Serenelli et al. 2017) with comparable accuracy (Zinn et al. 2019), and ages to about 10%.

The quality of the asteroseismic results has opened the path for precision exoplanet science. An example is shown in Fig.1, which confirms the existence of the theoretically predicted radius valley in rocky planets due to the loss of the planet atmosphere induced by the stellar irradiation (Van Eylen et al. 2018). Analogously, the combination of precise exoplanets masses and radii allow tests of mass-radius theoretical relations.

With very good asteroseismic data, it is also possible to determine the angle between the star's rotation angle with respect to the observer by measuring the relative amplitude of the components of dipole triplets, enabling the characterization of the orbital-stellar spin axis alignment. The next big revolution in asteroseismology will happen with the launch of PLATO, in 2026, the ESA M3 mission for exoplanet and stellar characterization. PLATO is the first mission that, by design, will incorporate asteroseismic analysis as part of its standard pipeline. It will observe tens of thousands of stars as part of its core program dedicated to characterization of the exoplanet-host star (FGKM) system. CSIC has a strong participation in the preparation of PLATO and its exoplanet and stellar science programs through several institutes.

Stellar non-thermal emission is dictated primarily by the activity level of a star. This is ultimately related to the presence, strength, and topology of magnetic fields on the star which, in turn, are the interplay of timescales of stellar convection and stellar rotation. Characterization of non-thermal radiation can be done, for example, by observations in radio, in extreme UV and X-rays. Low mass stars —which are the targets where terrestrial planets can be found more easily— retain high levels of activity for much longer than more massive stars, and it is likely to have a strong impact on habitability conditions for such red-dwarf planets. The habitability condition of exoplanet atmospheres needs to consider the past evolution of the star to the current day. A deeper understanding of the non-thermal radiation requires the development of simulations of magnetic field generation in stars, which is a very underdeveloped field. Probably the best example is the —yet unsolved— paradox of the faint young Sun according to which the young Earth had to be in a snowball state, contrary to what fossil and geological evidence show.

Planetary magnetic fields are also key elements in understanding the evolution and state of planetary atmospheres. Despite our incomplete understanding of Earth's magnetic field long-term behaviour, we know that its uninterrupted presence, detectable by paleomagnetism during the last 3.5 Gyr at least has been and still is a fundamental piece in the biosphere. Planetary magnetic fields provide shielding against cosmic rays and solar wind and (at the very least) is essential to provide a safe harbour to current Earth life. The key factors that allow a long-living magnetic field on terrestrial planets need to be identified in order to assess the best Earth-like candidates. One requisite is arguably the presence of strong heat fluxes, which could maintain a long-lived dynamo, so that long-thermal magneto-thermal evolutions, considering the thermal-magnetic interactions, could shed light on this issue. However, the main problem is that terrestrial planets are intrinsically more difficult to detect, and so are the signals of their magnetic fields: it is unlikely to detect radio emission from Earth-like planets or infer their inner structure in the foreseeable future. Radio emission from magnetic exoplanets has been proposed long ago, in analogy with Jupiter, known since 1955 to be the major planetary source of radio signals below 40 MHz. The observed auroral emission is thought to come from the cyclotron-maser instability and depends on the magnetospheric interaction with the Solar wind and/or the planetary rotation. Since many M-dwarf stars have large magnetic fields, it is possible that the interaction between the host star and the exoplanet may yield measurable radio emission at significantly larger frequencies, where current and future radio interferometers, e.g., the SKA, may crucially contribute. Auroral radio emission, in the last two decades at least, has been proposed as one of the most interesting possible exoplanetary observables.

