CAB Annual Report 2021

Memoria Anual

CENTRO DE ASTROBIOLOGÍA · CAB

ASOCIADO AL NASA ASTROBIOLOGY PROGRAM

EXCELENCIA MARÍA DE MAEZTU

CSIC Consejo Superior de Investigaciones Científicas

INTA

Centro de Astrobiología (CSIC-INTA)

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Portada: MEDA en Marte.

Conjunto de antenas de ALMA, el proyecto de astronomía más grande que existe, ubicado en la meseta de Chajnantor en los Andes chilenos. © Clem y Adri Bacri-Normier (wingsforscience.com) / ESO

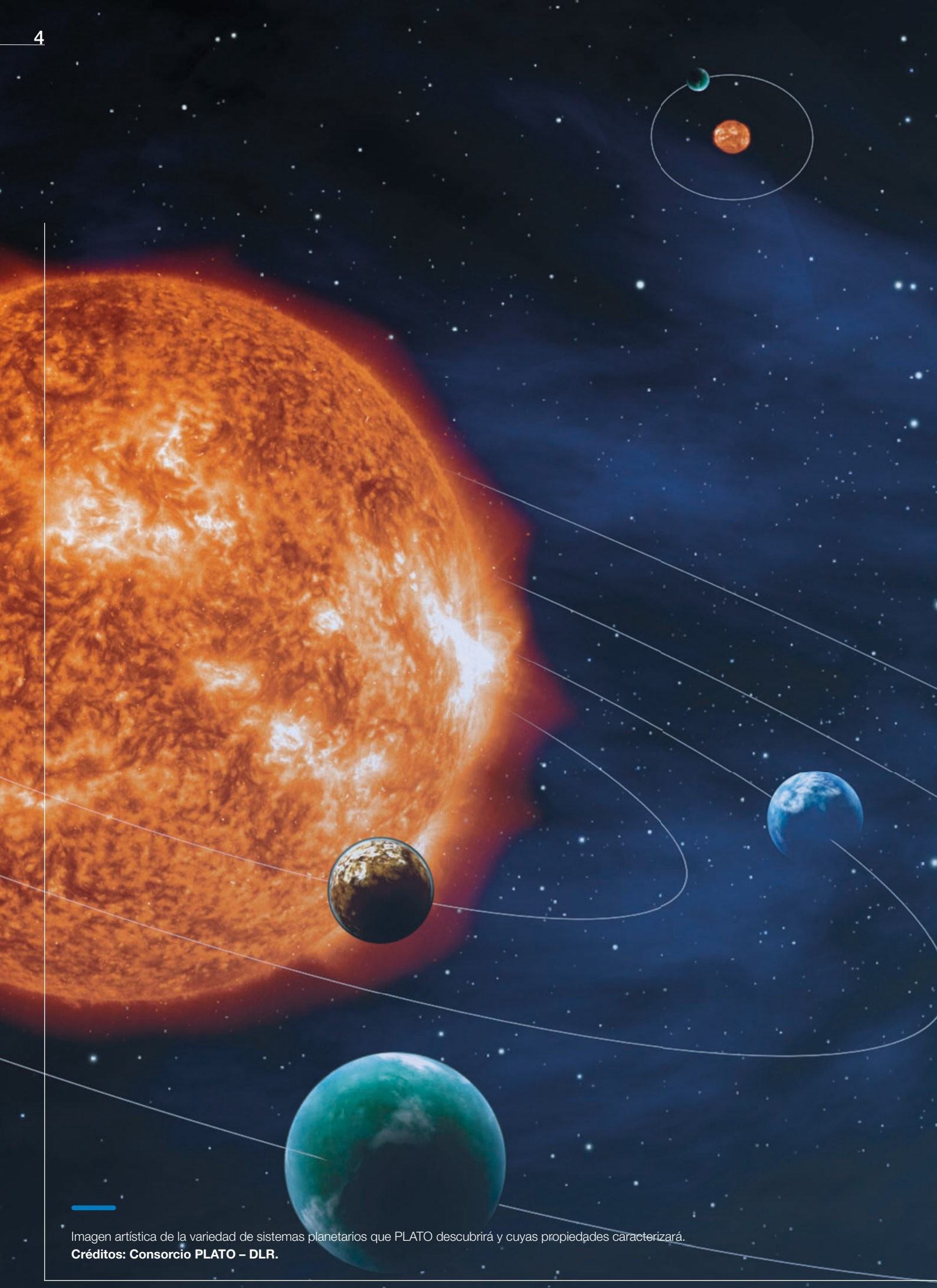

Imagen artística de la variedad de sistemas planetarios que PLATO descubrirá y cuyas propiedades caracterizará.
Créditos: Consorcio PLATO – DLR.

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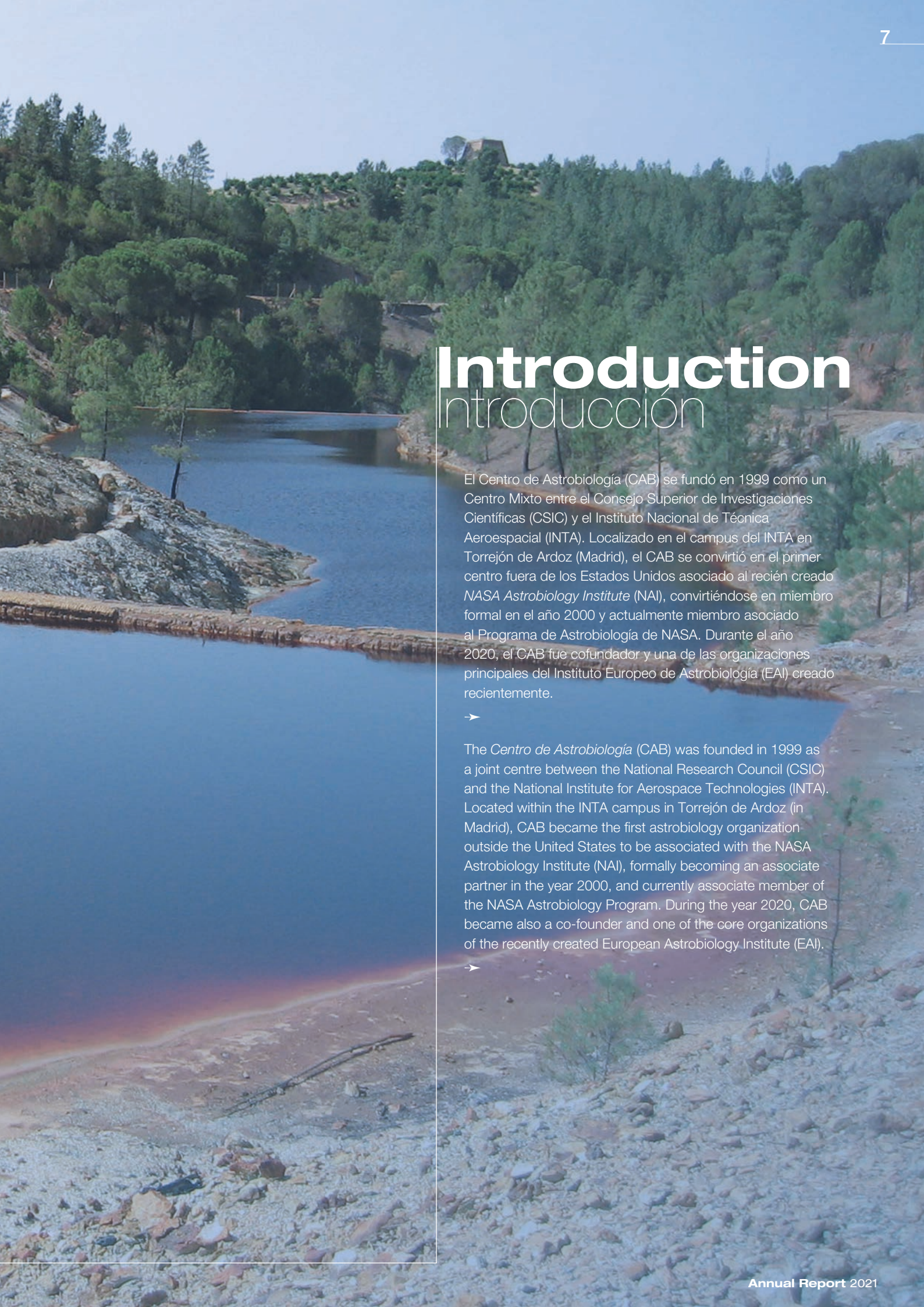
Imagen del río Tinto. **Crédito: CAB**



Introduction
Introducción

El Centro de Astrobiología (CAB) se fundó en 1999 como un Centro Mixto entre el Consejo Superior de Investigaciones Científicas (CSIC) y el Instituto Nacional de Técnica Aeroespacial (INTA). Localizado en el campus del INTA en Torrejón de Ardoz (Madrid), el CAB se convirtió en el primer centro fuera de los Estados Unidos asociado al recién creado *NASA Astrobiology Institute* (NAI), convirtiéndose en miembro formal en el año 2000 y actualmente miembro asociado al Programa de Astrobiología de NASA. Durante el año 2020, el CAB fue cofundador y una de las organizaciones principales del Instituto Europeo de Astrobiología (EAI) creado recientemente.

The *Centro de Astrobiología* (CAB) was founded in 1999 as a joint centre between the National Research Council (CSIC) and the National Institute for Aerospace Technologies (INTA). Located within the INTA campus in Torrejón de Ardoz (in Madrid), CAB became the first astrobiology organization outside the United States to be associated with the NASA Astrobiology Institute (NAI), formally becoming an associate partner in the year 2000, and currently associate member of the NASA Astrobiology Program. During the year 2020, CAB became also a co-founder and one of the core organizations of the recently created European Astrobiology Institute (EAI).

La astrobiología considera la vida como una consecuencia natural de la evolución del Universo, y el CAB tiene como objetivo estudiar el origen, evolución, distribución y futuro de la vida en el Universo, a través de investigaciones en la Tierra y en ambientes extraterrestres. Muchos pasos aún son desconocidos o poco comprendidos en esa sucesión de eventos y se requiere de un gran esfuerzo interdisciplinar para estudiar el único caso de vida que conocemos. En el CAB nos enfocamos principalmente en lo que consideramos los aspectos más críticos. Por ello, nuestros objetivos científicos de alto nivel son:

- **Objetivo 1:** Caracterizar los componentes básicos del Universo: Formación y evolución de galaxias y estrellas a través del tiempo cósmico.
- **Objetivo 2:** Comprender el ciclo de los elementos químicos: Del medio interestelar a las estrellas y planetas.
- **Objetivo 3:** Estudiar entornos planetarios potencialmente habitables.
- **Objetivo 4:** Identificar y analizar biomarcadores para la búsqueda de vida en ambientes planetarios.
- **Objetivo 5:** Comprender los principios básicos de la vida en ambientes planetarios, su evolución temprana y adaptabilidad a condiciones diversas y a menudo extremas.
- **Objetivo 6:** Desarrollar métodos e instrumentación avanzada para la exploración y caracterización in situ y remota de objetos cósmicos.

Durante 2021, el CAB ha mantenido una actividad de gran calidad y muy productiva. A destacar, por ejemplo, la llegada a Marte el 18 de febrero del instrumento MEDA (*Mars Environmental Dynamics Analyzer*) liderado por el CAB, uno de los instrumentos fundamentales de la misión Mars2020 de NASA. MEDA es una compleja red de sensores medioambientales, que empezaron a ser operativos a los pocos días del aterrizaje y puesta en marcha del *Rover Perseverance*, y que están midiendo las condiciones ambientales del lugar de aterrizaje, el cráter Jezero, así como estudiar el fino polvo marciano que es importante para la exploración humana en el futuro. En concreto, MEDA consta de sensores para medir la dirección y velocidad del viento, la temperatura del suelo y del aire, la humedad relativa, la presión atmosférica, la radiación solar ultravioleta, infrarroja y visible, las propiedades del polvo en suspensión y, además, cuenta con una cámara para tomar imágenes del cielo marciano y estudiar las nubes. MEDA es el tercer instrumento español operativo en Marte, y es la tercera estación medioambiental liderada por el Instituto Nacional de Técnica Aeroespacial - Centro de Astrobiología (CAB) CSIC-INTA, que funciona en el planeta rojo junto a REMS (*Rover Environmental Monitoring Station*) en operación desde agosto de 2012 a bordo del *Rover Curiosity*; y TWINS (*Temperature and Wind for InSight*), que aterrizó en 2018 a bordo de la misión *InSight*. Por primera vez existen tres estaciones medioambientales operativas en tres puntos distintos del planeta y todas lideradas y operadas por España.

Mencionar, entre otras, algunas contribuciones relevantes lideradas por científicos del CAB durante 2021 como: la detección por primera vez de etanolamina en el espacio interestelar, un compuesto que forma parte de los fosfolípidos que constituyen las membranas celulares y que ayudará a entender la evolución de las membranas de las primeras células; el primer informe meteorológico desde el cráter de impacto Jezzero en Marte gracias al instrumento MEDA; contribuciones al descubrimiento de nuevos planetas errantes dentro de nuestra galaxia; la detección y caracterización de biomarcadores lipídicos en rocas del Triásico-Jurásico del desierto de Atacama; experimentos pioneros en la caracterización de las interacciones entre la química y la mineralogía en cámaras de simulación de ambientes planetarios; o la caracterización de la diversidad microbiana en ambientes extremos como en glaciares y nunataks antárticos, o depósitos minerales de la Faja Pirítica Ibérica.

Finalmente, el telescopio espacial JWST (*James Webb Space Telescope*) de NASA, ESA, y CSA, que cuenta con importante participación española liderada por el CAB, se lanzó con éxito el 25 de diciembre. Fue uno de los acontecimientos más esperados en la exploración espacial y supondrá una revolución en el conocimiento del universo, en la que el CAB quiere estar y seguro formará parte de ella.

El Centro de Astrobiología (CAB) se fundó en 1999 como un Centro Mixto entre el Consejo Superior de Investigaciones Científicas (CSIC) y el Instituto Nacional de Técnica Aeroespacial (INTA).

The Centro de Astrobiología (CAB) was founded in 1999 as a joint centre between the National Research Council (CSIC) and the National Institute for Aerospace Technologies (INTA).

Astrobiology considers life as a natural consequence of the evolution of the Universe, and CAB aims to study the origin, evolution, distribution, and future of life in the Universe, through investigations on Earth and in extraterrestrial environments. Many steps are still unknown or poorly understood and it requires of a huge interdisciplinary effort to study the only case of life we know. At CAB, we mainly focus on what we consider the most critical aspects. Therefore, our high level scientific objectives are:

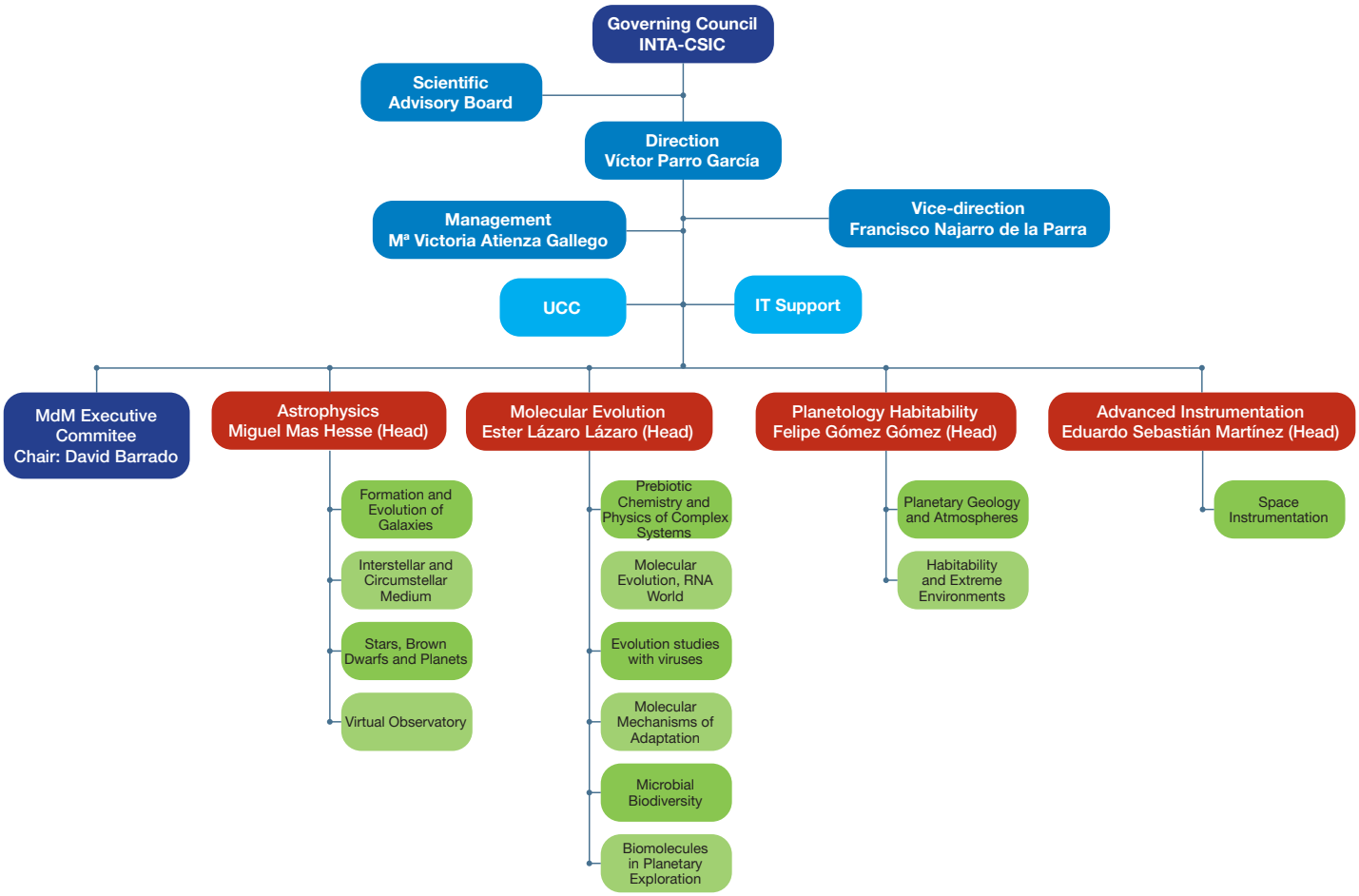
- **Objective 1:** To characterize the building blocks of the Universe: Formation and evolution of galaxies and stars through cosmic time
- **Objective 2:** To understand the cycle of chemical elements: From the interstellar medium to stars and planets.
- **Objective 3:** To study potentially habitable planetary environments. Objective 4: To find and analyze biomarkers for the search for life in planetary environments.
- **Objective 5:** To understand the basic principles of life in planetary environments, its early evolution and adaptability to diverse and often extreme conditions.
- **Objective 6:** To develop methods and advanced instrumentation for in situ and remote exploration and characterization of cosmic objects.

Over 2021, the CAB has maintained a high quality and very productive activity. To highlight, for example, the arrival on Mars on February 18th of the MEDA instrument (Mars Environmental Dynamics Analyzer) led by the CAB, one of the fundamental instruments of NASA's Mars2020 mission. MEDA is a complex network of environmental sensors, which became operational a few days after the Perseverance rover's landing, and which are measuring the environmental conditions at the landing site, the Jezero crater, as well as studying the fine dust Martian that is important for future human exploration. Specifically, MEDA consists of sensors to measure the direction and speed of the wind, the temperature of the ground and the air, the relative humidity, the atmospheric pressure, the UV light, infrared and visible radiation, the properties of the dust in suspension and, in addition, it has a camera to take images of the Martian sky and study the clouds. MEDA is the third Spanish instrument operating on Mars, and it is the third environmental station led by the National Institute of Aerospace Technology - Astrobiology Center (CAB, CSIC-INTA) that works on the red planet together with REMS (Rover Environmental Monitoring Station) in operation since August 2012 aboard the Curiosity rover; and TWINS (Temperature and Wind for InSight), which landed in 2018 aboard the InSight mission. For the first time there are three operational environmental stations in three different parts of the planet and all led and operated by Spain.

Mention, among others, some relevant contributions led by CAB scientists during 2021, such as: the detection for the first time of ethanolamine in interstellar space, a compound that is part of the phospholipids that make up cell membranes and that will help to understand the evolution of the membranes of the first cells; the first weather report from the Jezero crater on Mars thanks to the MEDA instrument; contributions to the discovery of new *free-floating* planets within our galaxy; the detection and characterization of lipid biomarkers in Triassic-Jurassic rocks of the Atacama desert; pioneering experiments in the characterization of the interactions between chemistry and mineralogy in simulation chambers of planetary environments and prebiotic chemistry experiments; or the characterization of microbial diversity in extreme environments such as Antarctic glaciers and nunataks, or mineral deposits in the Iberian Pyrite Belt.

Finally, the space telescope JWST (James Webb Space Telescope) of NASA, ESA and CSA, which has a significant Spanish participation led by the CAB, was successfully launched on December 25. It was one of the most expected events in space exploration and will mean a revolution in the knowledge of the universe, in which the CAB wants and will surely be part of it.

Center organization



Centro de Astrobiología is a joint institute participated by *Agencia Estatal Consejo Superior de Investigaciones Científicas* (CSIC) and *Instituto Nacional de Técnicas Aeroespaciales* (INTA). Its Governing Council is therefore chaired by CSIC President and INTA Director General, to whom the CAB Director and Deputy Director report.

Organization of *Centro de Astrobiología* in 2021. *Centro de Astrobiología* was organized in four Research Departments (red), each of them having different research groups (green). Additional units such as the *Unidad de Cultura Científica* (UCC), the Informatics Support, or the DNA Sequencing service, provide the required support for the operations of CAB. The departments operate a number of laboratories and facilities covering the very different areas of activities.

Members of the Governing Council 2021

D. Rafael Rodrigo Montero,

Secretario General de Coordinación de Política Científica, Ministerio de Ciencia e Innovación

Dña. Esperanza Casteleiro LLamazares,

Secretaria de Estado de Defensa, Ministerio de Defensa.

Dña. Rosa Menéndez,

Presidenta Agencia Consejo Superior de Investigaciones Científicas (CSIC)

D. Jesús Marco de Lucas,

Vicepresidente de Investigación Científica y Técnica (CSIC)

D. José María Salom Piqueres,

Director General, Instituto Nacional de Técnica Aeroespacial (INTA)

D. Julio Ayuso Miguel,

Subdirector General de Coordinación y Planes, INTA

D. Victorino Parro García,

Director, Centro de Astrobiología (CAB)

Advisory board

The former Directors of CAB constitute its Advisory Board:

Prof. Juan Pérez Mercader (CSIC): 1999-2008:

Prof. Álvaro Giménez Cañete (CSIC): 2008-2010

Dr. Javier Gómez Elvira (INTA): 2010-2015

Dr. Miguel Mas Hesse (CSIC): 2015-2019

External scientific advisory board

Paola Caselli,

Director and Scientific Member at the Max Planck Institute for Extraterrestrial Physics, Garching, (Germany)

Muriel Gargaud,

CNRS Research Director, Laboratoire d'Astrophysique de Bordeaux, Université de Bordeaux, (France)

Rosaly Lopes,

Directorate Scientist, NASA's Jet Propulsion Laboratory (JPL), Pasadena, CA, (USA)

Michel Mayor,

University of Geneva, Geneve. Nobel Prize in Physics 2019

Christopher McKay,

Space Science Division - NASA Ames Research Center, (USA)

Gian Gabriele Ori,

Universita d'Annunzio, Pescara, Italy - Ibn Battuta Centre, (Marrakech)

Direction and Center executive board

Victorino Parro García

Francisco Najarro de la Parra

Name	Position
Victorino Parro García	Director
Francisco Najarro de la Parra	Deputy Director
Victoria Atienza Gallego	Administrative Manager
Miguel Mas Hesse	Head of Astrophysics
Felipe Gómez Gómez	Head of Planetology and Habitability
Ester Lázaro Lázaro	Head of Molecular Evolution
Eduardo Sebastián Martínez	Head of Advanced Instrumentation
Benjamín Montesinos Comino	Senior Researcher
Ángeles Aguilera Bazán	Senior Researcher
Consuelo Moncayo Ortega	Administration

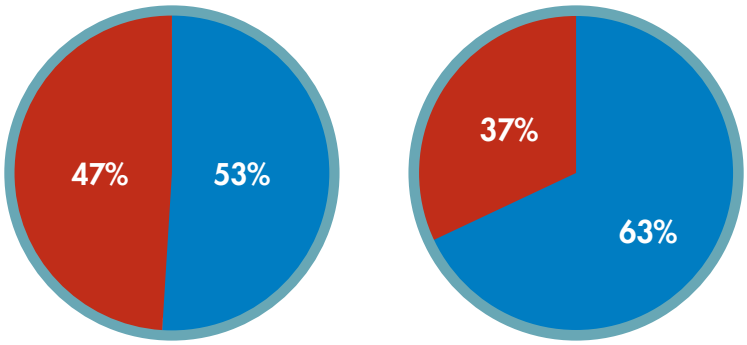
Management and support

Name	Position
Victoria Atienza Gallego	Administrative Manager
Margie Guitart Martín	Administration
Consuelo Moncayo Ortega	Administration
Esther Bermúdez Castillo	Technical management
Virginia Suarez Marsá	Technical management
Natalia Ruiz Zelmanovitch	UCC support

external support in 2021

María Pilar Alonso del Val	Technical support
Rosa del Olmo Andrés	Technical management
Tatiana Fraile Noriega	Technical management
Inmaculada García Climent	Technical management
María Teresa García Martín	Technical management
Macarena Gutiérrez Ortega	Technical management
Carmen Martínez de Llera	Technical management
Antonio Parras Rico	Computing support
Sergio Suarez Carrasco	Computing support
Juan Ángel Vaquerizo Gallego	Outreach support
Ignacio Barranquero	Scholarship student

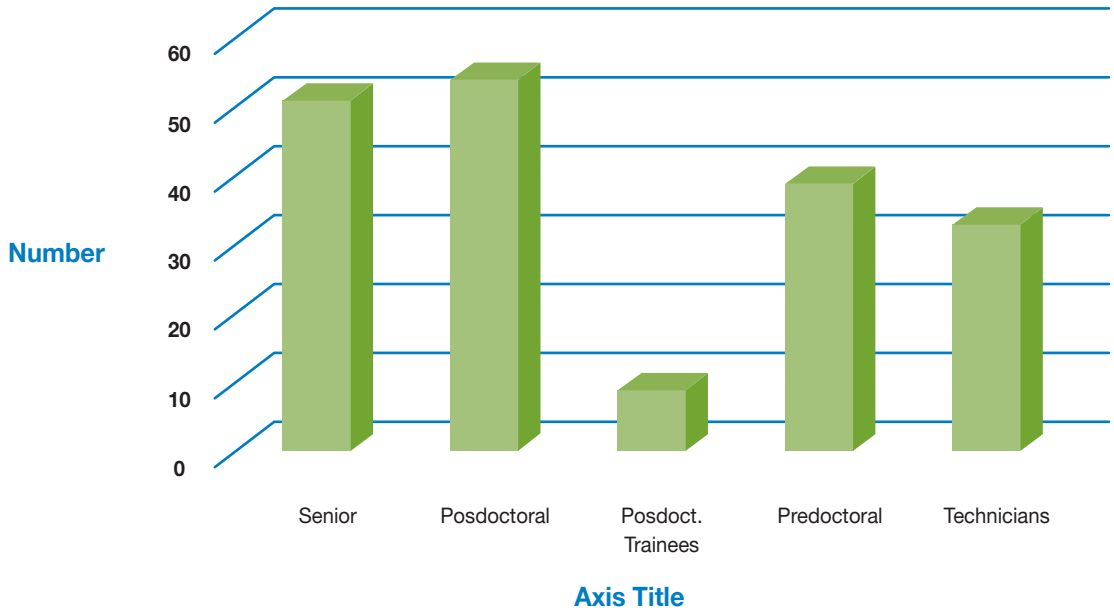
Personnel
by gender December 2021



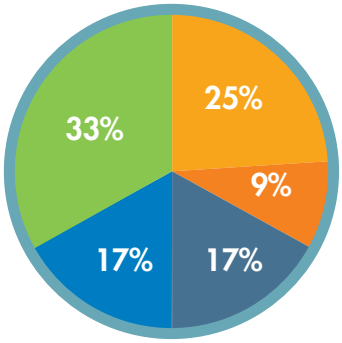
Gender Balance: (left) Total, (right) Scientific scales.

Women **Men**

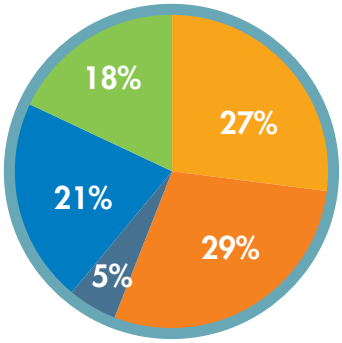
Personnel
by category (including 12 full time equivalents from other entities)



by type of contract



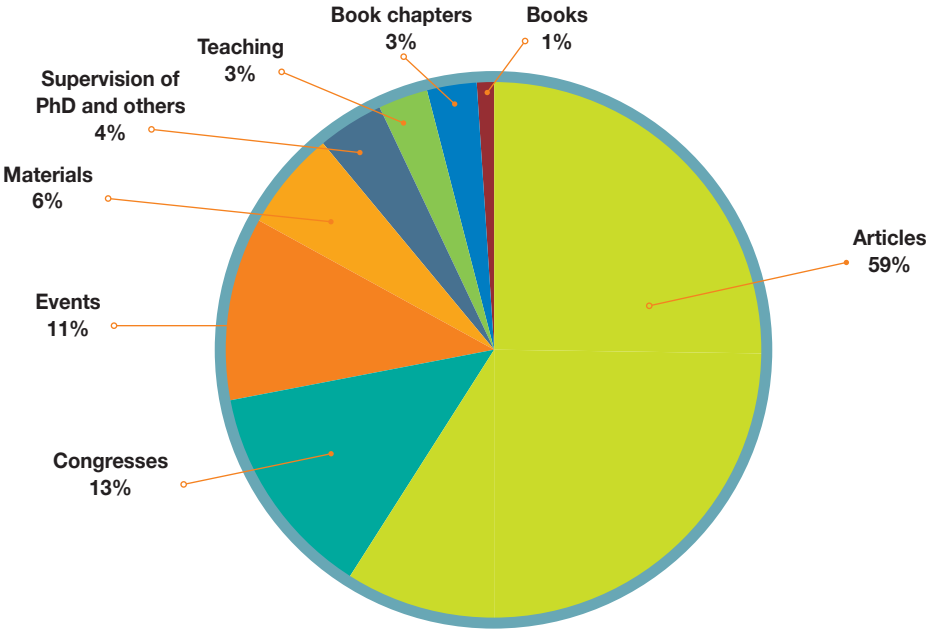
- Others contracs
- Predocts
- Doctors (Hired)
- Others Civil Servants
- Scientific Scales



- Tecnicians
- Predocts
- Post trainees
- Contrat. Pos.
- Seniors

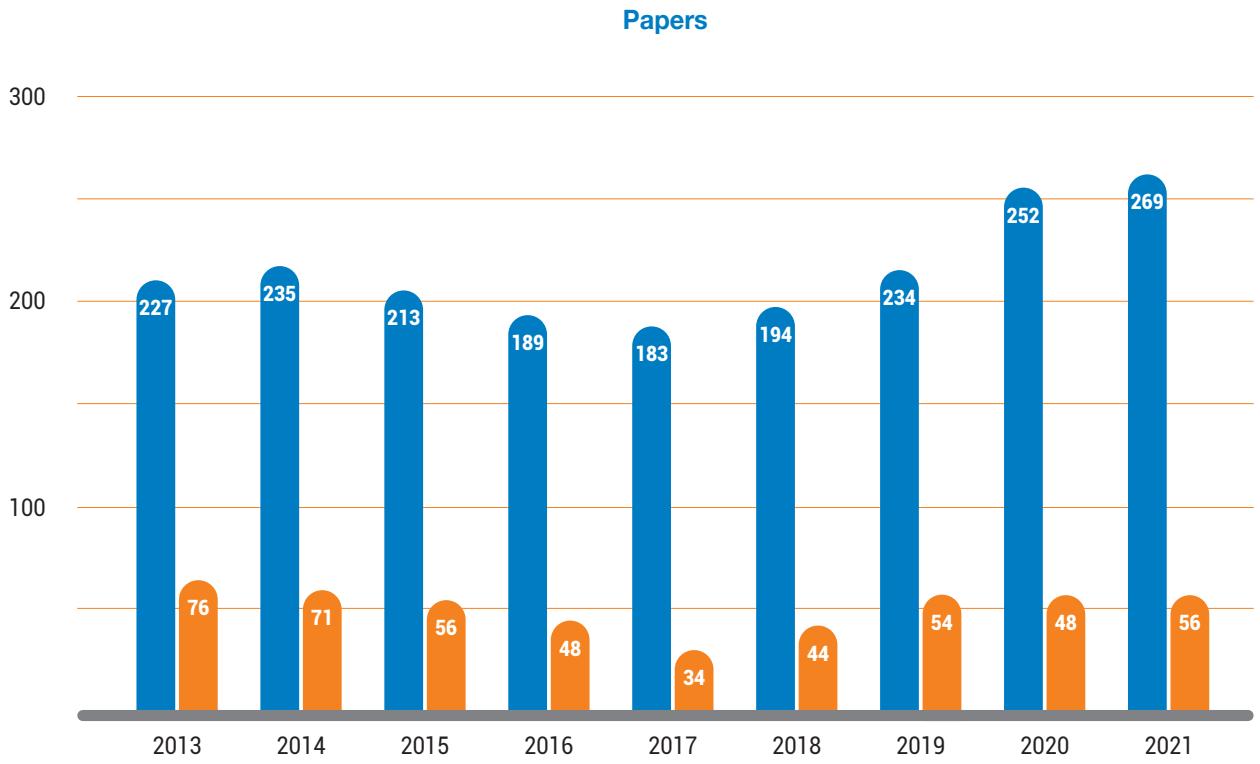
Scientific Production

Different indicators of the scientific production in 2021 (internal sources)

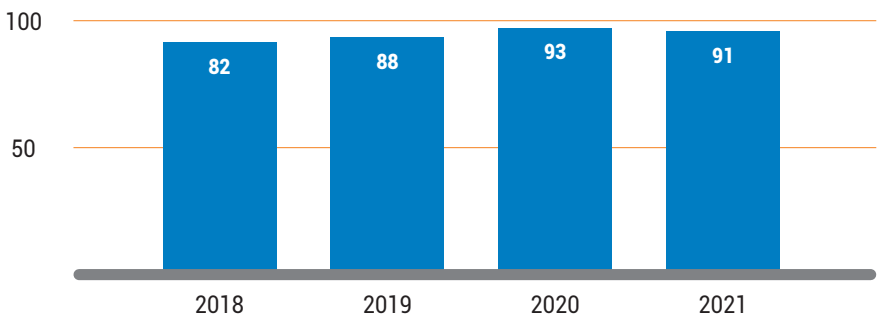


Research Articles

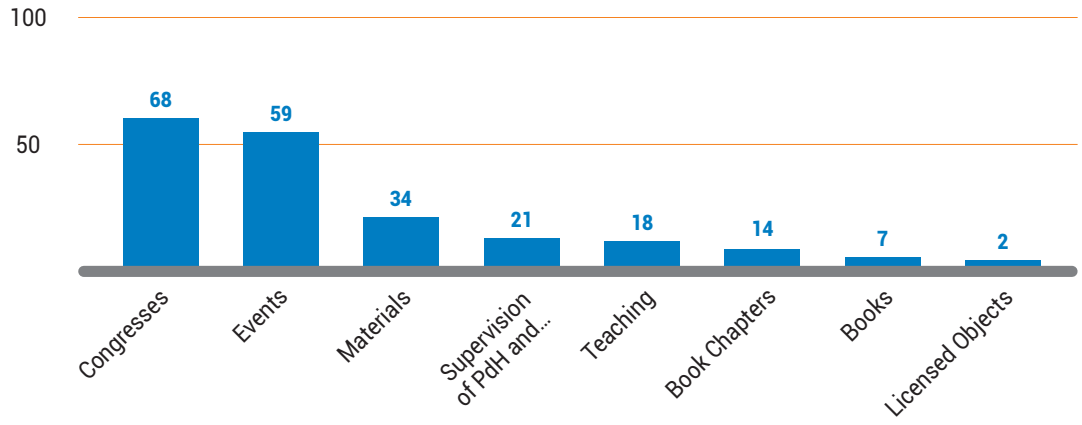
Evolution of the number of articles by year: total (blue) and led by CAB (red)



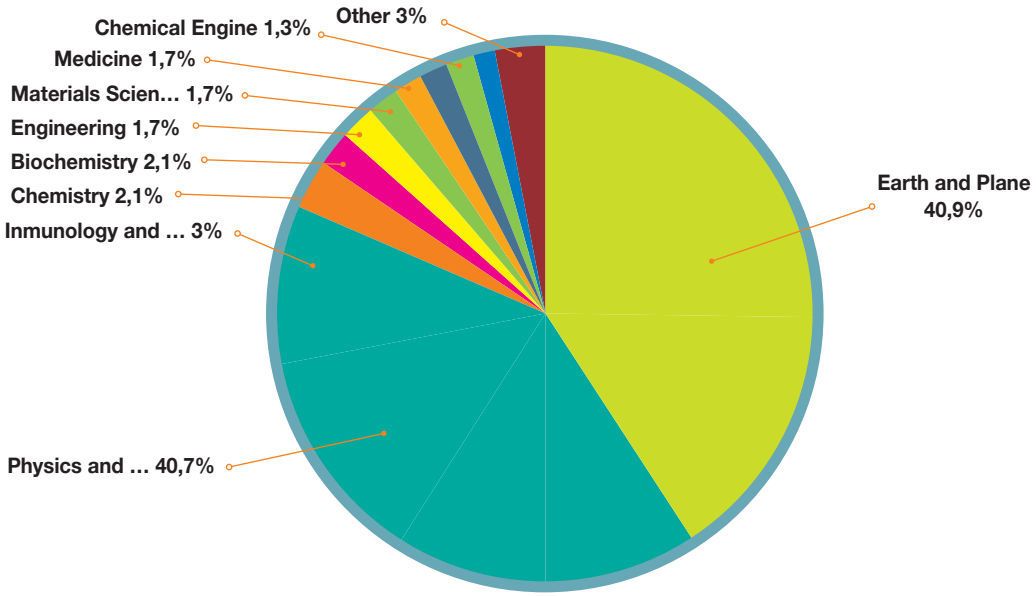
Evolution of the article production in quartile Q1 (%)



Other scientific production (internal sources)

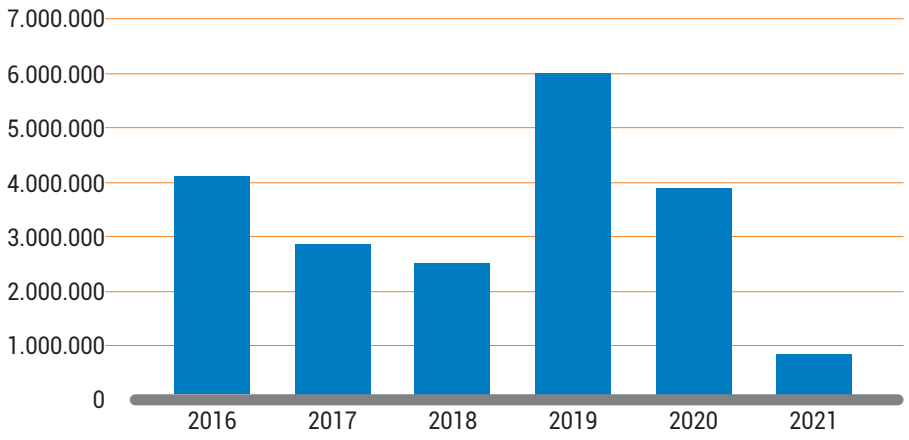


by subject area 2021 (source Scopus)



Documents by subject area

Funds from competitive calls (€ per year)



Espejo principal del telescopio JWST, formado por 18 segmentos individuales con un diámetro total de 6.5 metros. **Crédito: NASA**

Una imagen de las antenas de ALMA nevado en el llano de Chajnantor en el desierto de Atacama en Chile. **© ESO**

Astrophysics department of

Heads of Department:

J. Miguel Mas Hesse

The research at the Department of Astrophysics is focused on the formation and evolution of galaxies, stars and planets and their interplay with the interstellar medium, providing so the large-scale context in which Life emerged and evolved. The objectives are organized around the following questions:

To characterize the building blocks of the Universe: Formation and evolution of galaxies through cosmic time.
Our research is based on the general hypothesis that Life is a consequence of the evolution of matter and energy in the Universe, aiming to link the studies on the origin and evolution of the Universe with the emergence and potential spread of life.

To understand the cycle of chemical elements: From the interstellar medium to stars and planets.
The focus will be on the details of the cycle of chemical elements, from their production by stellar evolution to the formation of complex molecules and dust, the formation of stars, brown dwarfs and planets and the development of prebiotic chemistry in the interstellar space and protoplanetary disks. All this provides the boundary conditions to study the emergence of life in the solar System (at least) around 4 billion years ago.

To study potentially habitable environments.
We aim to connect the efforts from the point of view of Astronomy to discover (exo)planetary systems, analyze their components -planets and minor bodies- architecture and evolution, with those from the side of Biology and Planetary Science to assess their potential habitability.

To develop methods and advanced instrumentation for the characterization of cosmic objects.

Including the development ground and space- based instrumentation for observing objects within and beyond the Solar System

The Department of Astrophysics is constituted by 4 research groups:

- Formation and Evolution of Galaxies (FEG)
- Formation and Evolution of Stars, Brown Dwarfs and Planets (FESBDP)
- Interstellar and Circumstellar Medium (ICM)
- Virtual Observatory: Scientific exploitation of astronomical archives (VO)

Formation and Evolution of Galaxies (FEG)

Coordinator: Giovanni Miniutti

Senior Researchers:
Almudena Alonso Herrero
Santiago Arribas Mocoroa
Miguel Antonio Cerviño Saavedra
Luis Colina Robledo
José Miguel Mas Hesse
Pablo Guillermo Pérez González
Montserrat Villar Martín

Posdoctorals:
Javier Álvarez Márquez
Marianna Annunziatella
Heribert Argelaguet Vilaseca
Enrica Bellocchi
Luca Costantin
Alberto Estrada Piqueras
Margherita Giustini
Álvaro Labiano Ortega
Luis Peralta De Arriba
Miguel Pereira Santaella
Ana María Pérez García
Michele Perna
Javier Piqueras Lopez
Bruno Rodrigues Del Pino
Héctor Vives Arias

Posdoctoral trainees (1-3 years since PhD thesis):
Isabella Lamperti

Predoctorals:
Rosa María Mérida González
Alejandro Crespo Gómez
María Sánchez García

Technicians:
--

Students (Master, TFG, others):
Alejandro Gorgues Valenciano
Adrián Hidalgo Pinilla

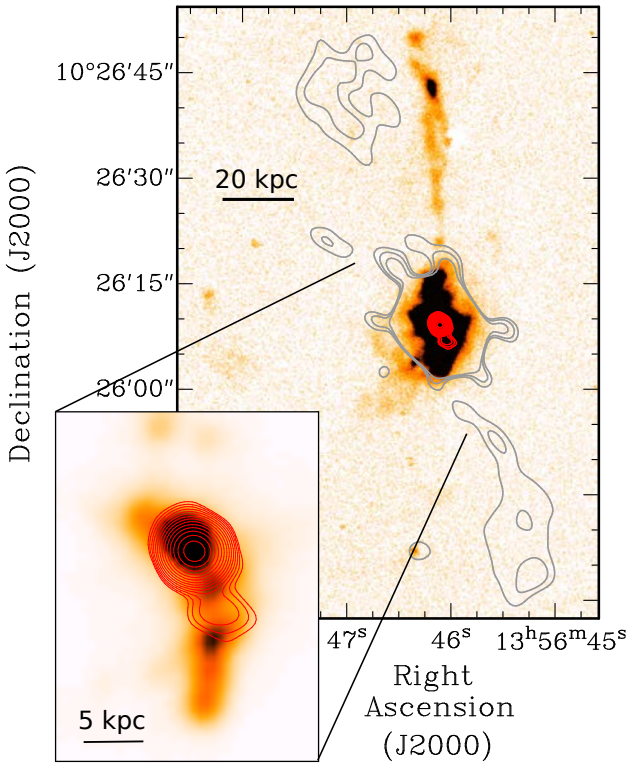
Summary

The Galaxies Formation and Evolution group contributes to objectives O1, O2 and O6 of the Center Strategic Plan. The group aims at providing a global view of the processes of galaxy formation and evolution across cosmic time. The research interests and expertise of the group members cover a wide range of physical phenomena: interacting/merging galaxies, superwinds and feedback, gas outflows from millimteric and infrared to optical and X-rays, as well as nuclear activity and its relation with the overall host galaxies properties. The group routinely collects, analyzes, and publishes astronomical data from radio and millimetric to infrared, optical and X-rays, making use of state of the art ground and space-based facilities. The group is heavily involved in technological projects for astronomical instrumentation both in space and on the ground in the framework of the ESA and ESO programs. Group members participate in the instrument teams of the MIRI and NiRSpec instruments for the recently launched James Webb Space Telescope (JWST), they take part in the team responsible for the development of HARMONI, a first light instrument for the European Extremely Large Telescope (EELT), and they participate to the definition of the next ESA large X-ray observatory Athena, among other projects. The following research highlights exemplify some of the most relevant recent investigations and results led by the group during the course of 2021.

Research Highlights (RH) 2021

RH1: Can radio jets of moderate power affect the evolution of galaxies?

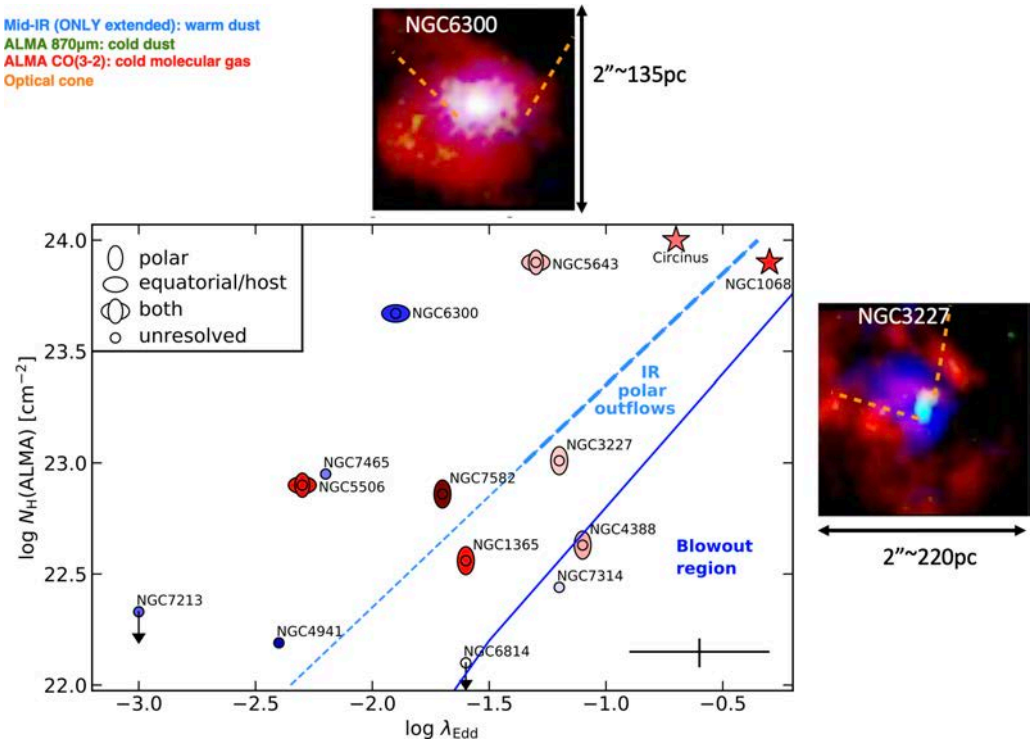
The activity of the supermassive black hole in galaxies can trigger extremely energetic phenomena, such as relativistic jets and lobes that advance at very high speeds through the host galaxies. In their way out, they can interact with the ambient medium modifying its properties dramatically and even pierce the galaxy to then expand into the circumgalactic medium. These structures, which emit preferentially at radio frequencies, can in this way provide a feedback mechanism whose impact on the evolution of galaxies is not totally understood. This is specially the case in active galaxies where the radio source has moderate to low power. It has been often believed that the feedback induced by the radio structures in these systems is negligible. We demonstrate in this work that this idea needs to be revised. Making use of radio maps obtained with VLA and optical images obtained with the GTC 10m Spanish telescope, we find that large-scale low to modest power radio sources can indeed provide a source of feedback across different scales through the galaxies and well into the circumgalactic medium [Villar Martín et al. 2021, A&A, 650, id. A84]. It is necessary to study in depth the potential impact of this phenomenon on the evolution of their host galaxies.



GTC Hα image (in color) of the quasar SDSS J1356+10 with overlaid radio contours. This very luminous active galaxy is associated with a rich reservoir of gas that extends over a huge volume, beyond the galaxy boundaries and well into the circumgalactic medium. The moderate power large scale radio source, discovered by us in this work, has managed to expand at huge distances. It provides a feedback mechanism whose impact on the evolution of the host galaxy is unknown [Villar Martín et al. 2021, A&A, 650, id. A84].