Star formation and the study of protoplanetary disks is another topic closely related to the origin of life as it includes the processes transporting matter from the interstellar medium to the planets. In the past two decades, there have been significant advancements in both observational and theoretical arenas. A theoretical understanding of the growth and migration of solids in gas-rich protoplanetary disks is emerging from advanced numerical modelling of high-resolution dust observations with long-baseline radio interferometers such as ALMA. General model predictions are qualitatively sound, but quantitative estimates of dust evolution timescales are hampered by simplistic assumptions about gas small-scale substructure (Andrews and Birnstiel, 2018). Dust coagulation barriers at centimetre scale are surmounted by pebble traps and gravitational collapse of pebble clouds (Blum, 2018) which are generated by instability mechanisms consistent with the formation of large-scale structures observed in disks around young stars. As planetesimals start to form they also collide and grow to larger objects, with further help of turbulence. Additionally, accretion of pebbles from the disk may facilitate the formation of planetary embryos. These then may migrate, with the outcome (outwards or inwards migration) depending on the viscous properties of the disk (Nelson, 2018)

In terms of finding evidence of intelligent life, Drake's equation could be updated by the addition of one term quantifying our ability to detect and identify (intelligent?) life as such. To quantify this term, one would need to examine more broadly the parameter space search in dimensions what we might not even consider. In these searches, the general strategy is looking for features are not commonly shared by the rest of the observed sample or by our theoretical expectations. Given that radio is the most energy efficient way to transmit information over long distances, the mainstream branch of these *Searches for Extraterrestrial Intelligence* (or SETI, see Tarter 2001) consists of scanning stars for anomalous radio emission. Along these lines, there are several initiatives (mostly privately funded) that have been operating for some decades now. Other SETI approaches consist in searching from excesses of infrared radiation from stars (and even galaxies), which could be indicative of civilizations operating at star-system (or galaxy) level from space (infrared radiation would be the waste product of such activity). In summary, and despite the fringe nature of the field, SETI searches is an active research. These programmes are also very popular and their use to engage the public into scientific discussion should not be underappreciated.

1.3. Interstellar Medium and Astrochemistry

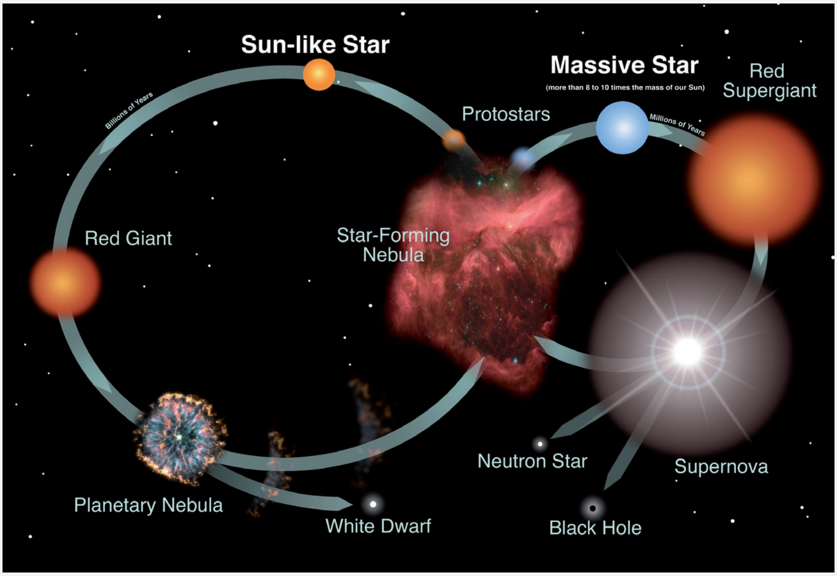
The life cycle of molecules in the interstellar medium (ISM) begins in stars. Most chemical elements are transported and created there by stellar winds and (sometimes) by supernova explosions and its aftershocks. The material dispersed from these processes forms diffuse clouds that eventually coalesce into denser dark (also called dense or molecular) clouds, where new stars and solar systems are formed, ready for the next cycle (see Figure 2)

While molecular complexity builds up at each stage of the Sun-like star formation process (Caselli and Ceccarelli, 2012), it is unclear whether the building blocks of life (i.e., prebiotic species) are inherited from the dense and cold molecular core material prior to the Sun's formation; or they are products of the different physical processes undergoing within the solar nebula protoplanetary disk. On the other hand, it is well known that massive and low-mass protostars undergo the so-called hot core/corino phase, with T~100-200K, that displays a very rich chemistry in interstellar complex organic molecules (iCOMs) because of the evaporation of ices from dust grain mantles. This raises the question of what happens to prebiotic species during the next evolutionary stage.