RH2: Torus and polar dust emission in GATOS Seyfert galaxies

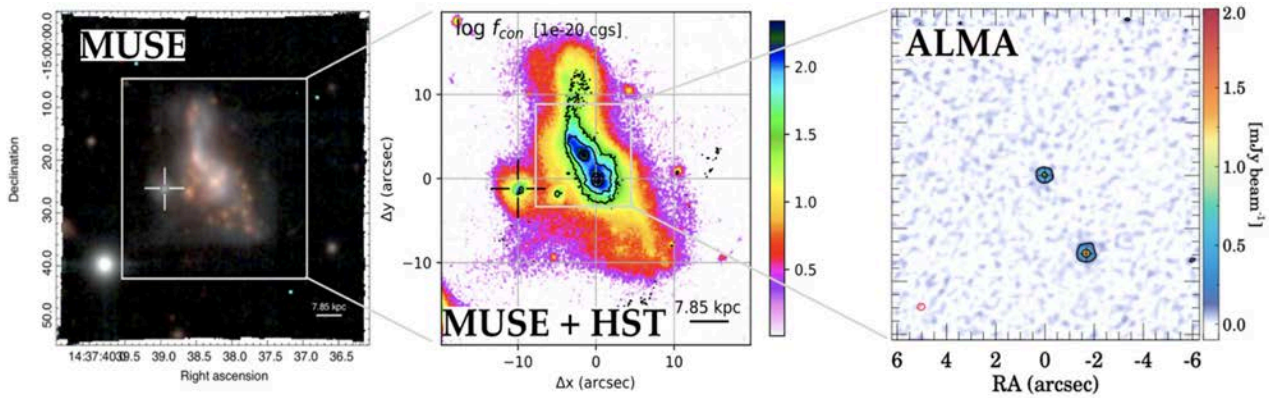
We used ~0.3" resolution mid-IR observations of nearby Seyferts selected from the Galaxy Activity, Torus, and Outflow Survey (GATOS) and compared them with ALMA far-IR continuum and CO(3-2) observations from García-Burillo et al. (2021). We detected extended mid-IR emission, typically in the polar direction and perpendicular to the ALMA torus, in more than half the sample. The unresolved mid-IR component contributes more than 60% of the emission of these galaxies. The observed Eddington ratios and the ALMA nuclear hydrogen column densities (NH) of ~50% of the sample are favorable to launching polar and/or equatorial dusty winds, according to numerical simulations. We generated new radiative transfer CAT3D-WIND disk+wind model (Hoenig & Kishimoto 2017) images at 8, 12 and 700μm, tailored to the properties of the GATOS Seyferts. When convolved to the typical angular resolution of our observations (0.3" in the mid-IR and 0.1" with ALMA), the CAT3D-WIND model images reproduce qualitative aspects of the observed mid -and far- IR morphologies. Low to intermediate values of the wind to disk cloud ratio are required to account for the large fractions of unresolved mid-IR emission observed in our sample. For more details see Alonso-Herrero et al. 2021, A&A, 652, id. A99.



Nuclear hydrogen column densities from ALMA CO(3-2) observations against the Eddington ratios for the GATOS Seyferts. Below the solid curve (Fabian et al. 2008) is the blowout region, where outflows are likely to clear material in the nuclear regions. The dashed line from Venanzi et al. (2020) indicates the limit where the AGN radiation acceleration balances gravity and the IR radiation pressure dominates, giving rise to polar dusty outflows. Also shown are two GATOS Seyferts: NGC6300 presents mostly extended mid-IR emission along the torus direction, while NGC3227 has an extended mid-IR component along the polar direction and a nuclear molecular gas outflow [Alonso-Herrero et al. 2021, A&A, 652, id. A99].

RH3: The incidence and origin of nuclear outflows in PUMA galaxies

As part of the PUMA project (Physics of ULIRGs with MUSE and ALMA) we analyzed the ULIRG nuclei taking advantage of MUSE optical data-cubes in combination with near-infrared HST, and millimeter ALMA data. We inferred (i) the ionization state of the ISM gas through standard optical line ratio diagnostics, and (ii) the presence of powerful outflows in both atomic ionized ([O III], Hα) and neutral (Na ID) gas. Broad and asymmetric [O III], Hα and Na ID profiles are found in almost all nuclear spectra, with line widths in the range 300 - 2000 km/s and ionization states compatible with AGN -and SB- driven winds. This result reinforces previous findings that indicated that outflows are ubiquitous in ULIRGs, and can affect the ISM conditions during the pre- and post-coalescence phases of major mergers. A further ALMA study investigated the origin of these outflows finding compact and obscured nuclei suggesting the presence of AGN. More details can be found in Perna et al. 2021, A&A, 646, id. A101 and in Pereira-Santaella et al. 2021, A&A, 651, id. A42.



Left: IRAS F14348-1447 color composite optical image from MUSE/VLT, showing Hα clumpy emission (reddish structures); center: zoom-in showing the MUSE optical (map) and the HST near-infrared (contours) continuum emission; right: zoom-in showing the ALMA emission (at ~250 GHz) from the two nuclei of this merging ULIRG.

RH4: A duality in the formation of bulges and spheroidal galaxies

In a recent work [Costantin et al., 2021, ApJ, 913, id. 125], we studied the assembly history of the spheroidal structures within massive galaxies at redshift z < 1, selected by the SHARDS survey in GOODS-N field. We characterized the formation scenarios of bulges in disk galaxies (upper and central panel in the figure below) and of pure spheroidal galaxies (lower panel). Firstly, our analysis reveals that these systems form in two waves. Indeed, we distinguish a fraction of very old bulges, which are formed at high redshift (z>3) and a dominant population of spheroids (bulges and pure spheroids) that formed at *z*~1. In particular, we argue that first-wave bulges could evolve through a blue and red-nugget phase and grow an extended stellar disk at later times (upper panel of the figure below). Furthermore, spheroids not only form in two waves but also form in two modes. At higher redshift, they assemble their mass fast (timescale around 200 Myr), while at lower redshift a slower mode starts to became relevant (with timescales ranging from 200 Myr to 1 Gyr and longer). These results provide a comprehensive picture of the morphological evolution of massive galaxies, extending to late-type galaxies the two-phase formation scenario currently accepted for early-type galaxies.

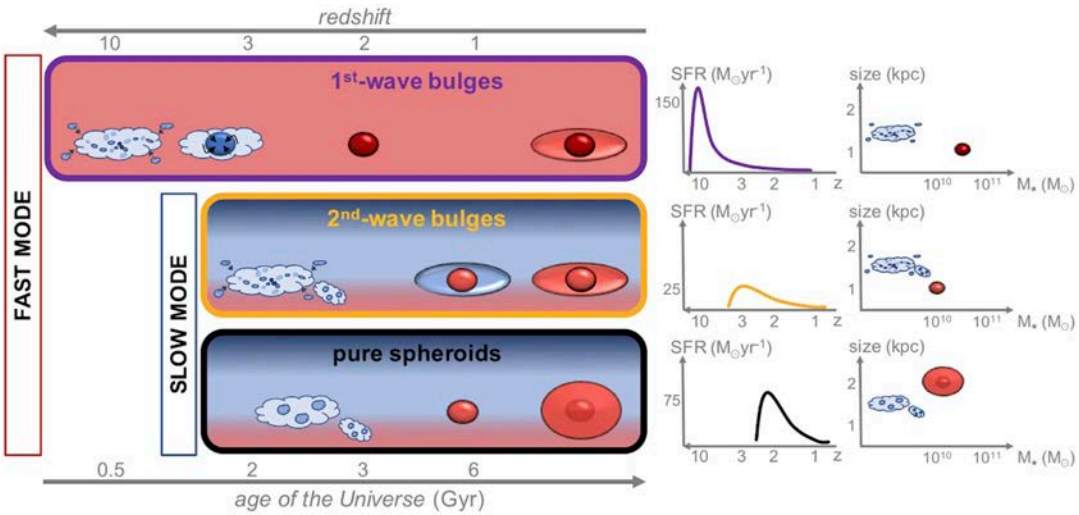
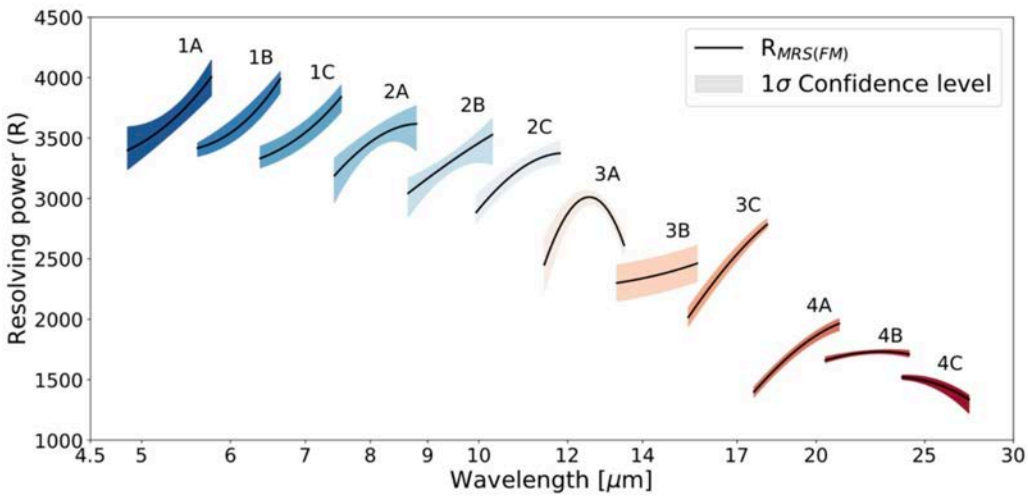


Illustration of the proposed formation scenario for the spheroidal component of massive galaxies at redshift 0.14 < z < 1, see text for details.

RH5: Spectral characterization of Webb's mid-infrared integral field spectrograph.

The Medium-Resolution Spectrometer (MRS) is the mid-infrared integral field spectrograph of the James Webb Space Telescope. It provides diffraction-limited spectroscopy between 4.9 and 28.3 µm, within a FOV varying from ~13 to~56 arcsec square. We used ground-based observations of discrete spectral features in combination with Fabry-Perot etalon spectra to characterize the wavelength solution and spectral resolving power of the MRS. Our results show that the MRS will cover the wavelength ranges from 4.9 to 28.3 µm with an accuracy below 1/10th of a pixel, and a resolving power varying between 4000 and 1500 depending on wavelength. We also presented the commissioning strategies we have designed, that will be used to refine these results on-orbit. These measurements guarantee that the MRS complies with the spectral requirements (resolution and accuracy) for which it was designed. More details can be found in Labiano et al. 2021, A&A, 656, id. A57.



Measurement of the MRS resolving power, based on ground test data. Black line: median MRS resolving power. Colored area: 1σ confidence level.

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Formation and Evolution of Stars, Brown Dwarfs and Planets (FESBDP)

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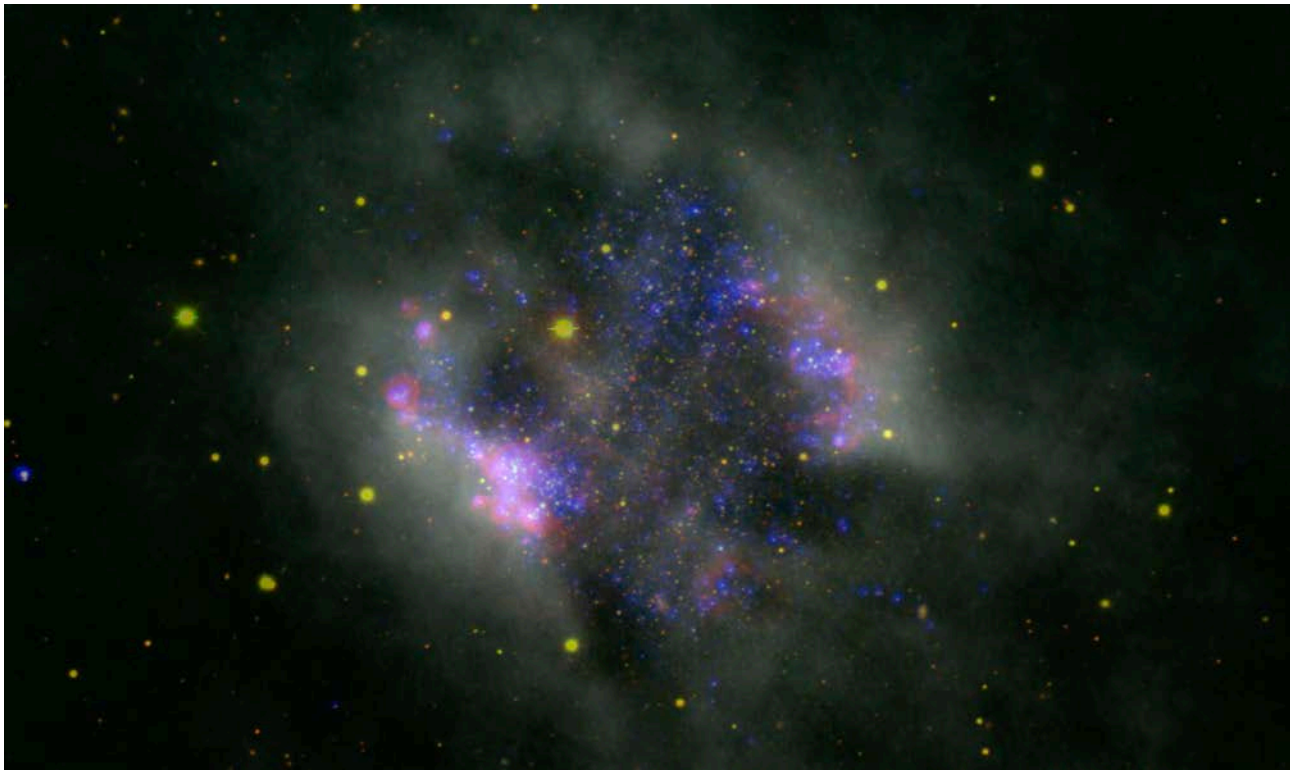
Summary

The Formation and Evolution of Stars, Brown Dwarfs and Planets group contributes to objectives O1, O2 and O3 of CAB (CSIC-INTA) Strategic Plan with the following scientific cases:

- Formation and evolution of high-mass and low-mass stars, brown dwarfs and isolated planets in star-forming regions, young star clusters and the field.
- Low-metallicity, massive stars. Synthesis processes, chemical mixing and structure of the interstellar medium.
- Stellar and substellar initial mass functions: maximum and minimum masses and dependency on environment.
- Protoplanetary disks around young stars and brown dwarfs, proto-brown-dwarfs.
- Formation of planetary systems.
- Debris disks.
- Atmospheres of stars, brown dwarfs and isolated planets.
- Exoplanets orbiting stars (direct imaging, transits and radial velocity).
- Exoplanetary atmospheres, planet-star interactions.

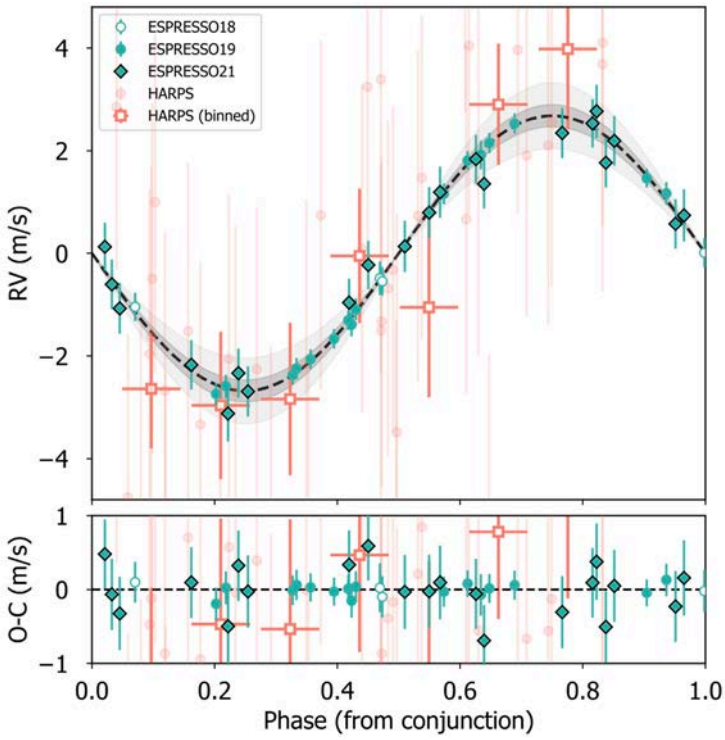
Group members are part of various scientific international consortia with access to either guaranteed time observations (CARMENES, ESPRESSO, Cheops) or secured long-term programs at highly competitive facilities (PanCET on the HST, HADES on the TNG). Scientific and technological highlights are given below. All of them are presented and detailed in the 105 refereed papers produced by the group in 2021.



Research Highlights 2021

RH1: First exoplanet "blind" detection with ESPRESSO.

We led the first detection of an extrasolar planet, HD 22496 b, resulting from the "blind" planetary search with the new ultra-stable high-resolution spectrograph ESPRESSO. The mass measured through radial velocities corresponds to a planet right between rocky and gaseous planets.



ESPRESSO phase-folded radial velocities (green) and HARPS (red) and the median Keplerian model (black line) of planet HD 22496 b. Figure extracted from Lillo-Box et al. (2021).

RH2: Non-transiting planets detected by photometric time series.

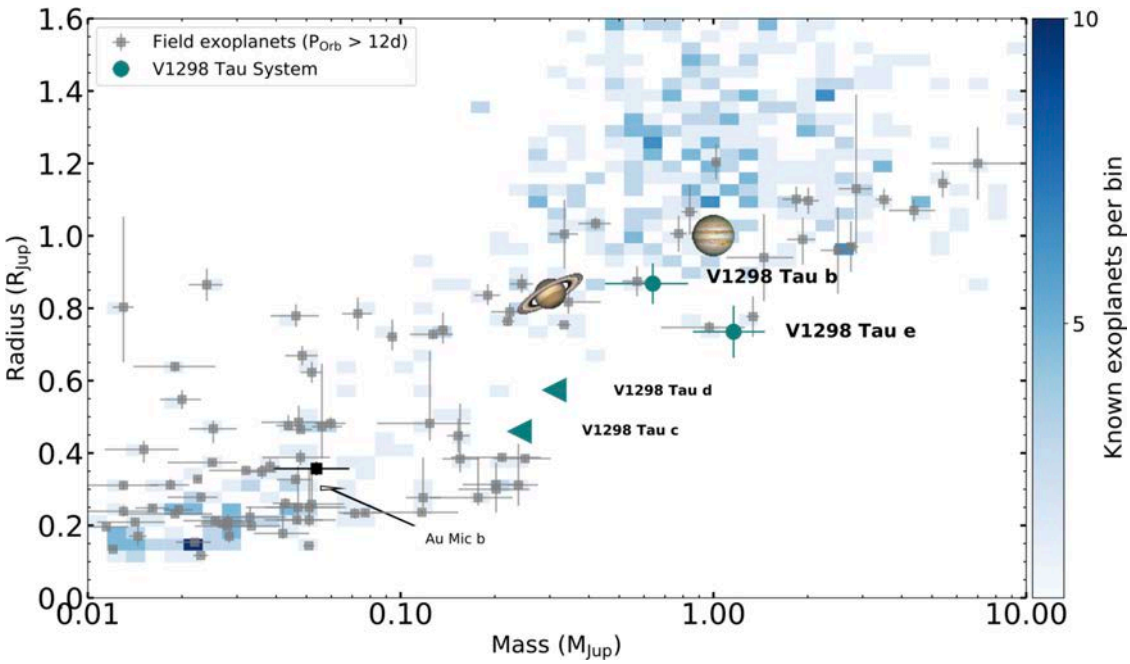
We identified and confirm new planets using the Kepler dataset. Interestingly, in this case, the planets do not transit their star but are so close to it that produced tidal deformations detectable with this telescope. We confirmed a total of 5 planets and perform radial velocity follow-up.

RH3: ϕ Leo revisited: Uncovering an exocomet-host impostor.

Previous observations of this star (A7 IV) showed variability, apparently associated to intense exocometary activity, only second to the prototype β Pic. Dedicated monitoring campaigns showed that the actual scenario is that of a pulsating δ Scuti star surrounded by an edge-on disc, the variability in the circumstellar lines being similar to that observed in rotating Be-shell stars. This configuration is the first one spotted in a late-A star.

RH4: Giant gas planets contract faster contradicting the theory of planetary evolution

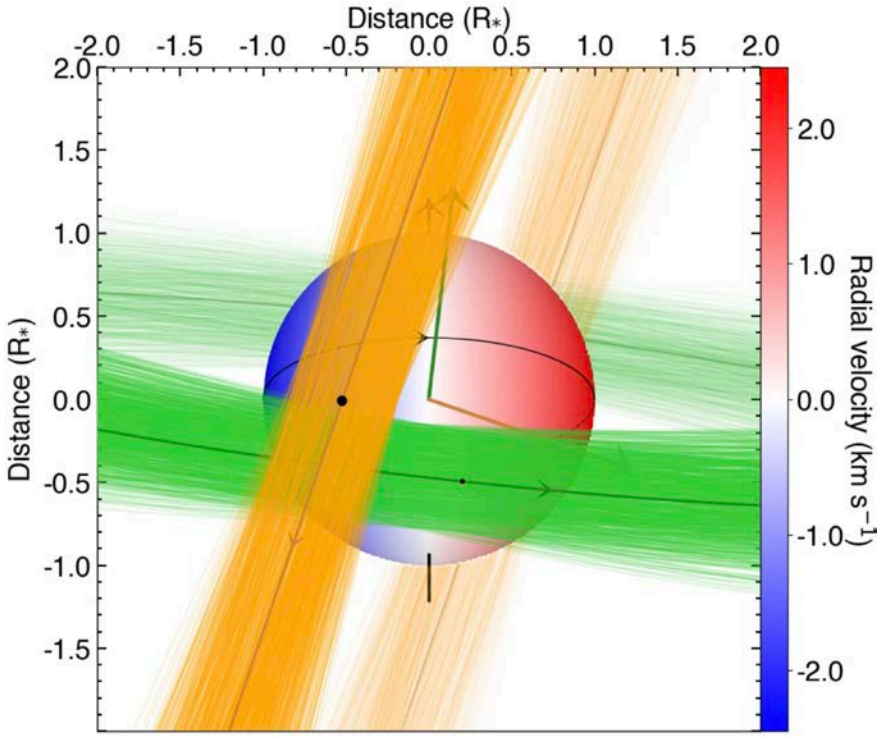
Radial velocity observations obtained with the CARMENES and HARPS-N spectrograph by an Spanish-Italian collaboration have shown that the giant planets, once formed, evolve to reach their final mass and size in less than 20 Myr (see figure below), which is at least a factor of ten much quicker than what current theories predict. This is a breaking result in the planetary field published in Nature Astronomy, with a significant impact on our understanding of the evolution of planets and planetary systems.



The 20-Myr planets V1298 Tau b and e have masses and radii very similar to those of Jupiter (4.5 Gyr), thus providing direct evidence that giant, gas planets form in much shorter time scales than predicted by the theory. Figure extracted from Suárez Mascareño et al. (2021).

RH5: Architecture of planetary systems

ESPRESSO observations of the multiple planetary system HD 3167 have shown that planets can co-exist on perpendicular orbits. The mini-Neptune HD 3167 c (orbital period of 29.8 d) has a high sky-projected spin-orbit angle (known from the literature), while the super-Earth HD 3167 b (with a short orbital period of 0.96 d) lies on an aligned orbit. Both planets show a mutual inclination of 102.3 deg (see figure below). HD 3167 b is the smallest exoplanet with a confirmed spectroscopic Rossiter-McLaughlin signal thanks to the ESPRESSO data quality.



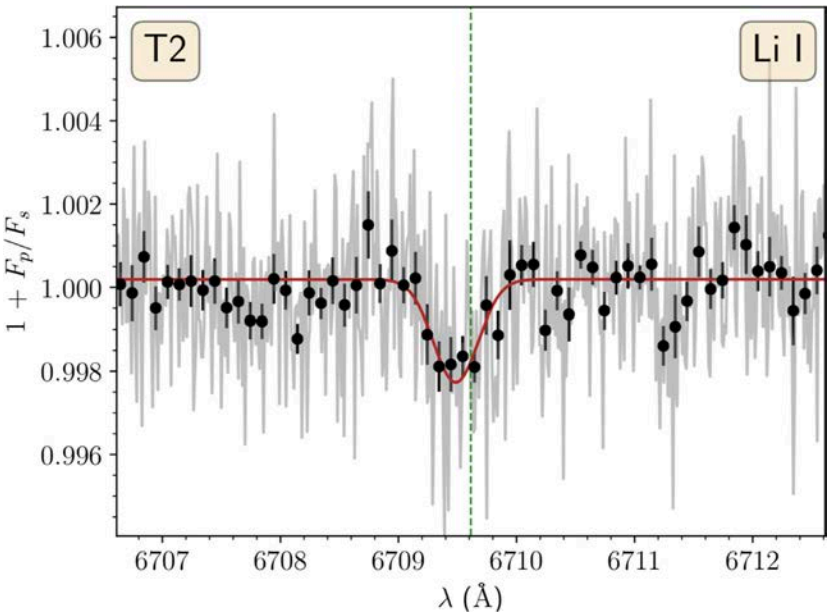
Projection of HD 3167 in the plane of sky. The orbits of planets HD 3167 b (green) and c (orange) are shown. The stellar disk (in the centre) is colored as a function of its surface rotation. Figure extracted from Bourrier et al. (2021).

RH6: Discovery of the first warm terrestrial planet with half the mass of Venus

ESPRESSO spectroscopic data combined with TESS photometry have led to the finding of the smallest planet confirmed with radial velocity measurements. Its mass is half of the mass of Venus; it is orbiting a nearby star, L 98-59, and its high density hints at a bulk composition with a small iron core.

RH7: Discovery of multiple species in the atmosphere of an ultra-hot Jupiter-mass planet

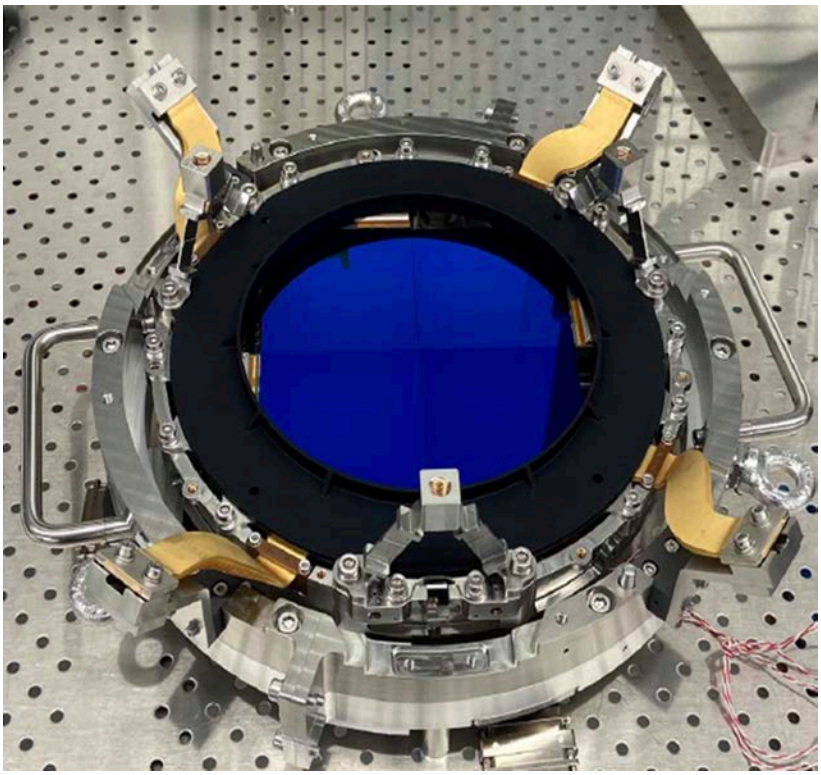
Using ESPRESSO data we announced the finding of numerous atomic species in the atmosphere of WASP-76 b, which has become a reference planet ever since. All of these species can be directly seen in the planetary visible spectrum: Li I, Na I, Mg I, Ca II, Mn I, KI and Fe I. Of particular interest is the detection of Li I (see Figure below), which has an intensity as strong as that of K I, thus indicating an unexpected high lithium abundance with strong implications on various astrophysical fields.



The Li I feature in the atmosphere of the Jupiter-mass planet WASP-76 b. Figure extracted from Tabernero et al. (2021).

RH8: Significant progress on the Spanish contribution to PLATO

CAB and INTA are responsible for the development of the Focal Plane Assemblies of the 26 telescopes of the PLATO Mission, as well as contributing to the scientific preparation of the operations. During 2021 several relevant milestones were accomplished: delivery of the Engineering Model (see RH4 figure) and the Structural and Thermal Model, successful completion of the Critical Design Review and the Critical Milestone Review at ESA Mission level, start of the manufacture of the first flight units, and publication of the first version of the PLATO Input Catalogue (PIC).



Engineering Model of the PLATO Telescopes Focal Plane Assembly (March 2021).

RH9: Tracking Advanced Planetary Systems (TAPAS) with HARPS-N. VII. Elder suns with low-mass companions

We present the current status of and new results from our search for exoplanets in a sample of solar-mass evolved stars observed with the HARPS-N and the 3.6 m Telescopio Nazionale Galileo (TNG), and the High-Resolution Spectrograph (HRS) and the 9.2 m Hobby-Eberly Telescope (HET). We present the analysis of RV measurements with the HET/HRS and the TNG/HARPS-N of four solar-mass stars, HD 4760, HD 96992, BD+02 3313 and TYC 0434-04538-1.

RH10: Do instabilities in high-multiplicity systems explain the existence of close-in white dwarf planets?

We investigate the origin of close-in planets and related phenomena orbiting white dwarfs (WDs), which are thought to originate from orbits more distant from the star. We find that planetary multiplicity is a natural condition to explain the presence of close-in planets to WDs, without having to invoke the specific architectures of the system, their migration or their survival through the common envelope phase.

RH11: Faint objects in motion: the new frontier of high precision astrometry

The goal of this White Paper is to address the fundamental science questions that are at stake when we focus on the motions of faint sky objects and to briefly review instrumentation and mission profiles.

RH12: The A-shell star ϕ Leo revisited: its photospheric and circumstellar spectra

We previously suggested that variable red- and blueshifted absorption features observed in the Ca II K line towards the A-type shell star ϕ Leo are likely due to solid, comet-like bodies in the circumstellar (CS) environment. We revisit the issue and suggest that ϕ Leo is a rapidly rotating δ Scuti star surrounded by a variable, (nearly) edge-on CS disk possibly re-supplied by the δ Scuti pulsations.

RH13: Homogeneous study of Herbig Ae/Be stars from spectral energy distributions and Gaia EDR3

Herbig Ae/Be stars (HAeBes) have so far been studied based on relatively small samples that are scattered throughout the sky. Their fundamental stellar and circumstellar parameters and statistical properties were derived with heterogeneous approaches before Gaia.

RH14: Title: Massive stars in massive Galactic clusters

Using data from KMOS-VLT, SINFONI-VLT and EMIR GTC, we have made significant progress in our studies of massive stellar clusters in the Galactic Center (Arches and Quintuplet) and inner disk of the Milky Way (Westerlund-1).

RH15: Title: Clumping in the winds of massive stars

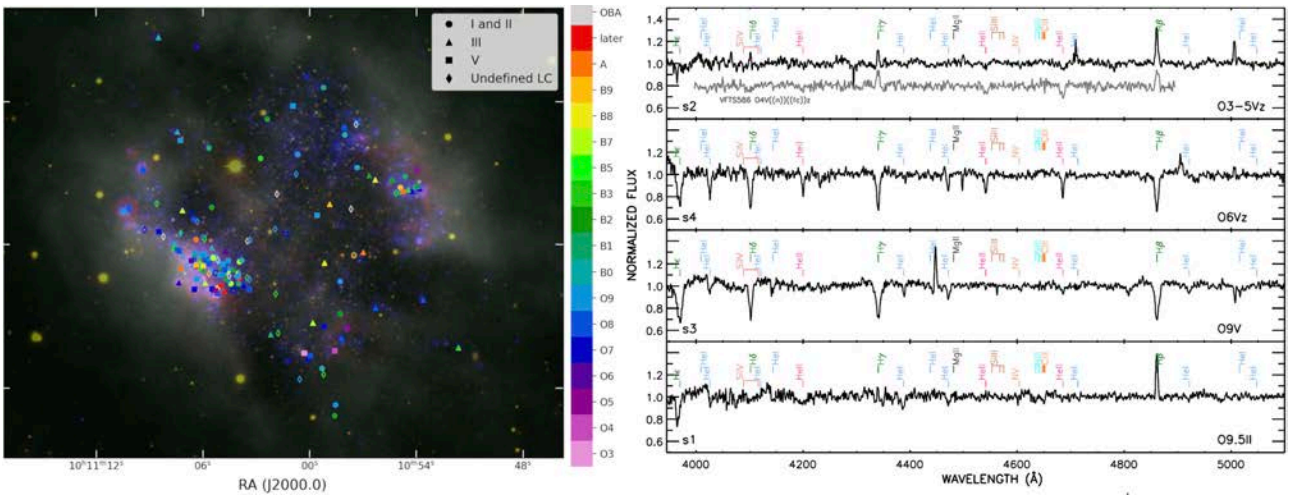
Using multiwavelength optical and near, medium and far infrared photometric data we characterized the stratification of inhomogeinities (clumping) throughout the winds of massive stars (Rubio-Díez et al. 2022).

RH16: Title: Radiatively driven winds of massive stars

A new formalism of radiation driven winds, consisting on a self-consistent solution of the extended atmospheres, has been implemented in the FASTWIND code (Björklund et al. 2021). We also contributed to this line of research with the stellar atmosphere code CMFGEN (Gormaz-Matamala et al. 2021).

RH17: Low metallicity, massive stars as a proxy for the first stars

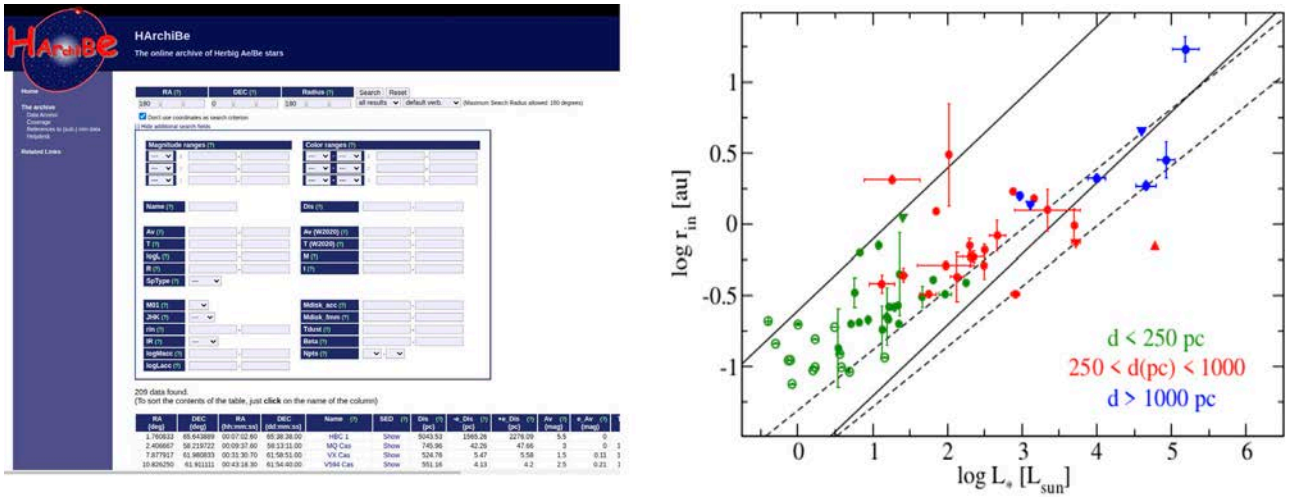
We have finished the first comprehensive census of very metal-poor massive stars with ~150 OB stars in Sextans-A (see RH17 figure). We have begun exploratory studies of metal poor massive stars in other uncharted dwarf irregulars such as Leo A and Sextans-B.



(Left) Massive stars in Sextans a discovered by our 5 observing campaigns with GTC-OSIRIS. (Right) GTC-OSIRIS spectra for a selected group of stars. (Adapted from Lorenzo et al., in preparation).

RH18: The most complete characterization of intermediate-mass young stars surrounded by protoplanetary disks

The most complete sample to date of intermediate mass "Herbig Ae/Be" stars has been characterized. This has been made both from a "large scale" approach, by providing their stellar and circumstellar parameters based on Gaia data, and from a "small scale" perspective, by resolving the innermost regions of their disks through GRAVITY/VLTI interferometry.



(Left): Except from "HArchiBe", we provide the online archive of Herbig Ae/Be stars compatible with Virtual Observatory (http://svo2.cab.inta-csic.es/projects/harchibe, Guzmán-Díaz et al. 2021). (Right): Observed inner disk size-stellar luminosity relation (circles) and models aiming to explain it (solid and dashed lines). Adapted from Marcos-Arenal et al. (2021).

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Principal Investigator: Ignacio Mendigutía

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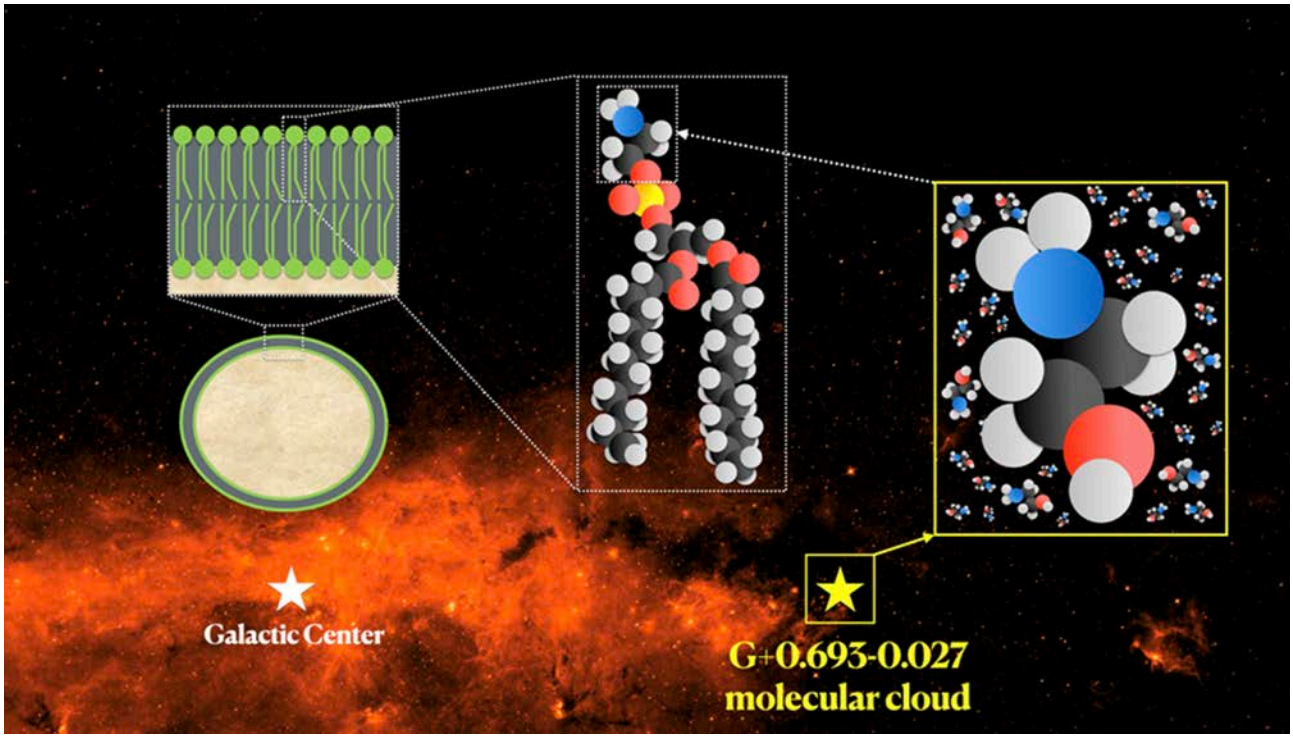
Summary

The chemistry in our Galaxy is often determined by UV fields from nearby stars, cosmic rays, shocks, turbulence and other phenomena. This group aims to obtain a detailed description of the physical and chemical properties of interstellar clouds, circumstellar environments around evolved stars and protoplanetary disks to understand the interplay between gas and dust, and to determine the limits of chemical complexity before life emerged on Earth. In particular, reactions leading to complex organic molecules (COMs) are of interest for Astrobiology (O1 and O2). This work is complemented by the development of instrumentation for airborne telescopes (O6).

Astrochemistry is studied following a four-fold approach: i) ***Observational*** (detection/mapping of simple molecules and COMs using single-dish telescopes, e.g. IRAM-30m, Yebes, APEX and Robledo de Chavela and interferometers, e.g. ALMA, ii) ***Theoretical*** (development of molecular excitation, radiative transfer, chemical models and MADCUBA code for data analysis), iii) ***Instrumentation*** (contribution to instrumentation on board future missions, development of KID detectors that operate in mm to far-infrared, and iv) ***Experimental*** (laboratory simulations of ice-covered dust processes leading to COMs in cold interstellar/circumstellar regions using the Interstellar Astrochemistry Chamber (ISAC) and radiation facilities, e.g. NSRRC synchrotron in Taiwan).

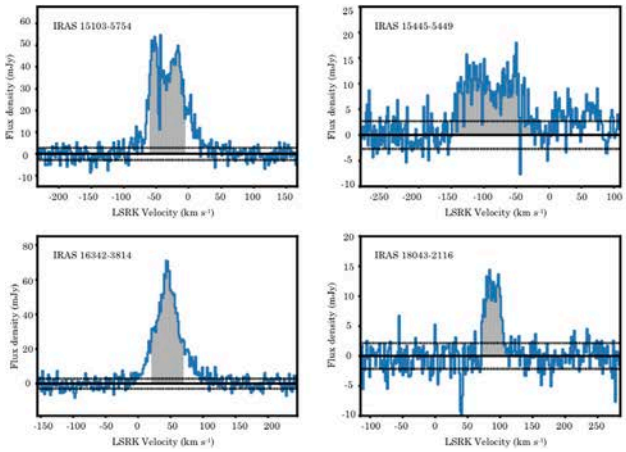
COMs were incorporated into comets and other minor bodies of the solar system. Impact of these objects on Earth delivered water and molecules of high astrobiological significance.

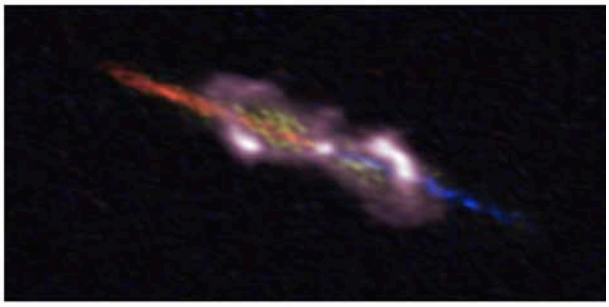


Research Highlights 2021

RH1: Observational identification of a sample of recent Common Envelope Events

One of the most poorly understood stellar evolutionary paths is that of binary systems undergoing common-envelope (CE) evolution, when the envelope of a giant star engulfs the orbit of a companion. Although this interaction leads to a great variety of astrophysical systems, direct empirical studies are difficult because few objects experiencing common envelope evolution are known. We present ALMA observations towards sources known as water fountains that, in contrast to the previous belief, reveal they had low initial masses (< 4 Msun) and ejected a significant fraction of it over less than a few hundred years. We conclude that the high measured mass-loss rates are most likely the consequence of common-envelope evolution. Since water-fountain sources show characteristic fast bipolar outflows, this would imply that collimated outflows and jets likely play an important role right before, during or immediately after the common-envelope phase.



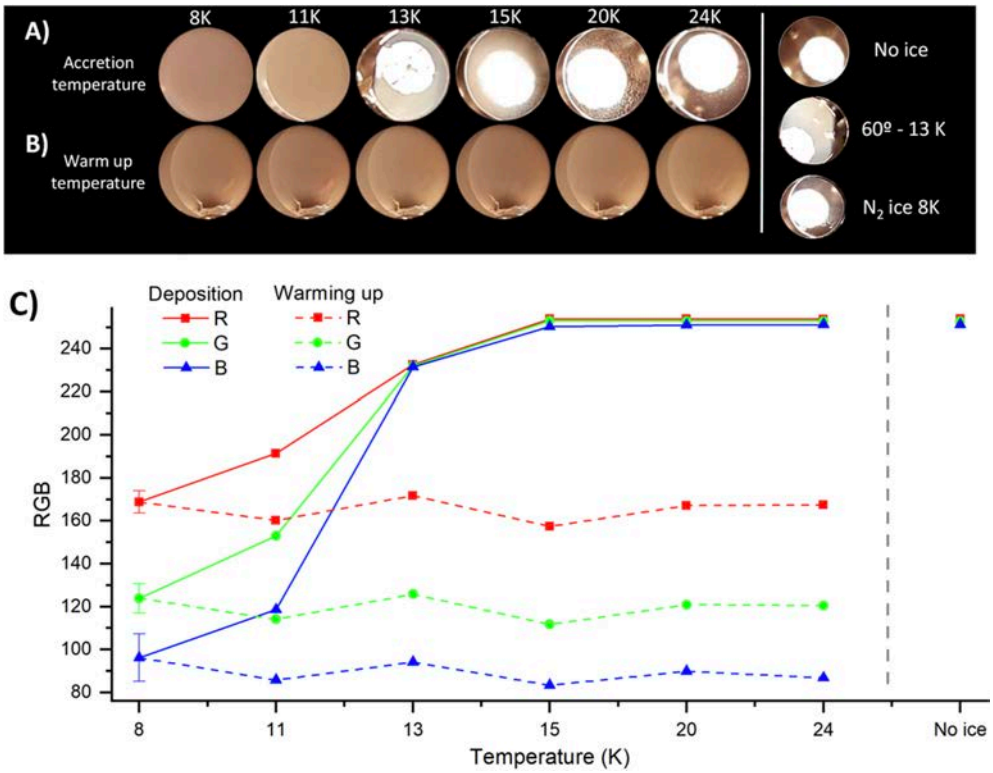


Left): $C^{18}O$ spectra of some of the water-fountain in our sample. The massive CO-emitting ejecta is most likely the consequence of CE evolution, after the giant star engulfed a binary companion. Adpated from Khouri et al. Right): ALMA's image of the water-fountain star system W43A. Credit: ALMA (ESO/NAOJ/NRAO), Tafoya et al. 2020.

RH2: Interstellar ice physics and chemistry highlights: First study of Ice Color Temperature and Synthesis of Nitrogen-heterocycles in UV-irradiated Ices

We used colorimetry to trace the relative orientations of CO ice molecules. For the first time, color variations were observed and depend on ice deposition temperature, ranging from brown to translucent or transparent when CO ice is deposited above 20 K and is nearly crystalline. As expected, apolar N_2 ice did not display color. This behavior of color temperature matches the photodesorption, i.e. the ejection of molecules from the ice surface when submited to UV-irradiation. Our method can monitor structural changes in molecular solids. The albedo of icy bodies can thus be low in CO patches. A brownish color is not only indicative of organic matter, as it may be due to disordered solid CO grown at temperatures near 10 K.

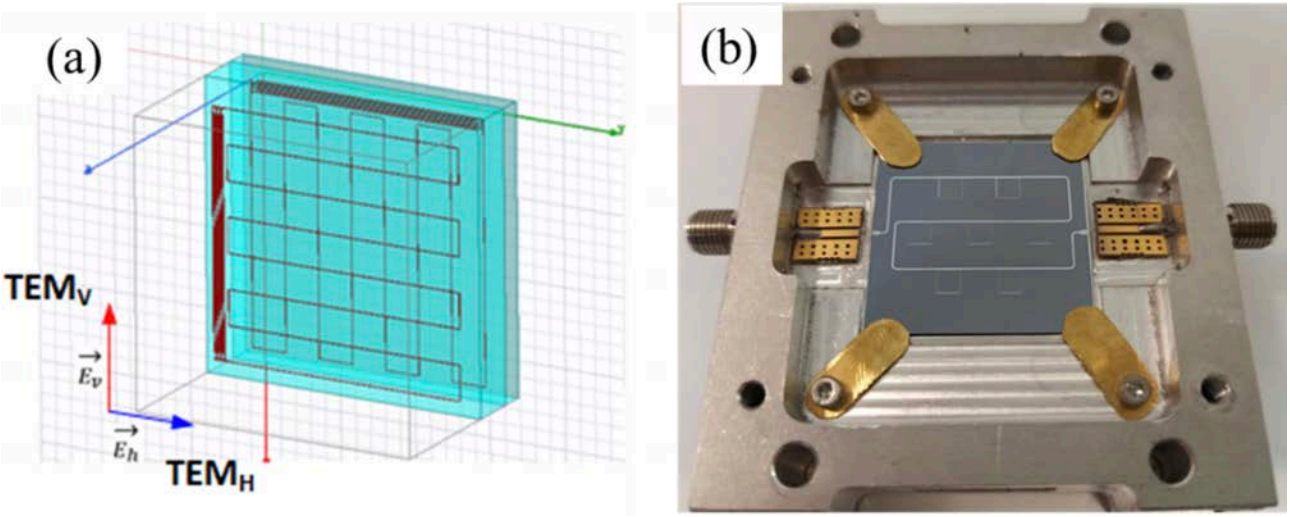
Nucleobases are N-heterocycles formed under simulated interstellar ice conditions. We used methylamine (CH_3NH_2) as precursor of N-heterocycles in UV-irradiated ices. N-heterocycles were also formed in H_2O:CH_3OH:NH_3 ice mixtures, but methylamine simplified the reaction network. Among the ice photoproducts are 12 species detected in space, 4 are COMs: formamide ($HCONH_2$), methyl cyanide (CH_3CN), CH_3NH and CH_3CHNH. During ice warmup the formation of 2 heterocycles, trimethylentriamine (c-[-CH_2-NH]$_3$) and hexamethylenetetramine (HMT, $[CH_2]_6N_4$) was observed. Their role as nucleobase precursors deserves further investigation.