We know that there are many polyatomic molecules in the ISM. Contrary to early beliefs, the diffuse ISM is chemically rich, albeit dilute. Many ion-molecule reactions and radiative association processes proceed without energy barriers and are important mechanisms of molecule formation in the ISM. Since the first detection of molecules in space in the late 30 's, currently around 200 molecules have been discovered in space thanks to the advent of radio astronomy (see Cologne Database for Molecular Spectroscopy, CDMS), indicative of the rich chemical complexity of ISM. A very significant part of unidentified lines in survey spectra of dense clouds are certainly due to vibrationally excited states and/or isotopologues of COMs and molecules with low-lying vibrational states and/or large amplitude can give raise to hundreds of lines, many of them not yet identified in the laboratory.

The search for prebiotic species in the ISM has been a huge effort over the last few years. Key species for the development of life of increasing complexity, such as formic acid (HCOOH), glycolaldehyde ($HOCH_2CHO$), amino

FIGURE 2—Diagram illustrating the life cycles of Sun-like and massive stars. (Credit: NASA and the Night Sky Network)



acetonitrile (NH_2CH_2CN), formamide (NH_2CHO), urea (NH_2CONH_2) or phosphorus-bearing species (PN and PO) have also been detected in massive star-forming regions and in Solar-type systems, mainly in the so-called hot core/hot corino phase (e.g., Fuente et al. 2014, Rivilla et al. 2020). Cold chemistry on ice surfaces, and the processing of ices and dust grains by shocks and radiation are thought to be largely responsible for the COM production.

There is a number of key molecules that are subject to intensive research in relation to the origin of life. One of them is glycine (NH_2CH_2COOH), which is the simplest amino acid that plays a role in the synthesis of proteins in known living organisms. Although it has not been detected in the ISM (yet), glycine and other simple amino acids have been found in meteorites and comets Regarding the phosphorus-bearing molecules, phosphorus (P) is a crucial chemical biogenic element for the development of life (Maciá, 2005) as it is one of the key components of deoxyribonucleic acid (DNA) and ribonucleic acid (RNA), phospholipids (the structural components of all cellular membranes) and the adenosine triphosphate (ATP) molecule, which transports chemical energy within cells (Pasek and Lauretta, 2005). Therefore, phosphorus plays a vital role in three essential aspects (replication, structure, and energy transfer), and it could also be fundamental for life in other planets besides Earth. Phosphorus is thought to be synthesized in massive stars and injected into the ISM by supernova explosions. As shown by Jiménez-Serra et al (2018), PN and PO molecules can be formed in quiescent and cold gas, although it remains undetected toward solar-type system precursors.

The delivery process of chemically complex material into planets and their survival through the protoplanetary phase remains unclear. However, comparisons of the C, N, O isotopic fractionation in the ISM and meteorites or pre-solar dust grains suggest that, at least, some material of interstellar origin has been delivered to Earth.

The study of pristine meteorites, like e.g., the carbonaceous chondrites, provides additional insight on the delivery of water (Trigo et al., 2019) and organics to the early Earth. Some of these meteorites have preserved ancient chemistry clues in the interior of their fine-grained matrixes and are also a source of valuable information studying other high temperature produced components like e.g. chondrules, refractory inclusions, clay minerals, etc... Carbonaceous chondrites retained water as hydrous minerals and organics in the fine-grained matrix that compacted the rest of chondritic components during the consolidation of these rocks. The organic compounds arrived in these meteorites are not so simple, as they include amino-acids, nucleobases, etc.

2. KEY CHALLENGES

2.1 Solar System exploration

Understanding the chemistry in different bodies ranging from planetesimals to icy worlds is important. For example, what is the minimum size to generate heat and stable liquid water? What is the role of salts? And radiation? How many different scenarios for the origin of life could have been created? How feasible could have been a second genesis of life elsewhere in the Solar System? Understanding the biochemistry and the biodiversity under such extremes is one of the major challenges of microbiology and molecular biology.

The exploration about the interior, surface, atmosphere, and interaction with the interplanetary medium faces many open questions nowadays for every rocky planet with a gaseous envelope. For instance, what is the current climate on Mars and how has it changed along its history? How wet and hot was the early Mars 3.8-3.5 Ma? Did life have the chance to thrive on early Mars? Is it there still today? What fingerprints did it leave? What lessons can we learn from terrestrial analogue environments? To address these questions new investigations and instrumentation must be developed.