(A) CO ice samples deposited at different temperatures, (B) a CO ice sample deposited at 8 K photographed at various temperatures during warm up. Substrate with no ice is shown for comparison on the right margin, along with a CO ice sample deposited at 13 K and 60° incidence angle, and the colorless N_2 ice deposited at 8 K. (C) RGB values of the CO ice samples. The spot of white light is the illumination from the back. CO ice samples deposited at 13 K and above are translucent and the spot of white light becomes apparent (A), while no color change is appreciated during warm up of ice deposited at 8 K (B). More info: Carrascosa et al. 2021, ApJ, 916, 1 (2021). AAS Journal Author Series: https://www.youtube.com/watch?v=He-CYJpguyQ

RH3: Analysis and Performance of Lumped-Element Kinetic Inductance Detectors for W-band

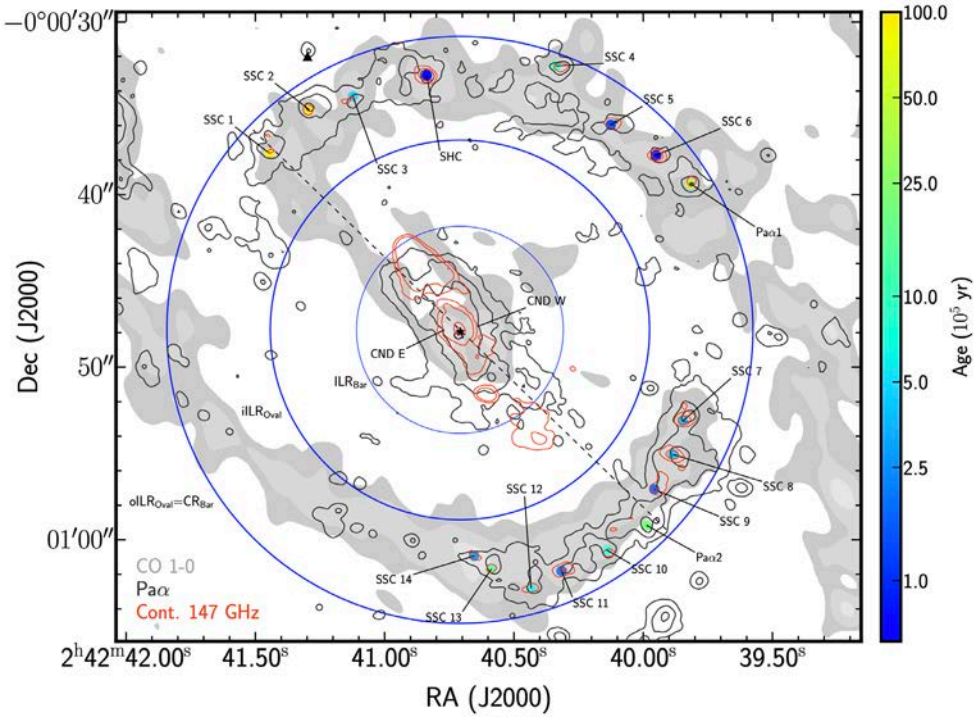
Lumped-Element Superconducting resonators are a promising technology for its use in millimeter-wave observations and quantum computing applications that require large arrays of extremely sensitive detectors. Among them, Lumped-Element Kinetic Inductor Detectors (LEKIDs) have shown good performance in the submillimeter band in several Earth-based telescopes. In this work, LEKIDs for their use as millimeter-wave receivers of astronomical applications are presented. LEKIDs arrays using a thin bilayer of superconducting titanium/aluminum (Ti/Al), deposited on silicon substrate, have been designed and fabricated. The design of a dual-polarization LEKID with the goal of detection at W-Band for two orthogonal polarizations is described and a fabricated array has demonstrated absorption at ambient temperature. Also, an approximate design methodology of the coupling parameter for LEKIDs readout, essential for dynamic range optimization of the detector under millimeter wave radiation, is proposed. In addition, resonance characteristics and coupling factor of the fabricated superconducting resonators using high-quality internal factor Qi under cryogenic temperatures have been analyzed. The design guidelines in this work are applicable to other LEKIDs arrays and the presented superconducting Ti/Al thin film LEKIDs can be used in future receiver arrays in millimeter bands.



(a) Dual-polarization LEKID and two incident TEM waves with electric fields orthogonal between them. Each LEKID is composed of a meander line inductor and an interdigital capacitor. (b) Fabricated LEKIDs array mounted for cryogenic testing.

RH4: Tracing the recent star formation in the starburst ring of the active galaxy NGC1068

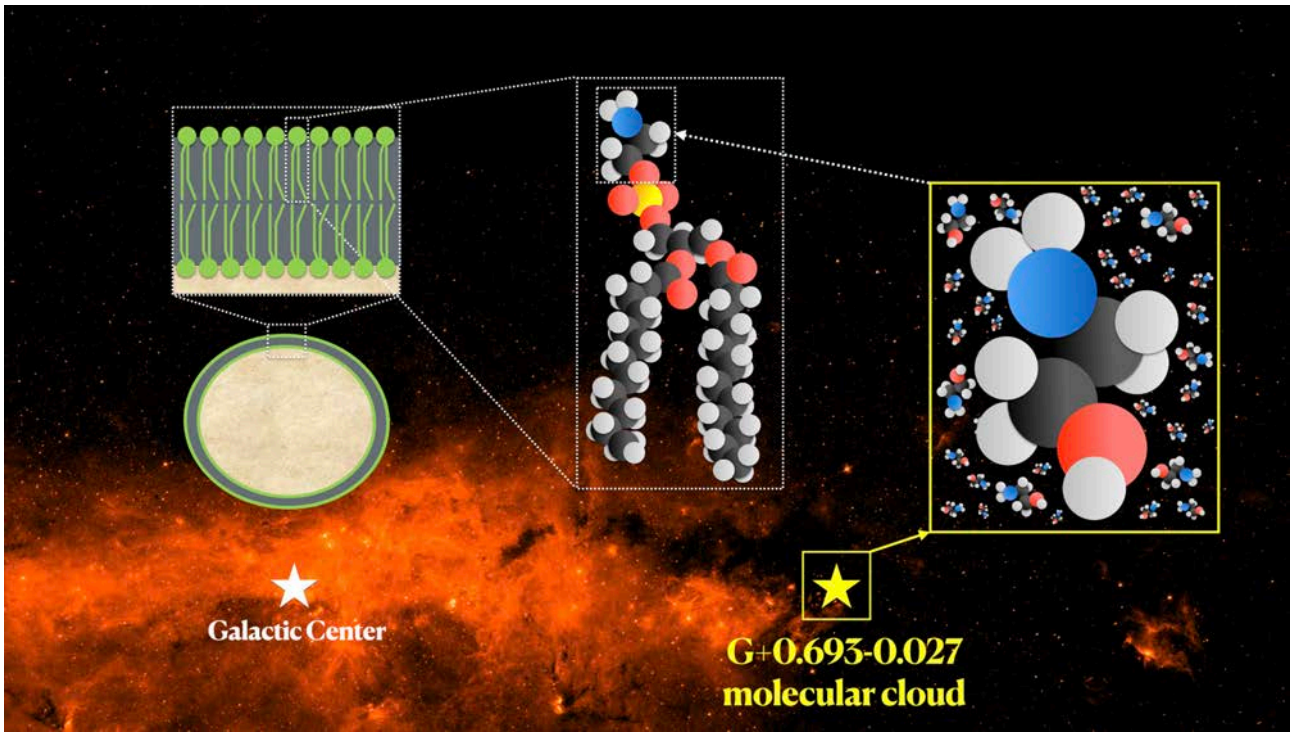
Using the ALMA data, we have studied the HC_3N and continuum emission in the starburst-ring and the circumnuclear disc (CND) of the active galaxy NGC 1068. Surprisingly, the vibrationally excited HC_3N (HC_3N^*) was detected only towards a very young star-forming region known as proto-Super Stellar Clusters (proto-SSCs) in the ring. Remarkably, HC_3N^* was not detected for the CircumNuclear Disk (CND) around the supermassive black hole, despite its large HC_3N column density. Combining the millimeter continuum emission with that of the Pa α, we have estimated the ages of other 14 SSCs in the ring. We find the SSCs to be associated with the region connecting the nuclear bar with the ring, supporting the inflow scenario. However, there is not a clear trend of the age with the location of the SSCs in the ring favoring the pop-corn scenario for the star formation. The analysis and the modelling of the HC_3N^*, shows very different dust temperatures (T_{dust}), of ~250 K for the proto-SSC and $T_{dust} \leq 100$ K for the CND. In spite of the large luminosity of the back hole in NGC 1068, the rather low dust temperature can be explained in the context of a system with low mid-IR opacity heated by the back hole.



NGC1068 map as seen in CO 1-0 (grey scale), Pa α (black contours) and 147GHz continuum emission (red contours). The AGN position is marked with a star. The stellar bar (seen in the IR) is indicated with a straight dashed black line. The gas is being accumulated in the SB pseudo-ring by the resonances between the ILRs of the outer oval and the stellar bar (indicated by solid blue lines). The estimated ages of the SSCs and the proto-SSC (i.e. the SHC) are indicated by the colorbar on the right.

RH5: Discovery in space of ethanolamine, the simplest phospholipid head group

Cell membranes are a key element of life because they keep the genetic material and metabolic machinery together. All present cell membranes are made of phospholipids, yet the nature of the first membranes and the origin of phospholipids are still under debate. We report here the presence of ethanolamine in space $NH_2CH_2CH_2OH$, which forms the hydrophilic head of the simplest and second-most-abundant phospholipid in membranes. The molecular column density of ethanolamine in interstellar space is $N = (1.51 \pm 0.07) \times 10^{13}$ cm^{-2}, implying a molecular abundance with respect to H_2 ***of (0.9–1.4)×10***$^{-10}$. Previous studies reported its presence in meteoritic material, but they suggested that it is synthesized in the meteorite itself by decomposition of amino acids. However, we find that the proportion of the molecule with respect to water in the interstellar medium is similar to the one found in the meteorite (10^{-6}). These results indicate that ethanolamine forms efficiently in space and, if delivered onto early Earth, could have contributed to the assembling and early evolution of primitive membranes.



Discovery of ethanolamine, a head group phospholipids, in the molecular cloud G+0.693-0.027 located in the center of our Galaxy. Credits: V.M. Rivilla and C. Briones (CAB) / IRAC4 camera onboard Spitzer Space telescope (NASA).

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Funded projects in 2021

Astrophysical ice processes, PI: G. M. Muñoz Caro, MICINN, PID2020-118974GB-C21, 3 years, 70.180 EUR.

Plataforma Temática Interdisciplinar, QTP2021-03-001: Tecnologías Cuánticas – Circuitos Superconductores, CSIC, PI: Juanjo Gacía-Ripoll, PI-CAB: Alicia Gómez Gutiérrez, 16/03/2021-31/12/2022, 105.374 EUR.

Linking ice, gas, and dust: Laboratory AstroChemistry (LI-LAC), MCIN, PI: B. Maté Naya, CSIC, LINKA20353, 2 years, 24.000 EUR.

Ramón y Cajal Grant (RYC2020-029387-I), PI: V.M. Rivilla, Title: Cosmic Origins of Life (COOL), 5 years, 42 kEUR

Virtual Observatory: Scientific exploitation of astronomical archives (VO)

Coordinator: Enrique Solano Márquez

Senior Researchers:

Ricardo Rizzo (External Support, ISDEFE)

Posdoctorals:

Alba Aller Egea

Miriam Cortés Contreras

Patricia Cruz Gamba

Francisco Jiménez Esteban

Belén López Martí

Posdoctoral trainees (1-3 years since PhD thesis):

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Predoctorals:

Pedro Mas Buitrago

Technicians:

Almudena García López (External support, ISDEFE)

Carlos Rodrigo Blanco

Almudena Velasco Trasmonte (External support, ISDEFE)

Students (Master, TFG, others):

Jaume Payeras Seguí (Prácticas en Empresas)

Enrique Moya (TFM)

Summary

This group contributes to objective O6 of Center Strategic Plan by addressing the question of the development of transdisciplinar mechanisms for data discovery and analysis (including Artificial Intelligence) in the framework of the Virtual Observatory, Big Data and the European Open Science Cloud. The group also plays an important role to fulfill the objectives O1 and O2. The following research highlights exemplify the most relevant investigations and results in the group.

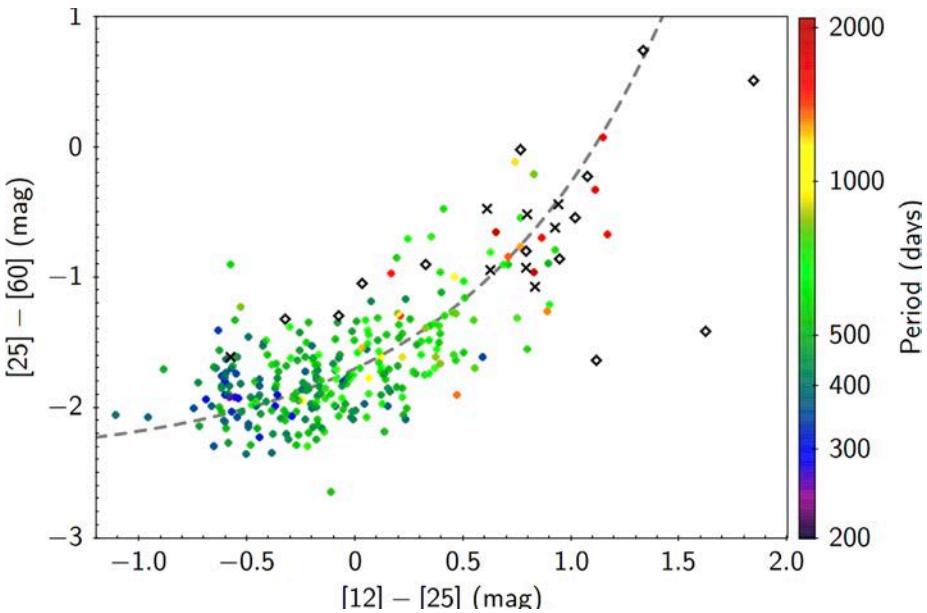
Research Highlights 2021

RH1: An infrared study of Galactic OH/IR stars - III. Variability properties of the Arecibo sample

This work is the result of a long-term near-infrared (NIR) monitoring programme carried out between 1999 and 2005 to determine the variability properties of galactic OH/IR stars (the Arecibo sample). The sample consists of 385 IRAS-selected O-rich Asymptotic Giant Branch (AGB) candidates heavily obscured by their circumstellar shell. Their O-rich chemistry has been proven by the detection of 1612 MHz OH maser emission. The monitoring data were complemented by data collected from public optical and NIR surveys within the Virtual Observatory. Periods were derived for 345 sources (~90 per cent of the sample).

Most of the sources were classified as long-period large-amplitude variable (LPLAV) stars. Their period distribution peaks at ~400 d, ranging from 300 to 800 d for most of the sources and having a long tail up to ~2100 d. Typically, the amplitudes are between 1 and 3 mag in the NIR and between 2 and 6 mag in the optical. We find correlations between periods and amplitudes, with larger amplitudes associated with longer periods, as well as between the period and the infrared colours with the longer periods linked to the redder sources.

This publication also has a catalogue accessible through the VO, and a dedicated website

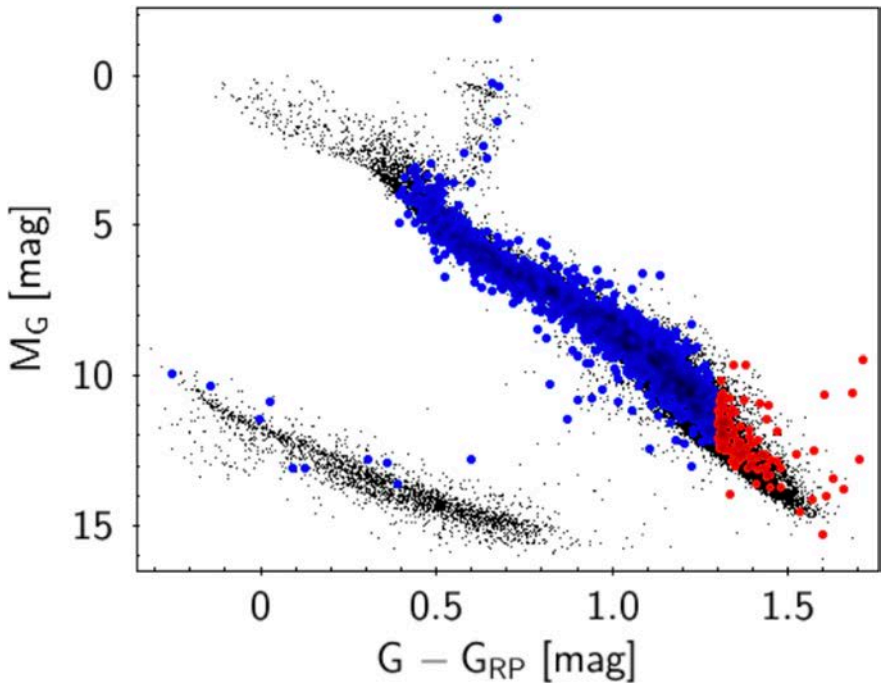


Mid/far-IR 2CDs of the Arecibo sample colour coded by period. LPLAVs are shown with full circles, post-AGBs with open diamonds, and unclassified sources with crosses.

RH2: Ultracool dwarfs in deep extragalactic surveys using the virtual observatory: ALHAMBRA and COSMOS

Ultracool dwarfs (UCDs) encompass a wide variety of compact stellar-like objects with spectra classified as late-M, L, T and Y. In this work we aim to validate a VO methodology designed to discover and characterize UCDs in deep extragalactic surveys like ALHAMBRA and COSMOS. Three complimentary searches based on parallaxes, proper motions and colours, respectively, were carried out. A total of 897 candidate UCDs were found, with only 16 previously reported in SIMBAD. Most of the new UCDs reported here are likely late-M and L dwarfs because of the limitations imposed by the utilization of optical (Gaia DR2 and r-band) data.

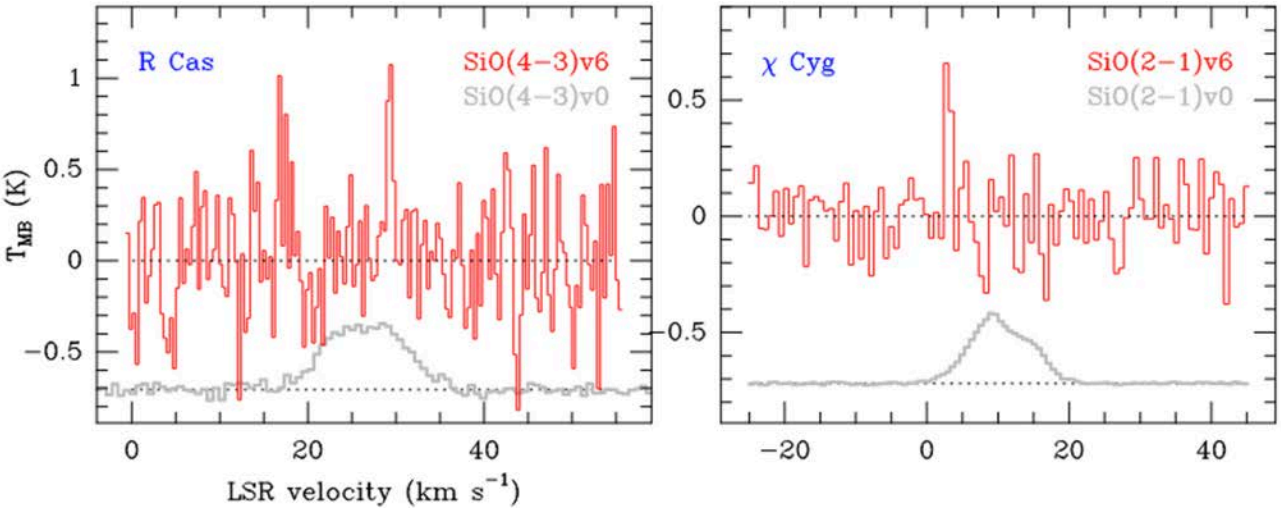
The agreement between the number of UCDs found in the COSMOS field and theoretical estimations together with the low false-negative rate (known UCDs not discovered in our search) validates the methodology proposed in this work, which will be used in the forthcoming wide and deep surveys provided by the Euclid space mission. Simulations of Euclid number counts for UCDs detectable in different photometric passbands are presented for a wide survey area of 15 000 deg2, and the limitations of applicability of Euclid data to detect UCDs using the methods employed in this paper are discussed.



Colour-magnitude diagram built using Gaia DR2 sources with parallaxes larger than 10 mas and good photometry (small black dots). Large blue dots indicate the position of the 1548 ALHAMBRA stellar (dwarfs, giants and white dwarfs) sources. Candidate UCDs defined as objects with G-Grp > 1.3 are overplotted in red.

RH3: SiO, 29SiO and 30SiO Emission from 67 Oxygen-rich Stars: A Survey of 61 Maser Lines from 7 to 1 mm.

Circumstellar environments of oxygen-rich stars are among the strongest SiO maser emitters. Physical processes such as collisions, infrared pumping and overlaps favor the inversion of level population and produce maser emission at different vibrational states. Despite numerous observational and theoretical efforts, we still do not have a unified picture including all of the physical processes involved in SiO maser emission. We present a survey of 67 oxygen-rich stars from 7 to 1 mm, in their rotational transitions from J = 1 → 0 to J = 5 → 4, for vibrational numbers v from 0 to 6 in the three main SiO isotopologs. The first tentative detection of a v = 6 line is reported, as well as the detection of new maser lines. The highest vibrational levels seem confined to small volumes, presumably close to the stars. The J = 1 → 0, v = 2 line flux is greater than the corresponding v = 1 in almost half of the sample, which may confirm a predicted dependence on the pulsation cycle. As a by-product, we report detections of 27 thermal rotational lines from other molecules, including isotopologs of SiS, H2S, SO, SO2 and NaCl. The results of this paper are publicly available through a VO-compliant archive.

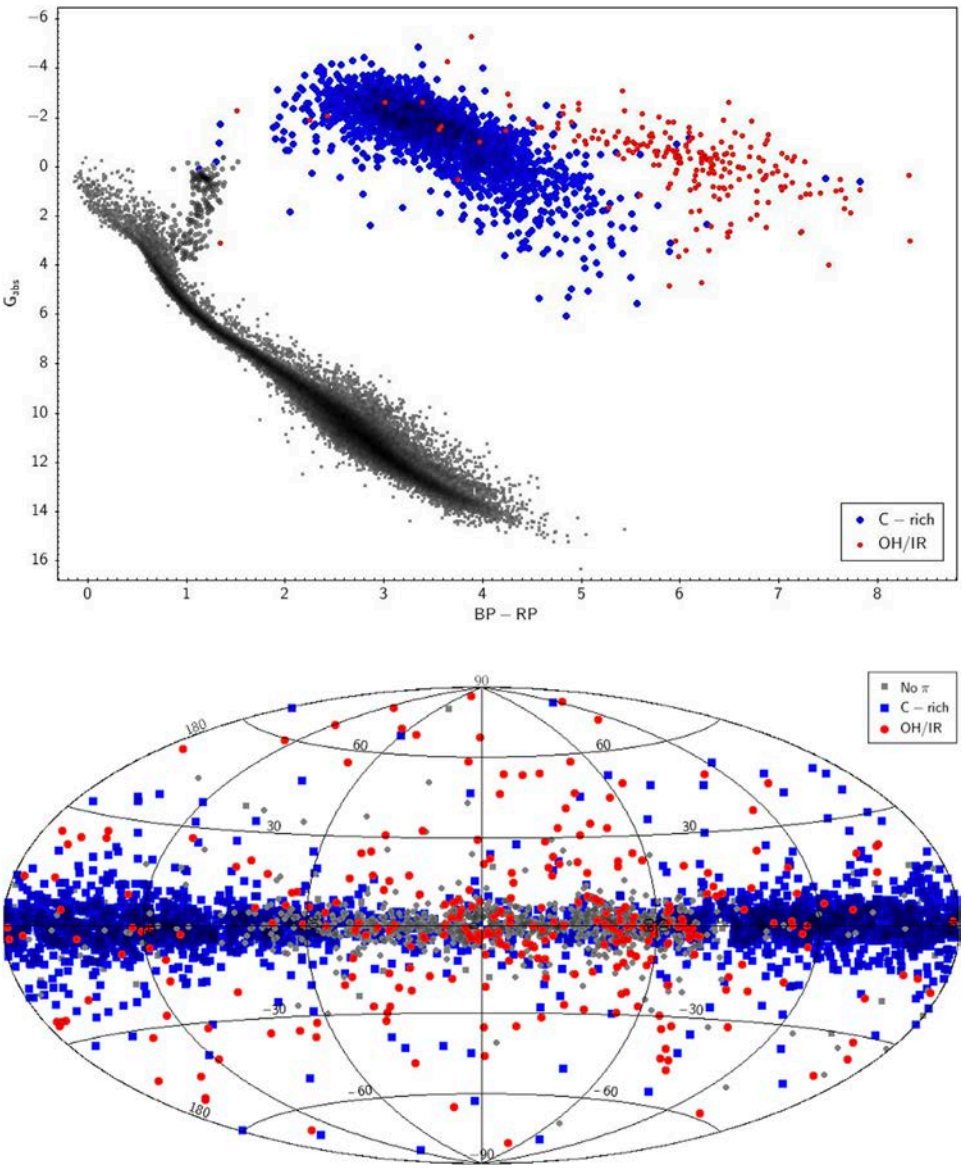


First tentative detections of v = 6 SiO maser line.

RH4: The Gaia Catalogue of Galactic OH/IR and C-rich AGB Stars

This research activity was performed in the framework of an ESA Express Procurement (EXPRO) contract. During 2021 we finished the construction of the Gaia Catalogue of Galactic OH/IR Stars and started its scientific exploitation. The catalogue contains 989 likely oxygen-rich AGB stars with OH masers and Gaia EDR3 counterparts; of them, 288 (26%) have good Gaia parallax measurements.

The previous work was extended with a Gaia Catalogue of Galactic C-rich AGB stars. While the OH/IR stars are thought to represent the largest mass fraction of AGB stars, the C-rich AGB stars represent an intermediate mass regime while the lowest-mass stars also have oxygen-rich envelopes, but their winds are not expected to be strong enough to produce OH maser emission. In 2021 a preliminary version of the catalogue was built through cross-matches of a literature compilation with several infrared catalogues and Gaia EDR3. Also, the Virtual Observatory tool VOSA was used to construct the spectral energy distributions of the sources to fit them with theoretical models in order to estimate their bolometric fluxes and, if a reliable parallax measurement was available, their absolute luminosities.



Gaia HR diagram for the OH/IR and the C-rich AGB stars with good parallaxes. Sky distribution of the samples

Other activities 2021

The CAB Astronomical Data Centre

The CAB Data Centre is the reference centre at national level for astronomical archives. A complete list of the archives managed by CAB Data Centre can be found here. All these archives are fully VO-compliant.

Among the activities carried out in 2021 we highlight the following ones:

Gran Telescopio Canarias Archive

- Definition of a procedure to handle spectropolarimetric data (CANARICAM).
- Improvement in the management of HIPERCAM data.
- Modification of the ingestion procedure for MEGARA data.

CARMENES Archive

- Improvement of the procedure to ingest off-line reduced spectra
- Improvement of the web application and its database. Error code management.
- Development of Technical Notes

New archives:

- EURD
- The SVO archive of white dwarfs from Gaia
- The SiO catalog towards 67 O-rich stars

Collaboration with other Spanish astronomical data centres

Assessment of the VO-compliance of the data obtained by the Yebes 40m radiotelescope.

VO-tools and services

In 2021 our group has continued working on the field of VO tools and services. New functionalities and data have been added to the already existing tools, and new tools have been developed.

Clusterix

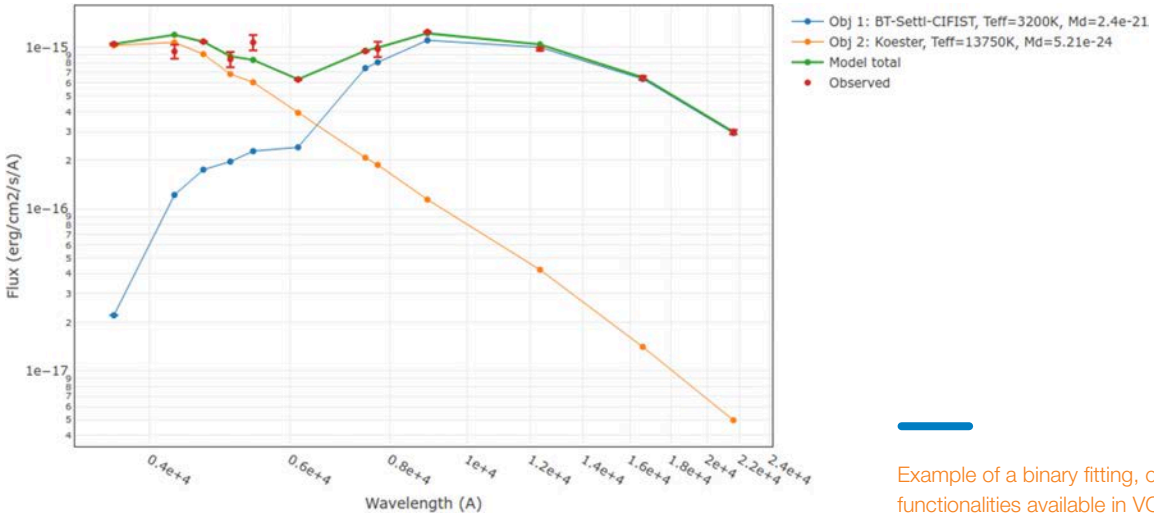
- Security reinforcement
- Ingestion of new catalogues (Gaia EDR3). New parameters (RUWE) in the query form.
- Stress testing. Implementation of warning/error messages for too demanding queries.
- Weekly removal of temporary files.
- Version control.

Others

- Ingestion of new collections of theoretical spectra (Pacheco et al. (2021)
- Technical assessment of the VO-compliance of MADCUBA
- New tools & applications
  - Empirical relations for estimating stellar masses and radii

VOSA

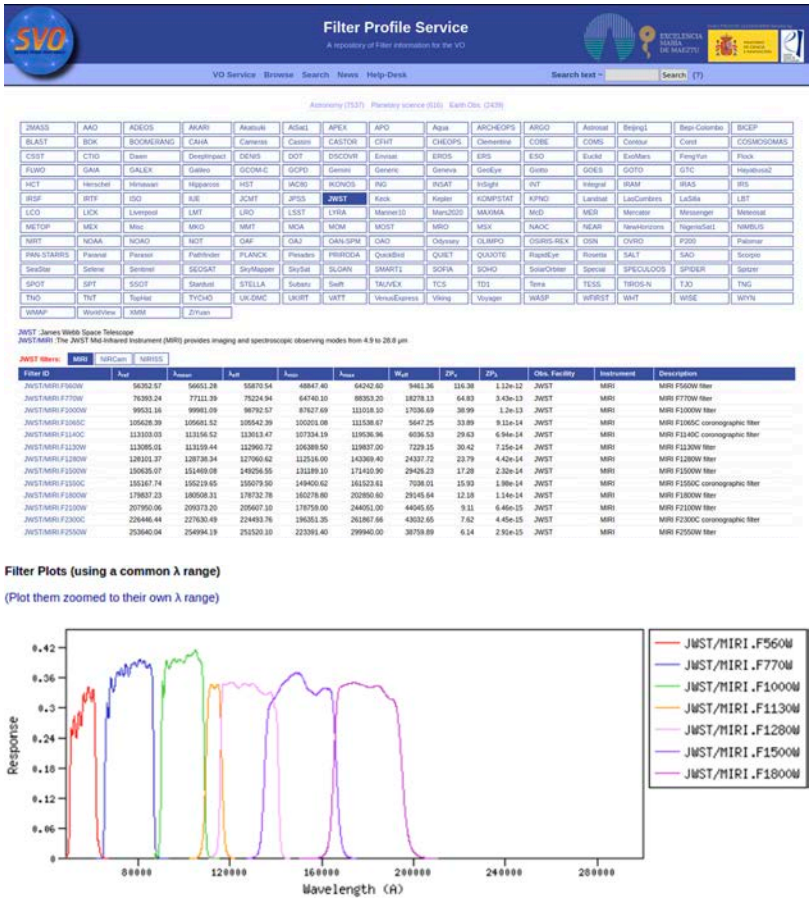
New release (VOSA 7.0).



Example of a binary fitting, one of the new functionalities available in VOSA 7.0

FPS

Ingestion of 1579 new filters. At present, the Filter Profile Service provides access to 10592 filters (7537 for astronomy, 616 for solar system and 2439 for Earth observation).



Screenshot of the *Information available at the Filter Profile Service on the JWST/MIRI filters*

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Molinaro M. et al. 2021. Supporting FAIR Principles in the Astrophysics Community: the European Experience. 2021arXiv211114468M

Balaguer-Núñez, L. et al. 2021. Clusterix2.0 for Gaia EDR3. 2021scgr.confE..26B

Barceló-Forteza, S. et al. 2021. The temperature, gravity, and frequency scaling relation for delta Scuti stars. 2021plat.confE..61B

Mendigutía, I. et al. 2021. Gaia EDR3 comparison of disk fractions from different spatial scales around young stellar clusters. 2021scgr.confE...6M

Passegger, V. et al. 2021. A deep learning approach to photospheric parameters of CARMENES target stars. 2021csss.confE.312P

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Miranda, L.F. 2021. The reactivation of water maser emission in the planetary nebula IRAS 18061--2505 through a born-again episode. 2021arXiv210505186M

Funded projects in 2021

El Observatorio Virtual Español. Explotación científico-técnica de archivos astronómicos

PI: Enrique Solano Márquez
Funding source: Ministerio de Ciencia e Innovación
Code: PID2020-112949GB-I00
Duration: 01/09/2021 – 31708/2024
Amount: 209935 euros (173 500 direct costs + 36435 indirect costs).

Education and Outreach

Virtual Observatory schools go virtual

Since 2009 the Spanish Virtual Observatory group has been actively participating in the organization of Virtual Observatory (VO) schools both at national and European level. These schools have two goals: to expose participants to VO tools and services, so they can efficiently use them for their research, and to gather feedback and requirements for VO tools and services and the schools themselves from the participants.

Due to the pandemic situation, the schools were moved online. Three schools were organised in 2021 with an attendance ranging from 49 to 112 participants (see below). This is quite relevant taking into account that "physical" schools were limited to 40 participants at most. The online VO schools represented a challenging experience but, at the same time, an opportunity to open new ways of spreading the VO knowledge and reach a broader audience.

List of VO schools:

Audience: Master/PhD students and early-career researchers

February. 49 participants (ESCAPE H2020 project)

October/December. 62 participants (PID2020-112949GB-I00 project)

Audience: Amateur astronomers

November. 112 participants (PID2020-112949GB-I00 project)

Other activities

Women promotion in STEM

Mentee for the Space4Women project (P. Cruz)

Public talks.

"Virtual Observatories" (P. Cruz)

"Descubriendo asteroides cercanos a la Tierra" (E. Solano)

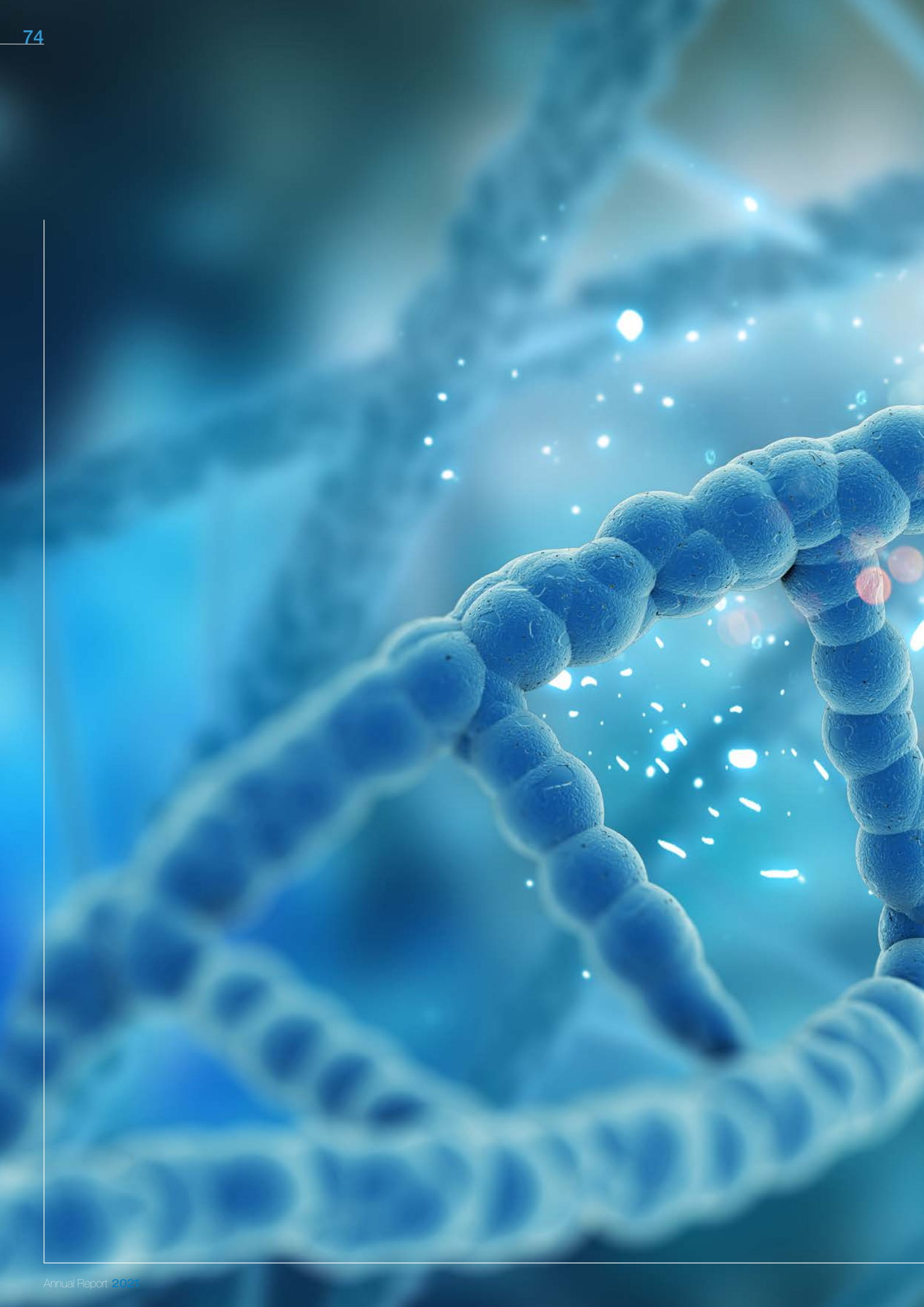
Contributions to Astroparsec (P. Cruz)

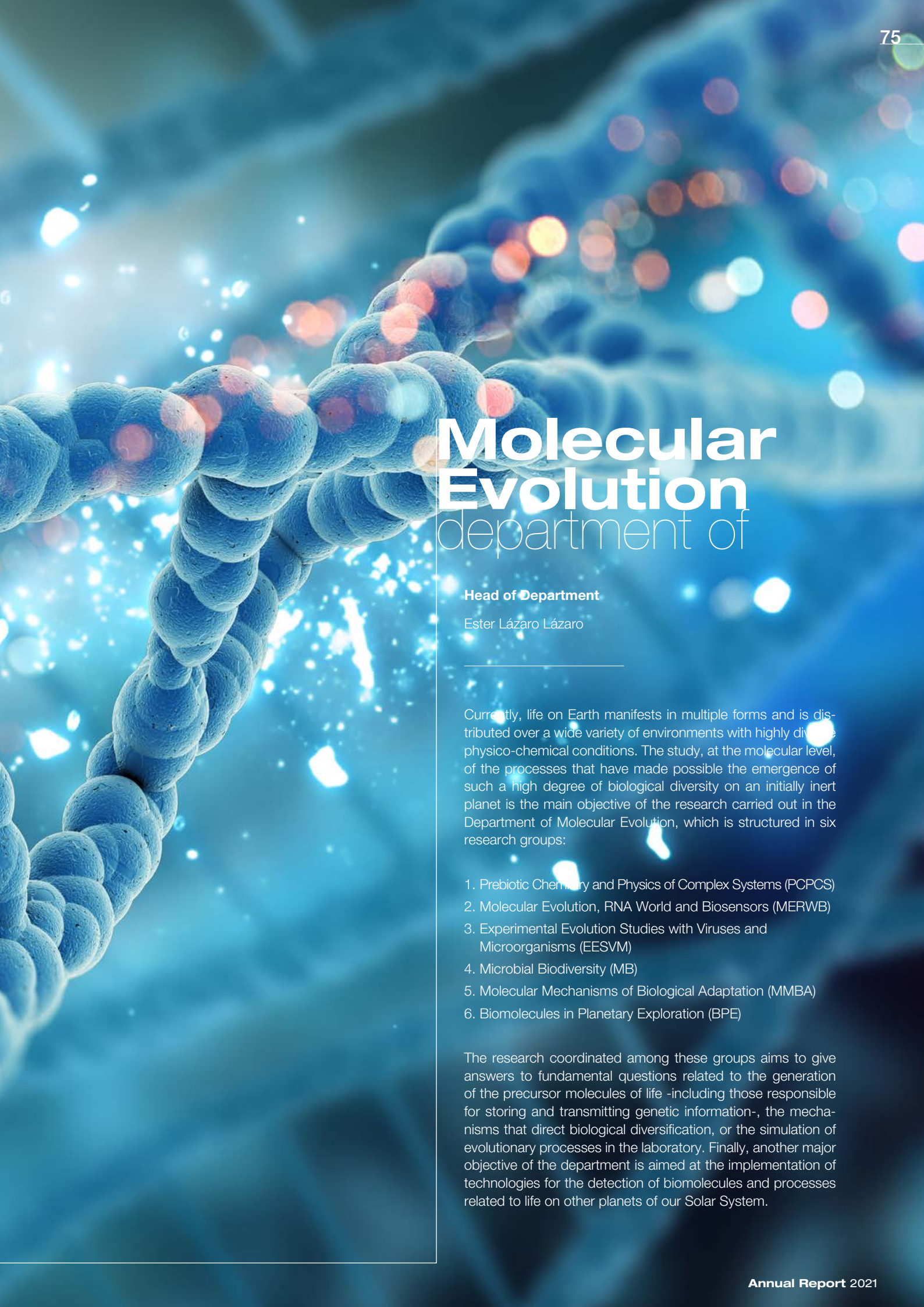
Citizen-science program:

Collaboration with high schools

Publication in "Ciel et Space"

Impresión artística de la misión PLATO. La carga útil consta de 26 telescopios. Dos cámaras más pequeñas, vistas en la parte inferior derecha, no forman parte de la carga útil, sino que se trata de cámaras de seguimiento de estrellas, utilizadas para la orientación. **Créditos: ESA/ATG Medialab.**





Molecular Evolution department of

Head of Department

Ester Lázaro Lázaro

Currently, life on Earth manifests in multiple forms and is distributed over a wide variety of environments with highly diverse physico-chemical conditions. The study, at the molecular level, of the processes that have made possible the emergence of such a high degree of biological diversity on an initially inert planet is the main objective of the research carried out in the Department of Molecular Evolution, which is structured in six research groups:

1. Prebiotic Chemistry and Physics of Complex Systems (PCPCS)
2. Molecular Evolution, RNA World and Biosensors (MERWB)
3. Experimental Evolution Studies with Viruses and Microorganisms (EESVM)
4. Microbial Biodiversity (MB)
5. Molecular Mechanisms of Biological Adaptation (MMBA)
6. Biomolecules in Planetary Exploration (BPE)

The research coordinated among these groups aims to give answers to fundamental questions related to the generation of the precursor molecules of life -including those responsible for storing and transmitting genetic information-, the mechanisms that direct biological diversification, or the simulation of evolutionary processes in the laboratory. Finally, another major objective of the department is aimed at the implementation of technologies for the detection of biomolecules and processes related to life on other planets of our Solar System.

Prebiotic Chemistry and Physics of Complex Systems (PCPCS)

Coordinator: David Hochberg

Senior Researchers
Marta Ruiz Bermejo
Eva Mateo-Martí
Jacobo Aguirre

Posdoctorals
Eduardo Cueto Díaz
Laura Jiménez Bonales

Posdoctoral trainees (1-3 years since PhD thesis):
Adrián Aguirre Tamaral

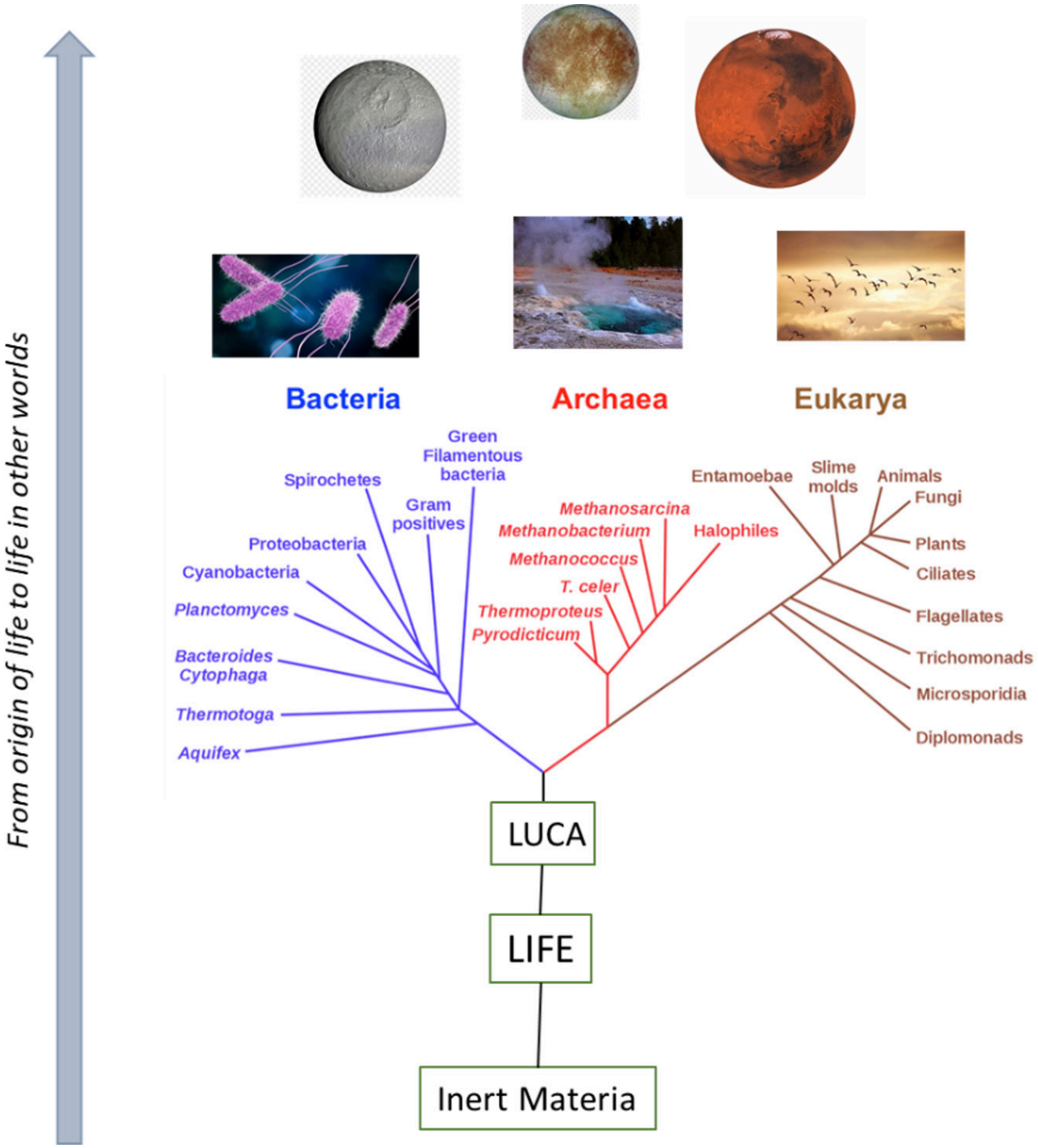
Predoctorals
Antonio López García
Cristina Pérez Fernández
Santos Gálvez Martínez

Technicians
Pedro Rayo Pizarroso

Students (Master, TFG, others):
Jorge Vega (TFG)
Marina Manjavacas (others)
Natalia Blanco Garcia (TFG)
Marina Fernández Ruz
Javier Gómez Sánchez
Sofia Backlund (Erasmus+University of Helsinki)

Summary

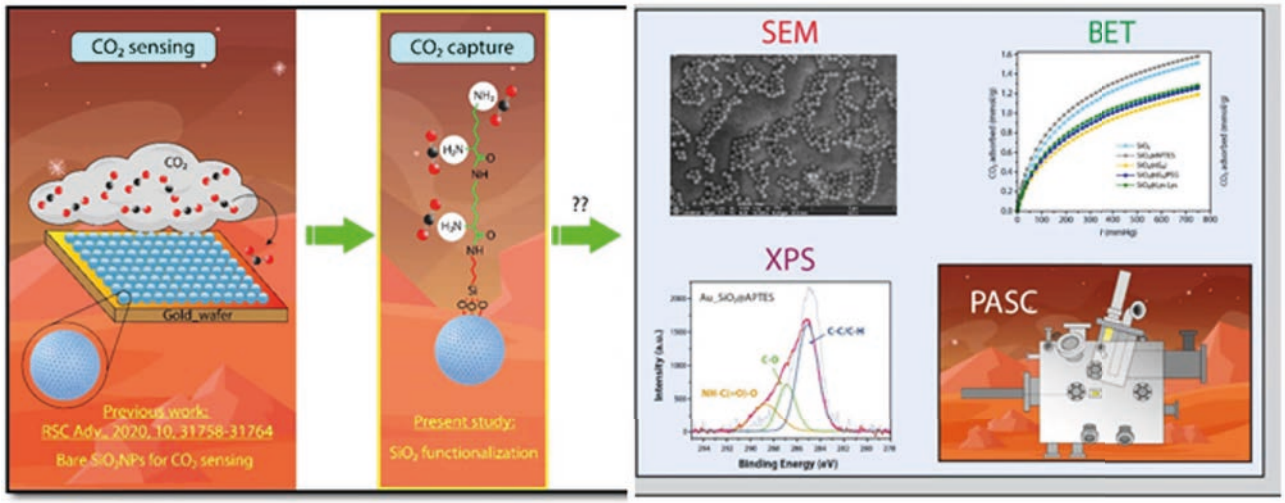
The Prebiotic Chemistry and Physics of Complex Systems group is concerned with the study of all aspects regarding the possible origins of life and its evolution on Earth, as well as with aspects related with the increase of molecular complexity and habitability on other planetary environments in the Solar System. These objectives are pursued from a completely transdisciplinary perspective, exploiting the connection between areas of expertise such as prebiotic chemistry, the physics and chemistry of surface science, non-equilibrium,stochastic thermodynamics and complexity theory, whose complementarity in the context of Astrobiology has not been sufficiently developed until only recently. Our methods range from experimental work simulating conditions on the primitive Earth to planetary environments in the Solar System, with an emphasis on liquid water interfaces, interaction of biomolecules on mineral surfaces and chemical reactivity to the mathematical modeling of complex processes, and supported by computation based on the use of experimental and observational data. The research carried out by our group contributes to objectives **O1, O2, O3 and O5.**