In the 50 's of the 21st century, it is foreseen the samples from Mars will be brought to Earth. To achieve this, technological challenges and planetary protection protocols must be established. Whether in-situ robotic exploration on the surface on Mars or through a Mars sample return, the CSIC can (and must) be an active part of this exciting chapter of science and human knowledge.

Liquid water is essential to Earth-like life, but this liquid water must have a minimum of physical-chemical conditions for supporting the development of physiological processes. These physicochemical minima are not well understood, requiring a considerable multi/inter-disciplinary effort to decipher them. The sensitivity of astrobiology-dedicated instruments must be high enough to guarantee the detection of a limited number of cell-like morphologies as well as low concentrations of biomolecules. Besides, studies on terrestrial analogues deploying instrument suites are critical to better understand what kind of morphological and biochemical diversity could be expected on other planets and moons of the solar system.

Plans of future biological exploration of ocean worlds (i.e., the icy moons at the outer Solar system) consider successive steps that advance by accessing the plume materials, exploring the subsurface by drilling the icy crust, and even bringing materials back to Earth for analysis. Underwater exploration would include reaching the seafloor where organisms could potentially concentrate around foci of hydrothermal activity. Drilling in the subsurface of any Solar System body different from the Earth will be the forthcoming challenge for the in-situ exploration searching for life (also on Mars). First attempts to drill within the regolith in Mars revealed the technological difficulties, and the needs for improved specific drilling equipment adapted to the actual geology and conditions at each target based on preliminary assessment by geophysical methods. Seismic sensors were deployed on Mars and have detected ongoing seismic activity (Giardini et al., 2020) are likely related to active geologic processes in the subsurface.

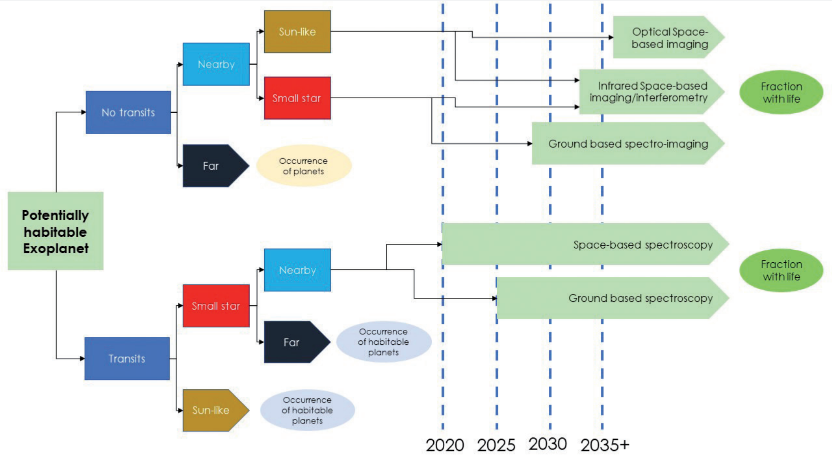
Data obtained by the Lunar Penetrating Radar have revealed a layered structure of the first 40 m section of the lunar subsurface (Li et al., 2020). These results indicate the presence of granular and porous rocks and outlines a layered structure of rock bodies underlying the 12m thick regolith on the Moon. Also, the internal textural properties consist of heterometric boulders embedded in finer grain granular material. This can be considered one of the first and successful exploration achievements and first results of exploration using conventional techniques developed and used on the Earth as *ground penetrating radar*. Following these advances in drilling, new downhole logging, sampling, and monitoring instrumentation will be necessary to extract new information, samples, and data.

2.2. Exoplanets and their host stars

Radial velocities and transits are, and will likely remain, the two most relevant techniques in the discovery of terrestrial exoplanets in the liquid-water habitable zone of stars. While Doppler spectroscopy can efficiently be done from the ground, transit searches are now being executed by space-photometry missions (like NASA's Kepler & TESS, and ESA's CHEOPS and PLATO). In addition, the traditional separation between Doppler spectrometry surveys and transit planet searches is blurring, as transit missions combined with coordinated ground-based spectroscopy follow-up are becoming an efficient way to nail down the most valuable planets for characterization. A scheme of the observational roadmap towards detection and characterization potentially habitable exoplanets for the next decades is shown in Figure 3.

In terms of radial velocity measurements, there are numerous visible and near-infrared high-resolution spectrometers from many countries (incl. Spain) at various stages of development, to the extent that it is difficult to keep track. Europe has had a clear leadership in this arena since the beginning. In the European landscape, several facilities in operation demonstrated ~1 m/s level precision on a sizeable sample of targets like HARPS (ESO), HARPS-N (Italy and others, incl. Spain), CARMENES (Spain + Germany) and ESPRESSO (ESO), the latter having reached precisions of tens of cm/s and thus allowing, in principle, for the detection of true Earth twins. Operational facilities outside Europe include HIRES at the Keck-1 telescope, APF at Lick Observatory, PFS at Las Campanas/Magellan-II, IRD at the Subaru Telescope, MINERVA-Australis, EXPRES at the 4.2-m Discovery Channel Telescope, Veloce and Veloce Rosso at the AAT, NEID just to mention the most relevant ones. It is also becoming clear that the gain to expand into the infrared is modest because of the diminished radial velocity content, and therefore the optical and far-red appear sufficient to reach down to

FIGURE 3–Decision tree for exoplanet detection and expected methodologies to become relevant in terms of characterization in the next two decades.



planetary close to the substellar domain boundary. To achieve the necessary long-term precision and stability in Doppler spectroscopy, ultraprecise devices such as Laser Frequency Combs has been developed and adapted to astronomical applications. Hardware innovation and filtering techniques based on Fabry-Perot interferometers, fibres, etc., are needed to overcome difficulties in terms of optimal spectral line densities and secure long-term (year scale) stability.

Regarding characterization, the most immediate big leap in exoplanet characterization is likely to happen on small transiting exoplanets around red dwarf stars observed with space observatories like the Hubble Space Telescope, JWST/NASA (launch planned in fall 2021), and possibly with ESA's Ariel mission (>2026). The same spectrometers used in precision radial velocity searches are also being used for atmospheric characterization, so investing on their development is also an investment in future relevant research. In the future (e.g. ESO's E-ELT instrumentation), the combination of adaptive optics with high-resolution spectroscopy could reach sufficient contrast (10^9-10^{10}) to allow for the measurement of atmospheric components of planets in the habitable zone of nearby stars. **High contrast large missions from space** for direct imaging of exoplanets in the optical and infrared are also being planned in the timeframe of 2030+, including the LIFE project (Quanz et al. 2019, mid-infrared interferometry, ESA context) and LUVOIR (Snellen et al. 2019, optical imaging, US/NASA + ESA context). It is key that CSIC keeps involvement in the international consortia being organized around these concepts.

Experiment and theory to obtain molecular opacities at the high temperatures of most known exoplanets are needed: laboratory observations at high spectral resolution test and validate the more extensive calculated line lists and can lead to improvements in the calculated line lists by empirical adjustment of the potential energy and dipole surfaces used in the calculations. It must be noted however, that the calculated line lists are far less accurate regarding line positions, while they can be more reliable regarding line strengths. Line positions should be validated in the extreme ranges of quantum numbers and temperatures. Data are needed for pressure-induced (collisional) effects: broadening coefficients for perturbers other than N_2 and O_2, as for example, H_2, CO_2, H_2O, CH_4, in broad temperature (70-2000 K) and pressure (up to 100 bar) ranges, way beyond HITRAN's (the most widely spread database for molecular line lists) coverage. This information is currently very scarce and encompasses a huge laboratory effort that may take decades to complete. Collision Induced Absorption (CIA, i.e., absorption through normally forbidden transitions induced by transient dipole moments occurring under frequent collisions), has been mainly studied for N_2 and O_2 under conditions relevant to Earth's atmosphere, and it should be extended to absorptions induced in H_2, N_2, CO_2, O_2 by collisions with relevant background gases in general exoplanetary environments such as H_2, He, N_2, CO_2, O_2, H_2O, CH_4, CO and NH_3. Even in the case of temperate atmospheres, since information about exoplanets atmospheric properties comes from interpretation of their spectra, efforts like the ExoMol computed line lists (Tennyson et al. 2016) are being developed.