From origin of life to life in other worlds
Bacteria
Archaea
Eukarya
Green Filamentous bacteria
Spirochetes
Gram positives
Proteobacteria
Cyanobacteria
Planctomyces
Bacteroides Cytophaga
Thermotoga
Aquifex
Methanosarcina
Methanobacterium
Methanococcus
T. celer
Thermoproteus
Pyrodicticum
Halophiles
Entamoebae
Slime molds
Animals
Fungi
Plants
Ciliates
Flagellates
Trichomonads
Microsporidia
Diplomonads
LUCA
LIFE
Inert Materia

Research Highlights 2021

RH1: Exploring functional silica nanoparticles as suitable for CO2 detection and storage, under well controlled experimental Martian conditions

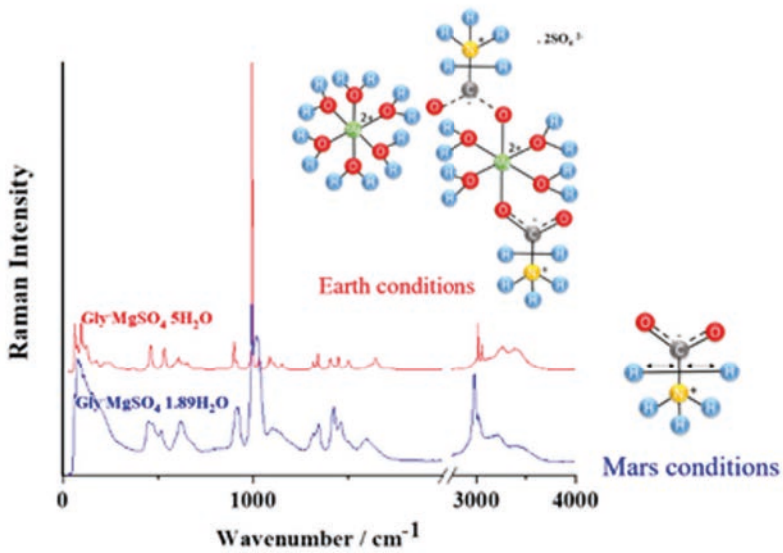
Here, we show how functional silica nanoparticles can be used for CO_2 physisorption and chemisorption. We analyze the system, both spectroscopically and morphologically, before and after exposure to an atmosphere of 7 mbar of CO_2, inside a planetary atmospheres and surfaces simulation chamber, (PASC) mimicking Martian atmospheric conditions. Our studies demonstrate that these clusters are suitable for CO_2 detection and storage, under well controlled experimental Martian conditions. The influence of functional chemical groups in the CO_2 retention was investigated using a battery of surface science techniques such as: FTIR, XPS, SEM and BET. Furthermore, our goal was to explore the influence of functional chemical groups (attached to the SiO_2NPs) on CO_2 sequestration. The observed results showed that at low and high CO_2 gas pressure conditions, typical APTES functionalized SiO_2Np surpassed the CO_2 adsorption capacities of dendritic and peptide-based nanoparticles bearing amine-polymer functionalities, a remarkable effect that was investigated in this work. In addition, a convenient and facile method to decorate and quantify SiO_2 nanoparticles with PAMAM and a short peptide was reported.

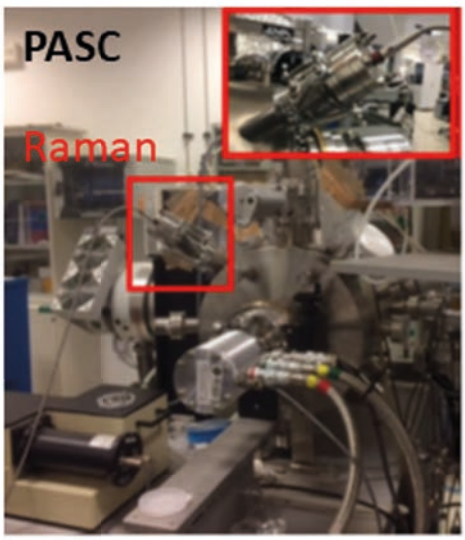


Functional silica nanoparticles for CO_2 adsorption inside PASC and their characterization by surface science techniques.

RH2: Exploring Raman molecular/mineral spectroscopic fingerprints under Mars conditions

Identifications of relevant Mars types of environments is crucial to search for unequivocally molecular/mineral spectroscopic fingerprints. Therefore, we study the stability of Gly.$MgSO_4$.$5H_2O$ under Mars-like surface conditions, compared to the behaviour of epsomite and glycine. Gly.$MgSO_4$.$5H_2O$ has been recently identified as a molecule with astrobiological interest since an amino acid and water molecules, which are essential for life, are part of its structure. Furthermore, this compound may form by interaction of sulphates minerals with glycine-bearing aqueous solutions, and both could be presents at Mars. The main analyses were performed by using *in situ* Raman spectroscopy, upcoming ground-breaking technique for NASA and ESA Mars planetary missions. Raman spectroscopy has been set-up into the Planetary Atmosphere and Surfaces Chamber allowing us to successfully identify and compare the process occurring in molecules exposed to Mars simulated conditions: atmosphere, UV irradiation and temperature. Ours results show that pressure is critical to provoke dehydration and amorphization of Gly·$MgSO_4$·$5H_2O$ and release of the glycine from a matrix compound; low temperature provides greater stability to Gly·$MgSO_4$·$5H_2O$ compared to glycine and epsomite individually. This strategy is designed to be able to evaluate by Raman spectroscopy how diverse Mars simulated environmental conditions favour or inhibit molecular preservation and their identification.

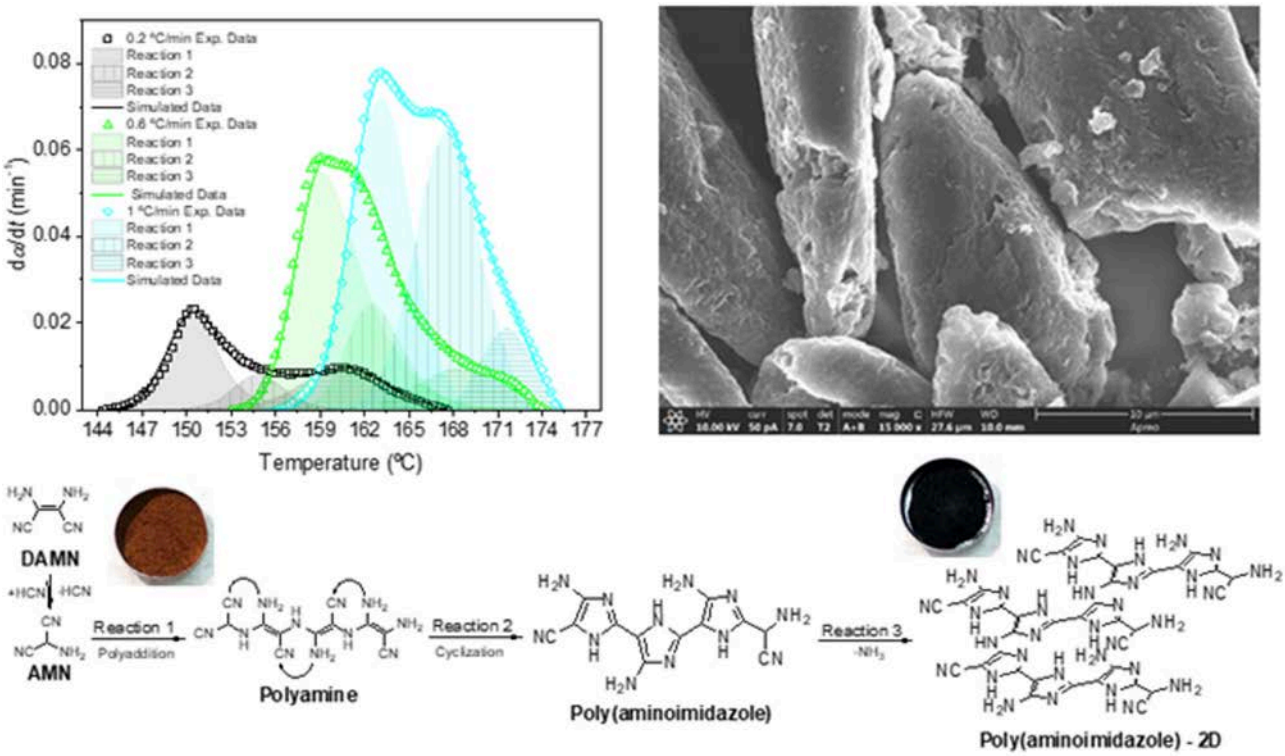




The evolution of Gly$MgSO_4$ $5H_2O$ is studied at Mars relevant conditions during its dehydration and UV irradiation by *in situ* the Raman spectroscopic inside planetary atmospheres and surfaces chamber (PASC).

RH3: Exploring the HCN chemistry

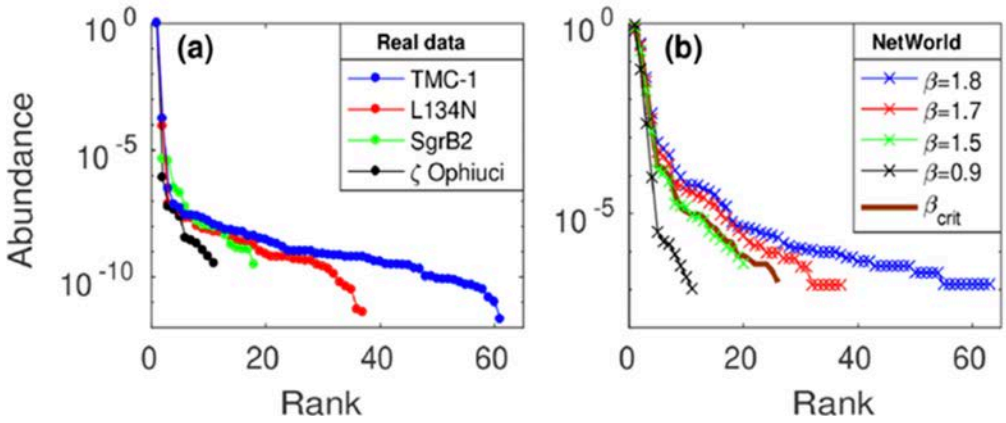
HCN polymers are a heterogeneous family of substances synthesized under different conditions using neat HCN, its soluble salts (NaCN, KCN, NH_4CN), its oligomers (aminomalononitrile or diaminomaleonitrile), or its hydrolysis product such as formamide. These complex macromolecular systems are astrobiologically interesting because they may be precursors of important bioorganics such as amino acids, purines, pyrimidines, pteridines and carboxylic acids. In addition, they present attractive redox properties and can act as protective films against corrosion, which offers completely unexplored new perspectives in the field of prebiotic chemistry and by extension in materials science.



Thermal activation of DAMN leads to the generation of HCN-derived polymers.

RH4: The emergence of interstellar molecular complexity explained by interacting networks

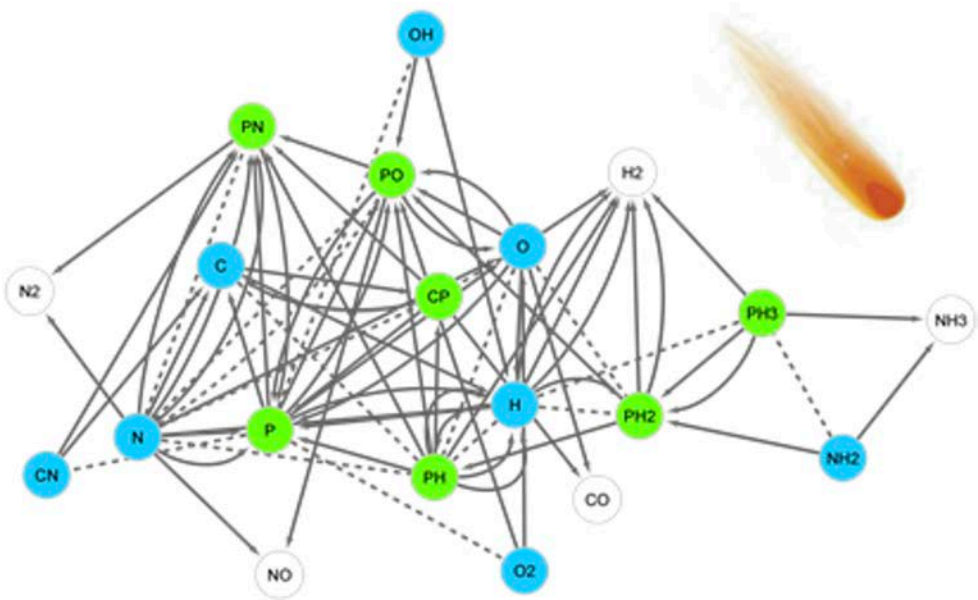
This work introduces the computational framework *NetWorld* to address how fruitful can complexity theory and network science be to disentangle the origin of the building blocks of life and their role in the long way from astrochemistry to biology. In our model, complex networks simulate interacting chemical compounds, and we describe the emergence of a transition from simple networks that mimic the most basic initial molecular ensembles towards chemical complexity when the parameter representing the environment reaches a critical value. Our results, while obtained in an abstract context that is totally different to that of real chemistry, predict the evolution of chemical complexity in the interstellar medium, proving the applicability of the conceptual scenario here presented and suggesting that the rules leading to the emergence of complexity may be universal.



Comparison between the predictions of the digital environment *NetWorld* and the evolution of chemical complexity in 4 real interstellar clouds, the astrochemical environments where the most basic bricks of life were created.

RH5: Study of astrochemical complex networks: the chemistry of the interstellar phosphorus

Phosphorus chemistry in the interstellar medium has become a topic of growing interest in astrobiology, as it is present in many organic molecules. In fact, it is plausible that some of these molecules were introduced in the early Earth during the *Late Heavy Bombardment* 4 billion years ago –inside asteroids or comets-, and importantly enrich prebiotic chemistry. Here we present a model of the P-chemical network for an interstellar diffuse cloud, focusing on the relevant molecules PO and PN. Making use of a novel and fruitful connection between complex network theory and astrochemistry, we totally solve the system obtaining explicit mathematical expressions for the evolution of the abundances of all the species involved, obtaining with an unprecedented precision the abundances of the chemical compounds and the reaction rate coefficients that are compatible with the observed values in different astrophysical environments. Our work could help to improve the existing astrochemical models significantly reducing their level of parameter uncertainty, and to a better understanding of the formation of the chemical precursors of organic macromolecules in space.



Interstellar phosphorus chemistry network.

RH6: A complexity theory approach to prebiotic chemistry in the early Earth: towards the first RNA replication

The *RNA world* hypothesis suggests that life was preceded by an environment in which RNA molecules were able to self-replicate. However, the minimum size for an RNA polymerase ribozyme is around 165 nt, 3-4 times longer than what is attainable through abiotic, random polymerization of RNA. This limitation could be solved with a *modular evolution* of RNA, but current models face the difficulty of obtaining many identical copies of a specific RNA sequence. In this line of research, started at the end of 2021, we combine the mathematical modeling of complex systems with the RNA biochemistry to develop a computational model to study the possible first replication of RNA molecules located in an adequate environment of the early Earth, and how it could depend on the parameters of the system (RNA length, size of genetic alphabet, strength of chemical bonds and probability of rupture, environmental conditions, etc.)

RH7: Study of complexity in the present biosphere

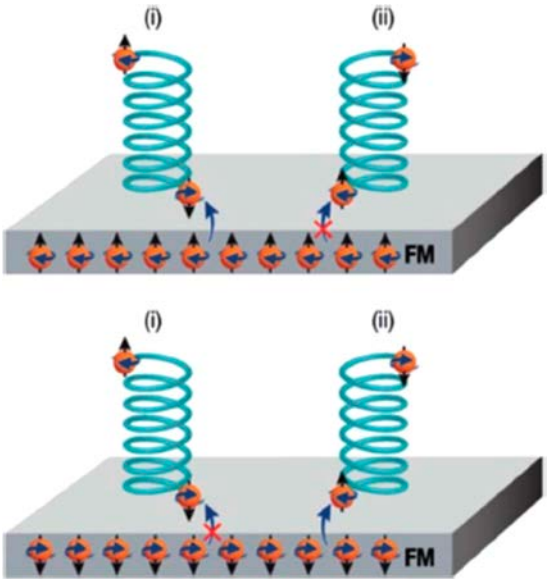
In this line of research we focused on three systems of different nature and scale:

- The interaction between the proteins of the Epstein-Barr virus, the Herpes virus and the Vaccinia virus with the proteins of a human cell at different moments of the infection. We have focused on the host-virus protein co-expression networks, and the correlation between the different topological communities detected in them and the biochemical function of their proteins.
- Application of complexity theory and artificial intelligence to the study of animal social networks.
- The review of the state of the art of a major missing piece in a fully predictive theory of evolution: understanding how genotypes map onto phenotypes, fitness and eventually organisms.

RH8: Spontaneous Deracemizations (A Review)

Chirality, or handedness, is a fundamental physical attribute, which spans the length scales ranging from the elementary particles to the asymmetry of galaxies. The way that chirality in chemistry, or molecular handedness, arose in a primitive terrestrial environment and how it can be triggered, amplified and transferred by chemists, are challenging problems with clear scientific and technological potentials for science and society. Chirality constitutes a unifying feature of the living world and is a prime driving force for molecular selection and genetic evolution.

This work is an authoritative review, which will be of particular interest for the communities of organic, inorganic and physical chemists who are interested in achiral-to-chiral transformations and for all researchers acquainted with conglomerates, spontaneous asymmetric synthesis, cryptochirality, chiral fields and forces, chirality at the nanoscale, mirror-symmetry breaking processes, nonstochastic behavior, autocatalysis, nonlinear chemical dynamics and the origin of biological homochirality.



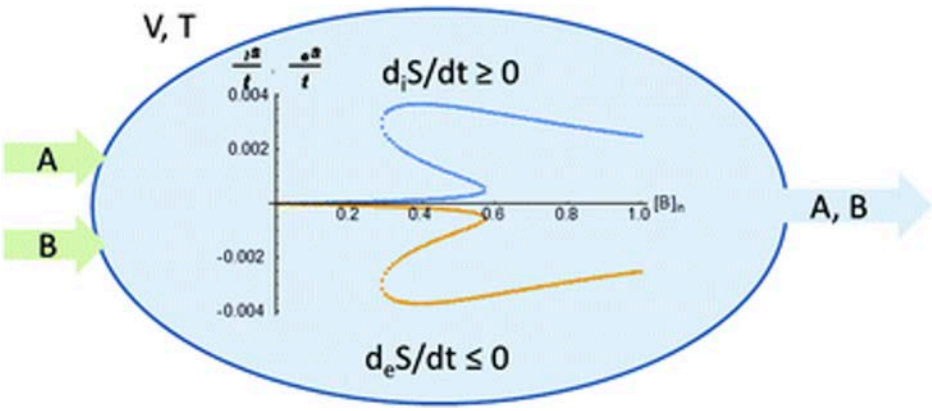
Enantioseparation by crystallization using magnetic substrates by chirality-induced spin selectivity (CISS). Spin-polarized ferromagnet interacts favorably with enantiomers that have antiparallel spin. Consequently, the longer residence time of one amino acid enantiomer on the surface, owing to its stronger interaction, increases its probability of crystallization. The left and right green helices indicate the handedness of each process.

Research Highlights 2021

RH9: Entropic analysis of bistability and the General Evolution Criterion

A reaction network has the ability for bistability when there exist combinations of parameter values, as for example, rate constants and substrate supply rates, such that corresponding reaction rate equations admit at least two different stable stationary states. Bistability and switch-like behavior has attracted considerable attention recently. Both theoretical and experimental evidence exist pointing to the capacity of metabolic pathways for bistability Bistability, multistability, and the associated patterns of bifurcation have been found in a number of biochemical networks, including cellular, genetic, metabolic, and catalytic networks. Such dynamical properties are believed to be at the core of the proper functioning of biochemical reaction networks and of living systems.

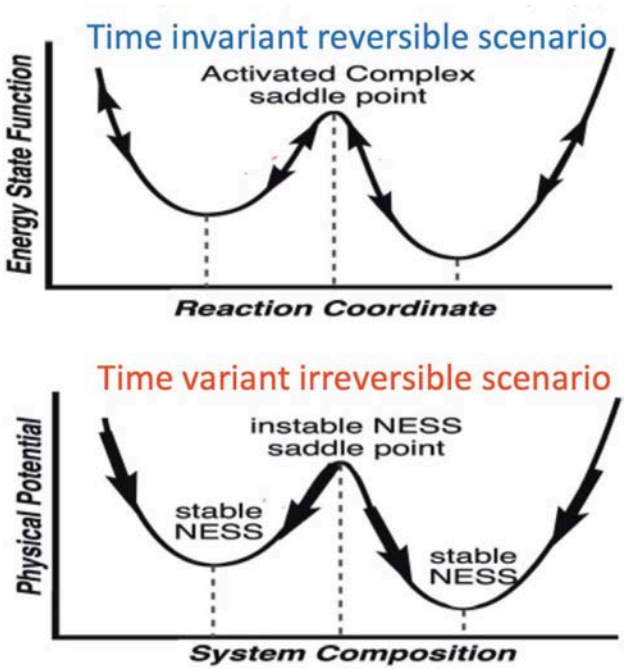
In this work we present a detailed study of the entropy production, the entropy exchange and the entropy balance for the Schlögl model of chemical bi-stability for both the clamped and volumetric open-flow versions. The General Evolution Criterion (GEC) is validated for the transitions from the unstable to the stable non-equilibrium stationary states. The GEC is the sole theorem governing the temporal behavior of the entropy production in non-equilibrium thermodynamics. We also use stoichiometric network analysis to calculate the distribution of the entropy production and the exchange entropy over the elementary flux modes of the clamped and open-flow models, and serves to reveal the underlying mechanisms of dissipation and entropy exchange.



An open flow bistable Schlögl model in a well-stirred isothermal reaction volume V showing the balance of the entropy production (upper blue curve) and the exchange entropy (lower brown curve) on the non-equilibrium stationary states. The system is maintained out of equilibrium by matter flow: species A, B flow in and flow out.

RH10: Interpreting the Emergence of Chemical Complexity

The way chemical transformations are described by models based on microscopic reversibility does not take into account the irreversibility of natural processes, and therefore, in complex chemical networks working in open systems, misunderstandings may arise about the origin and causes of the stability of non-equilibrium stationary states, and general constraints on evolution in systems that are far from equilibrium. In order to be correctly simulated and understood, the chemical behavior of complex systems requires time-dependent models, otherwise the irreversibility of natural phenomena is overlooked. Micro-reversible models based on the reaction-coordinate model are time invariant and are therefore unable to explain the evolution of open dissipative systems. The important points necessary for improving the modeling and simulations of complex chemical systems are: (a) understanding the physical potential related to the entropy production rate, which is in general an inexact differential of a state function; (b) the interpretation and application of the so-called General Evolution Criterion (GEC), which is the general thermodynamic constraint for the evolution of dissipative chemical systems.



Time-invariant models (top panel) are the basis of the molecular description of modern organic chemistry. However, applied to open systems far from equilibrium, they may lead to erroneous interpretations. In such systems, stationary states must be described, in both their stability and evolution (generalized evolution criterion), through irreversibility (time variant) by macroscopic systems methods (bottom panel). Even the ordinate, abscissa and curves, in reductionistic graphical descriptions; have quite different meanings, as exemplified above.

Publications

Muñoz Iglesias V, Fernández-Sampedro M, Gil-Lozano C, Bonales L J, Ercilla Herrero O, Valles González M.P., Mateo-Martí E, Prieto-Ballesteros O. 2021 Characterization of NH_4-montmorillonite under conditions relevant to Ceres. Applied Clay Science, 209, 106137.

Villafañe-Barajas, S. A.; Ruiz-Bermejo, M.; Rayo Pizarroso, P.; Galvez-Martinez, S.; Mateo-Martí, E.; Colín-García, M. 2021. A serpentinite lizardite-HCN interaction leading the increasing of molecular complexity in an alkaline hydrothermal scenario: Implications for the origin of life studies". Life, 11, 661.

Pérez-Fernández, C.; Ruiz-Bermejo, M.; Gálvez-Martínez, S.; Eva Mateo-Martí. 2021. A XPS study of HCN-derived films on pyrite surfaces: A prebiotic chemistry standpoint towards the development of protective coatings. RSC Adv., 11, 20109–20117.