Experimental and theoretical efforts in gas collision rates and their effects are also needed. JWST will likely produce a large amount of data in the near to mid-IR on the atmospheres of exoplanets (mostly hot planets, a handful of temperate ones). The spectral retrieval codes used in the interpretation of the observations need collision rates as input to cope with the far from equilibrium conditions in the outer layers of the atmospheres. Despite of their great importance, they are difficult to obtain experimentally, difficult to calculate and they are often neglected resulting in extrapolations to conditions too far from the experimental ones and scaling laws not fully validated. Experimental groups at CSICs IEM and theoretical experts at CSICs IFF have developed strategies to accurately measure or validate state to state rates in H_2:H_2, H_2O:He, N_2:N_2, and other relevant molecules. Efforts are currently underway to extend these measurements to higher temperatures.

Chemistry and atmospheric dynamics are often coupled, and therefore including chemistry in General Circulation Models is key for future characterization of exoplanets. Atmospheres targeted for transit are typically hot (500 K – 2500 K), with UV photochemistry influencing their disequilibrium chemistry. Room temperature photo-absorption cross-sections usually underestimate exoplanet UV photo-absorption and photo-dissociation rates. Thus, high temperature UV photo-absorption cross sections of key species such as CO_2, CO, CH_4 and H_2O are required (see e.g. Venot et al., 2018). Similarly, reaction rate constants for conditions not found on modern Earth (high and low temperatures, reducing atmospheres) are poorly constrained. There is a lack of data for reactions of elements other than C, H, O and N, some of them biologically important elements such as P and S. Data for heavier organic molecules and ions are also lacking. It is also important to obtain reaction rates for key species by exposing them simultaneously to VUV photons. While the supersonic expansion technique enables wall-less experiments in the very low temperature range (see Douglas et al., 2018; Ocaña et al., 2019), laboratory measurements of absorption cross sections and reaction rate constants at high temperatures are experimentally challenging and require substantial engineering and support.

Computational models should be used to expand the range of pressure and temperature covered by laboratory experiments also to include interactions between gas and solid phases. In-house expertise in computation of *ab-initio* spectra and photochemistry exists at several institutes of the CSIC. Hazes play central roles in the dynamics, radiative transfer, and chemistry of planetary atmospheres. Understanding formation chemistry and thermal stability of photochemical hazes is essential to interpret future spectroscopic data (Madhusudhan, 2019). This requires new advances in ion-neutral chemistry, gas-to-particle conversion, particle growth and loss rates, chemical and thermal stabilities of particles and coupled volatile-refractory chemistry under UV irradiation. The chemical coupling of CHON elements and more refractive elements such as S, P, Na, Si, Mg, Fe, etc. can generate particles whose properties are poorly known. Refractory condensates formed in high temperature atmospheres (500 K — 2000 K; 10^{-3} — 10 bar), such as magnesium silicates or iron are also poorly understood. There are essentially no laboratory experiments of grain growth under relevant exoplanet conditions: vapor pressures of refractory materials are needed to estimate formation of condensate clouds, and data is required to infer gas-to-particle conversion pathways and obtain surface reaction rates, for a wide range of conditions including temperature, pressure, metallicity, etc. There are suitable facilities at CSIC to study physical and chemical properties of hazes and aerosols. However, some engineering challenges will have to be addressed, including e.g., in-situ measurements of ice particles. Progress in this field can benefit from synergies among different existing laboratories within CSIC.

In terms of models for biosignatures, approaches in search for features related to life are based on the study of the photometric, spectroscopic and/or polarimetric properties of potentially habitable worlds. Schwieterman et al. (2018) classify features potentially useful to infer the presence of living processes into three broad categories: gaseous, surface, and temporal biosignatures. All of them are inevitably based on our knowledge of life on Earth, so substantial work needs to be done to extrapolate them outside Earth conditions. Typical surface biosignatures refer to vegetation and, together with atmospheric O_2, surface reflectance of vegetation is one of the most robust planetary scale biosignatures. The models to anticipate these signatures are based on identifying the metabolic process where light is transformed into chemical energy and used to drive biosynthesis of organic matter from CO_2. Pigments are a key component of that process and remotely detecting their spectral signature at 690-740 nm (red edge region) would allow speculating on expressions of life these worlds. However, new chlorophylls absorbing in different areas of the spectrum as well as other pigments should be also investigated, such as carotene and xanthophyll that are also structural elements of the photosynthetic apparatus related with photo-protection presenting distinctive absorption features. Models designed to understand light interaction with vegetation, can relate to other Radiative Transfer Models already available to simulate the planet's atmosphere and rock/soil background. This way we can add potential confounding factors to the planetary-scale surface biosignature so the spectral signal detected by ongoing or future space-based and ground-based missions could be interpreted with respect to environmental context.

Concerning the identification of biosignatures, there is a doubtless convergence between Earth and Space observation, including the study of chlorophyll fluorescence or sun induced fluorescence (SIF), a fast-responding regulatory mechanism that helps keeping the energy balance of the light-absorbing complexes (plant photosystems). For example, Chlorophyll exhibits SIF emission spectrum in the red and near-infrared regions characterized by two peaks at approximately 685 nm (red region) and 740 nm (far-red region) which are already used on Earth observation methods and can be searched during the spectroscopic characterization of exoplanets.

Magnetic fields in exoplanets (as well as in the solar system planets) are crucial to protect the planet of the harmful environment and could prevent the development and long-term survival of superficial life. Their detection can only come after the detection of the planets themselves, something that currently is happening at a steady pace. The expectation is that with current facilities we should be able to start detecting magnetic fields of hot giant planets, and slowly move towards detecting similar effects in smaller and more habitable ones. One key observational ingredient to discriminate between stellar and planetary emission is the polarized emission as for the exoplanet-star system will be generally unresolved. Cyclotron maser instability radiation is strongly circularly/ elliptically polarized and beamed anisotropically whereas stellar plasma radiation is basically unpolarized. Therefore, measurements at low frequencies (<=3 GHz) with circular or full *Stokes* polarization observations with the new era of low-frequency radio telescopes will represent a significant leap forward in the field.

2.3. Interstellar medium and Astrochemistry

The advent of the current centimetre and millimetre instrumentation opened the possibility to detect many species of biochemical interest in several astrophysical environments. The cutting-edge of radio interferometers such as Square Kilometre Array (see review on the topic in Acosta-Pulido et al. 2015) soon will open a new window to perform high-sensitivity molecular line observations toward the earliest stages of star formation pre-stellar cores on the verge of gravitational collapse. Data to be acquired with SKA, James Webb Space Telescope, Extremely Large Telescopes (ESO and others), etc., need more complete databases for rotational spectroscopy. To this end, increased efforts in developing sophisticated experiments to prepare and study highly reactive species (molecular ions, radicals), sensitive detection techniques, trained personnel and long-time commitment are needed.

The interpretation of the observations relies on laboratory experiments, simulations, and theoretical calculations, providing information about the respective astrophysical environments of gas, dust, and ices. The success of astrophysics is bonded to the development of Laboratory Astrophysics, and, specially, of spectroscopic techniques, to enable the full exploitation of the observational resources. Line frequencies, cross sections, and collisional data, rate coefficients of many chemical reactions over a large range of conditions (phase, temperature, pressure), *ab-initio* calculations of energy levels and spectra, and reaction rates and collision theories are needed. Many of these laboratory studies, experiments and computer models are similar (or made by the same groups) as those discussed in the previous section so they will not be repeated here for briefness.

It is the entanglement of astrophysics and spectroscopy what has led to the identification of more than 200 molecular species in the ISM. The study of exoplanet atmospheres is revealing their most abundant constituents, including water, and, of course, our own solar system has shown evidence of complex molecules in many objects beyond Earth. Paraphrasing the Nobel laureate *Harry Kroto*, a natural question arises: "*Where molecules are, can life be far behind?*"

As a closing remark, we want to highlight that the *search for life beyond Earth* is a hot and rapidly expanding topic, and it is likely to be one of the main driving forces shaping near and long-term instrumentation, international collaborations, and missions. CSIC has numerous teams working on different aspects of this endeavour. Maintaining leadership will require support and possible expansion to keep up at the cutting edge of this exciting field.

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