Hortelano, C.; Ruiz-Bermejo, M.; de la Fuente, J. L. 2021. Solid-state polymerization of diaminomaleonitrile: toward a new generation of conjugated functional materials. Polymer, 223, 123696.

Mas, I.; Hortelano, C.; Ruiz-Bermejo, M.; de la Fuente, J. L. 2021. Highly efficient melt polymerization of diaminomaleonitrile. Eur. Polym. J., 143, 110185.

Ruiz-Bermejo, M.; de la Fuente, J. L.; Pérez-Fernández, C.; Mateo-Martí, E. 2021. A comprehensive review of HCN-derived polymers. Processes, 9, 597.

Cueto-Díaz EJ, Castro Muñiz A, Suárez-García F, Gálvez-Martínez S, Torquemada-Vico MC, Valles González MV, Mateo-Martí E. 2021. APTES based silica nanoparticles as a potential modifier for the selective sequestration of CO_2 gas molecules. Nanomaterials (10.3390/nano11112893) 11, 2893, 1-19.

Manrubia S, Cuesta JA, Aguirre J *et al.* 2021. From genotypes to organisms: State-of-the-art and perspectives of a cornerstone in evolutionary dynamics. Physics of Life Reviews 38, 55-106.

Briones C, Jiménez-Serra I, Aguirre J *et al.* 2021. Challenge 1: The origins of life, from chemistry to biology. White Paper 2: Origins, (Co)evolution, Diversity & Synthesis of Life: 20- 53. Consejo Superior de Investigaciones Científicas (España).

Buhse T, et al. 2021. Spontaneous Deracemizations. CHEMICAL REVIEWS, 121, 2147-2229.

Hochberg D, Ribó JM. 2021. Entropic analysis of bistability and the general evolution criterion. PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 23, 14051-14063.

Ribó JM, Hochberg, D. 2021. The Coordinate Reaction Model: An Obstacle to Interpreting the Emergence of Chemical Complexity. CHEMISTRY-A EUROPEAN JOURNAL, 27, 13098-13106.

Funded projects in 2021

Operación técnica y explotación científica de datos en RSL de Exomars, y contribucion al RAX de MMX. PI: Olga Prieto Ballesteros / Daniel Carrizo Gallardo. Funding source: Ministerio de Ciencia e Innovación. PID2019-107442RB-C32. 01/01/2020-2021. 665.379 €.

Ciclo de aerosoles en Marte y la Tierra, estudio comparativo. Implicaciones para la vida y protección planetaria-atmosferas (CAMELIA-ATM). PI: Maria-Paz Zorzano Mier / Carmen Cordoba Jabonero. Funding source: Ministerio de Ciencia e Innovación. PID2019-104205GB-C21. 01/06/2020-2023. 75.000 €.

Title: MIRROR-SYMMETRY BREAKING IN CONTINUOUS FLOW CHEMICAL PROCESSES: THEORETICAL ANALYSIS AND APPLICATIONS TO CATALYSIS
PI: David Hochberg
Source: Ministerio de Ciencia e Innovación
Code: PID2020-116846GB-C22
Duration: 3 years
Amount: 23.800 €

Public Outreach Activities, TFG and TFM

1.- Tutor Dr. E. Mateo- Marti of the students' internships and the Final Degree Project (TFG): Ms. Natalia Blanco García. Degree in Experimental Sciences (Universidad Rey Juan Carlos) Date: 1/03/2021-30/06/2021. Title: "Reactivity of biomolecules on mineral surfaces in planetary simulation environments".

2.- Co-directors Dra. Marta Ruiz-Bermejo and Dr. José L. de la Fuente of the Final Degree Project (TFG): Jorge Vega Fernández. Degree in Chemical Sciences (Universidad de Alcalá de Henares). Date: 1/03/2021-15/07/2021. Títle: "Influence of the ammonium ion in the synthesis and properties of cyanide polymers".

3.- Invited Oral Presentation Dr. E. Mateo- Marti: Title: "Planetary Atmosphere and Surface Simulation Chamber (PASC): studies in astrobiology. Conference: Presentation of the Thermal Vacuum Chamber of the University of Malaga Planetary Exploration: research strategies in extraterrestrial environment chambers Faculty of Science, University of Malaga (Spain), 17 September 2021.

4.- Lecture Dr. E. Mateo- Marti: "Simulation chambers for planetary environments and astrobiology". Almirante Don Juan de Borbón Chair. Complutense University of Madrid. Centro Superior de Estudios de la Defensa Nacional ECTED 2021.

5.- Seminar Dra. Marta Ruiz-Bermejo: "HCN chemistry: From researches about the origins of life to materials sciences". Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden, 3 December 2021.

6.- During 2021 the work of Jacobo Aguirre was presented at 3 conferences (two plenary talks and one poster), was invited to give a plenary talk at the *Polish Astrobiological Society Meeting*, was member of the Program Committee of one international conference, and taught a 30-hour course on Astronomy at Universidad Rey Juan Carlos. Furthermore, he supervised 2 Master's Thesis students and 1 Erasmus+ student:

- Marina Fernández Ruz, Master's thesis at Universidad Autónoma de Madrid, JAE Intro ICU scholarship, *Interstellar phosphorus chemistry as a complex system: a theoretical approach to the formation of the simplest building blocks of life.* Sept 2020-Sept 2021.
- Javier Gómez Sánchez, Master's thesis at Universidad Autónoma de Madrid, *Application of complexity theory to the study of animal social networks*. Sept 2020-June 2021.
- Sofia Backlund, Erasmus+ scholarship, University of Helsinki, *The complex interaction between virus and host protein networks during a viral infection.* Feb. 2021-Sept 2021

7.- Invited Lecture, Dr. David Hochberg. Title: "General Evolution Criterion in Chemistry: Bistability and Spontaneous Mirror Symmetry Breaking". Conference: IV Simposio en Investigaciones en Quiralidad, Universidad del Estado de Morelos, Cuernavaca, Mexico, 11 November 2021.

8.- Invited Lecture, Dr. David Hochberg. Title: "Chemical Basis of the Origins of Biological Homochirality". Conference: Faculty of Science, University of Heidelberg (Germany), 17 May 2021. HIFOL Colloquium Series, Heidelberg, Germany.

Experimental evolution studies with viruses and microorganisms (EESVM)

Coordinator: Ester Lázaro Lázaro

Predoctorals

María Arribas Hernán

Mara Laguna Castro

Technicians:

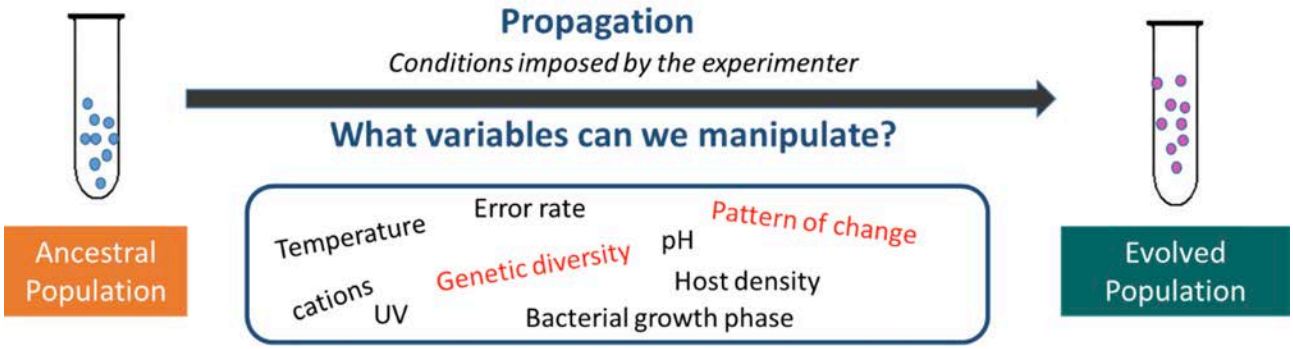
--

Students

Alicia González Moreno (TFM)

Blanca Martín Urdiales (TFG)

Sandra Pérez García (extracurricular practices)



Summary

This group contributes to objective O5 of Center Strategic Plan. In order to understand how life has diversified since its origin, it is necessary to know the basic principles that drive adaptation to different environments. In this sense, the re-creation of evolutionary processes in the laboratory, using simple organisms that evolve rapidly under controlled conditions, has allowed great advances in the identification of relationships between environmental parameters, genetic changes and specific adaptations. RNA viruses meet most of the requirements to be used as an experimental system in this type of studies. They have short generation times and replicate their genomes with very high error rates, giving rise to large, highly heterogeneous populations, composed by a dynamic ensemble of mutants which adapts rapidly to most changes in environmental conditions.

Our experimental system is bacteriophage Qβ. This virus has a single-stranded, positive-sense RNA genome of only 4217 nucleotides that facilitates the establishment of genotype-phenotype relationships. Evolutionary experiments carried out in our group are usually focused on analyzing the genotypic and phenotypic changes experienced by Qβ when it is propagated under the particular conditions whose influence on evolution we want to analyze. The following research highlights exemplify the most relevant investigations and results in the group.

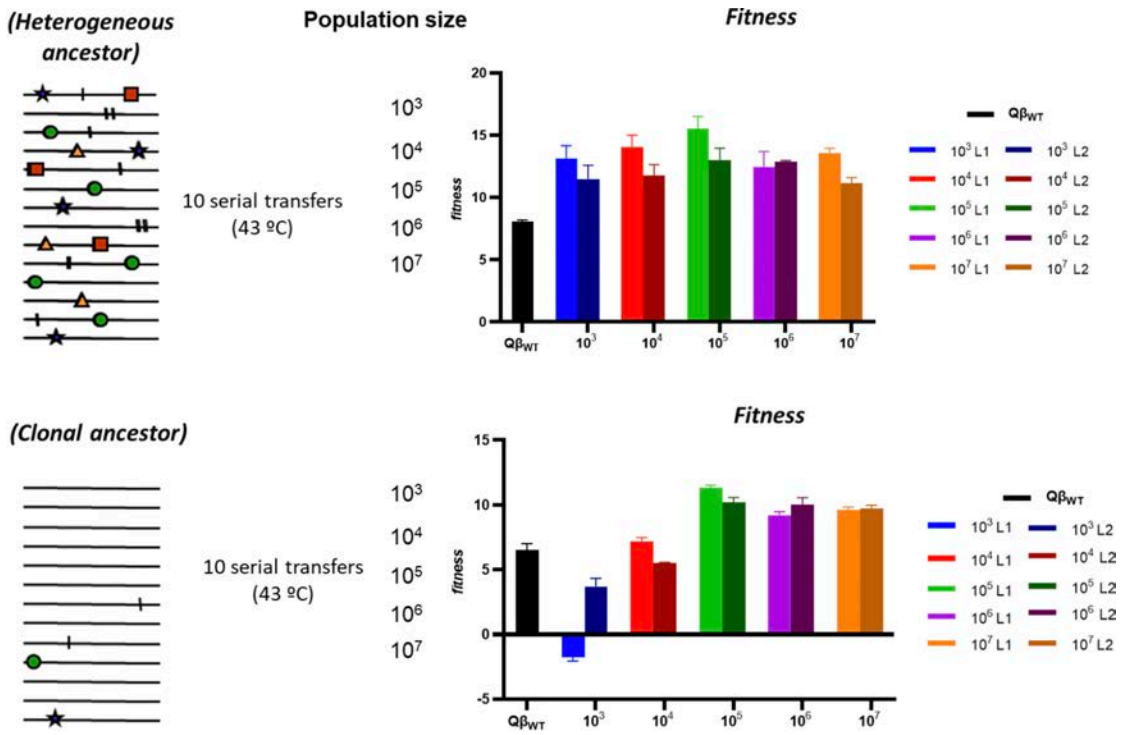
Research Highlights 2021

RH1: Propagation of Qβ at 37º C generates a mutant spectrum that contains low-frequency mutations relevant for adaptation to 43 °C

Massive sequencing analysis of the mutant spectrum of a Qβ population propagated at 37 °C shows the presence, at frequencies so low as to prevent its detection in the consensus sequence, of some mutations that had been previously identified as responsible for virus adaptation to 43 °C. These mutations, which remain in low proportion during evolution at 37 °C, could constitute the basis on which natural selection begins to act when the environment changes. Additional experiments are currently underway to confirm whether these mutations are also selected when the virus is exposed to selective pressures different of changes in temperature.

RH2: Relationships between population size and pre-existent genetic diversity on adaptation to increased temperature

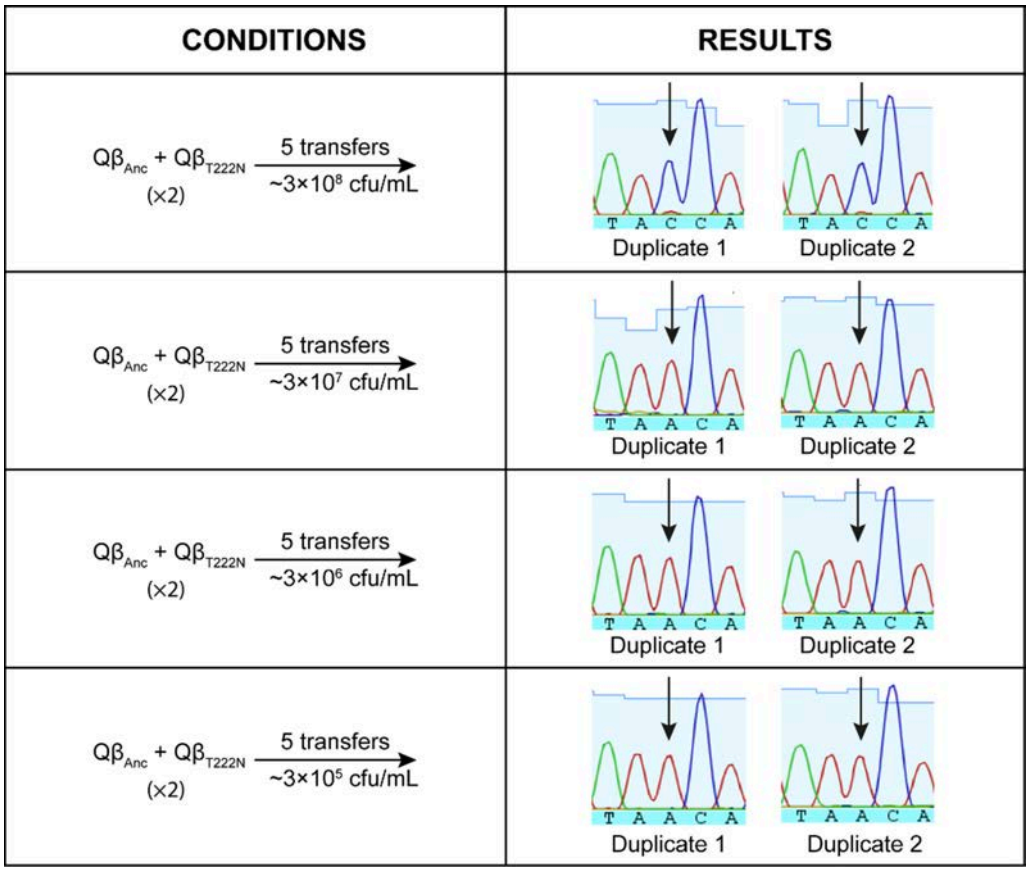
In this study, we focused on understanding the relationships between the genetic diversity contained in a virus population, the bottleneck size used for virus transmission during adaptation to a new selective pressure, and the magnitude of the change experienced in fitness. The experimental work consisted in the propagation of a Qβ population at 43 °C using different population sizes at each transfer that gave rise to different evolutionary lineages. The results showed that the adaptive pathways followed at 43 °C depended on the population size, although the growth rate values reached by the different evolved populations did not vary as a function of this parameter. In contrast to this, the change in the growth rate of a low diversity Qβ population (a biological clone), which was propagated in parallel, was clearly dependent on the population size, with small sizes being incompatible with adaptation. Our main conclusion was that the effect of the transmission bottleneck size on virus adaptation has a clear dependence on the pre-existent genetic diversity contained in the ancestral population.



Scheme showing the evolution experiment followed by two virus populations differing in their initial genetic diversity. The fitness values reached by the evolutionary lineages whose ancestor was the heterogeneous population did not depend on the population size, whereas when the ancestor was a clonal population, there was a clear dependence on the population size.

RH3: Analysis of evolutionary strategies followed by an RNA bacteriophage propagated in conditions of low host availability

The successful spread of a virus in a population is largely determined by host availability. The lower the host concentration, the longer the virus spends in the external environment between successive infections, thus increasing its probability of degradation due to physical-chemical variables, which ultimately could lead to its extinction. Nevertheless, the high error rate of viral replication, particularly in the case of RNA viruses, can lead to the emergence and subsequent selection of mutants that increase their probability of transmission under unfavorable conditions. In this work we have carried out an evolution experiment in which the bacteriophage Qβ was propagated at suboptimal host concentrations under conditions that prevent the selection of defense mechanisms in the bacteria. Our results show that there is a minimal host concentration that separates sustained propagation from extinction. After a certain number of generations, all lineages propagated at suboptimal host concentration selected a mutation in a minor capsid protein whose phenotypic effect was to favor the entry of the virus into the cell.



Competition between the ancestral virus and a mutant containing the mutation that was selected in the evolution experiment. The mutation was dominant at all host densities but the highest one assayed.

Publications

Arribas M, Lázaro E. 2021. Intra-Population Competition during Adaptation to Increased Temperature in an RNA Bacteriophage. *Int J Mol Sci*. 2021;22(13):6815.

Funded projects in 2021

Title: Experimental evolution of an RNA bacteriophage: Influence of contact networks, external environment, and pre-existing mutations (EVOLCEM)
PI: Ester Lázaro
Funding Source: Agencia Estatal de Investigación
Code: PID2020-113284GB-C22
Duration: 1-9-2021/31-08-2024
Amount: 91.960 €

Doctoral Thesis

"Influencia de la diversidad inicial y la pauta de cambio ambiental en la evolución del bacteriófago Qβ". Defended by Pilar Somovilla Crespo at Universidad Autónoma de Madrid (2021-06-29). Grade: Sobresaliente cum laude.

Master Thesis (TFM)

"Relaciones entre tamaño poblacional y diversidad genética en la adaptación a temperatura elevada del bacteriófago Qβ". Defended by Alicia Rodríguez Moreno at Universidad Complutense de Madrid (2021-09-30). Grade 8.8.

Final degree Projects (TFG)

"Caracterización del efecto de un mutante del bacteriófago Qβ en la adaptación a temperatura elevada". Defended by Blanca Martín Urdiales at Universidad Politécnica de Madrid (2021-07-12). Grade: 8.7.

Outreach (most relevant contributions)

Conferences

"Virus emergentes. Una amenaza global". A total of 4 conferences were given in the Science Evening Cycle of CaixaForum (CXF Girona, Lleida, Sevilla y Madrid)

"Virus: compañeros inseparables de la vida". VII edition of the San Lorenzo de El Escorial Conference on Science. 17-10-2021. San Lorenzo de El Escorial (Madrid)

"La Astrobiología: Un viaje al origen de la vida en el Universo". 30-04-2021. Universidad de Zaragoza (Zaragoza)

"Aproximaciones científicas a la búsqueda de vida extraterrestre". 04-10-2021. Institute for Integrative Systems Biology (Valencia)

"Pandemias virales". 01-10-2021. Universidad Autónoma de Madrid (Madrid)

"Los detalles. La Tierra como referencia". Cycle: El origen de la vida. 19-06-2021. Residencia de Estudiantes (Madrid).

"La vida: ¿un fenómeno singular?" 18-11-2021. Planetario de Madrid. (Madrid).

"Evolución experimental con bacteriófagos". 24-03-2021. Universidad Complutense de Madrid (Madrid)

Articles in specialized press

¿Por qué están apareciendo ahora tantas variantes del SARS-CoV-2? 26-01-2021. The Conversation. https://theconversation.com/por-que-estan-apareciendo-ahora-tantas-variantes-del-sars-cov-2-153739

¿Sabemos cómo comenzó la vida en la Tierra? 27-06-2021. The Conversation. https://theconversation.com/sabemos-como-comenzo-la-vida-en-la-tierra-162188

La evolución es un hecho tan indiscutible como que la Tierra no es plana. 14-06-2021. The Conversation. https://theconversation.com/la-evolucion-es-un-hecho-tan-indiscutible-como-que-la-tierra-no-es-plana-162135

Las incógnitas de la transmisión del SARS-CoV-2 en India. 29-04-2021. The Conversation. https://theconversation.com/las-incognitas-de-la-transmision-del-sars-cov-2-en-india-159947

¿Se vacunaría con Janssen o AstraZeneca? Ocho expertos tienen la respuesta. 15-04-2021. The Conversation. https://theconversation.com/se-vacunaria-con-janssen-o-astrazeneca-ocho-expertos-tienen-clara-la-respuesta-158971

¿Reaccionamos a la pandemia a tiempo? 8-03-2021. El Español. https://www.elespanol.com/el-cultural/opinion/dardos/20210308/reaccionamos-pandemia-tiempo/564445265_0.html

Molecular Evolution, RNA World and Biosensors (MERWB)

Coordinator: Carlos Briones Llorente

Senior Researchers

Yolanda Blanco López

Posdoctorals

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Posdoctoral trainees (1-3 years since PhD thesis):

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Predoctorals

Beatriz Torres Vázquez

Technicians

María Fernández Algar

Students (Master, TFG, others):

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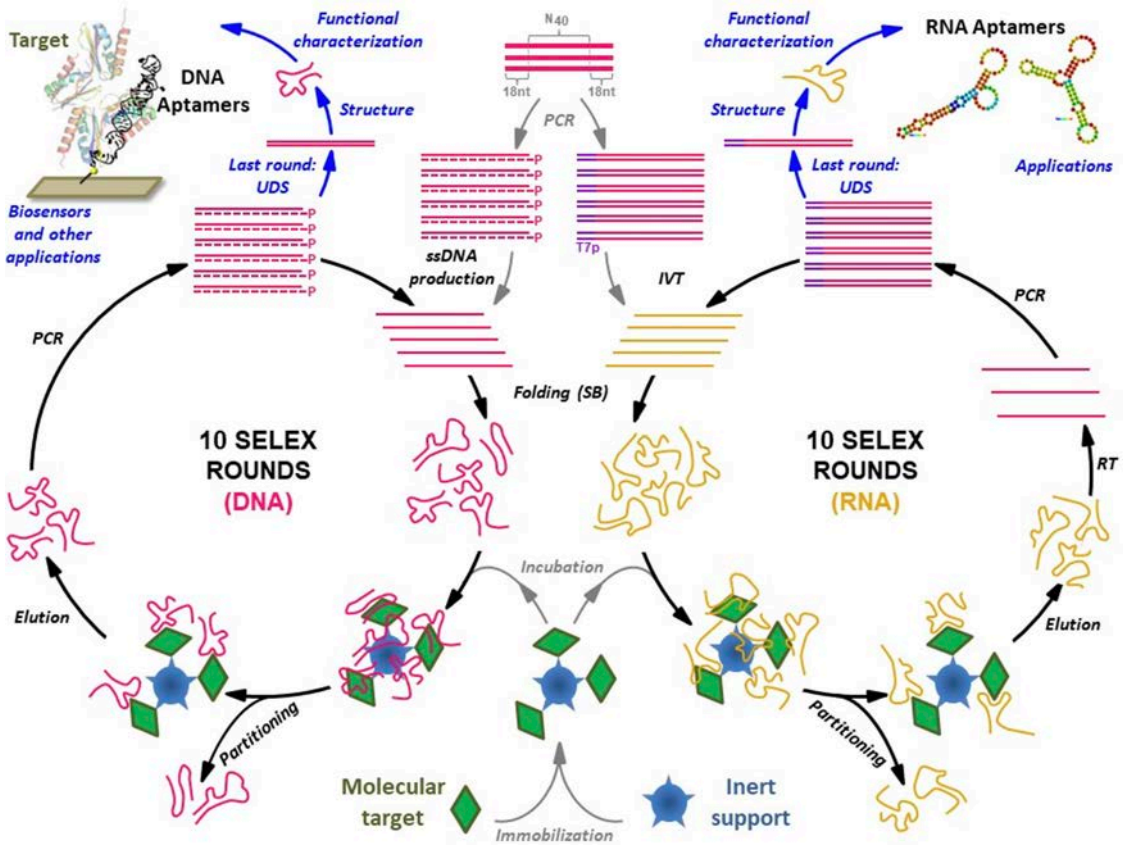


Summary

This group contributes to objectives O2, O4, O5 and O6 of Center Strategic Plan by addressing the following questions: collaboration with the Astrochemistry group in the search for and characterization of molecular precursors of the RNA world (including hydroxylamine) and early life (such as ethanolamine) in the interstellar medium (ISM); development of experimental approaches to polymerize ribonucleotides in mineral-water interfaces (including clay minerals) and other complex media; characterization of the dynamics and evolution of RNA virus quasispecies in different experimental conditions; *in vitro* selection of RNA and DNA aptamers against different molecular targets (low molecular weight biomolecules, astrobiologically-relevant peptides and proteins, viral proteins); development of aptamer-based biosensors with applicability in biotechnology and astrobiology.

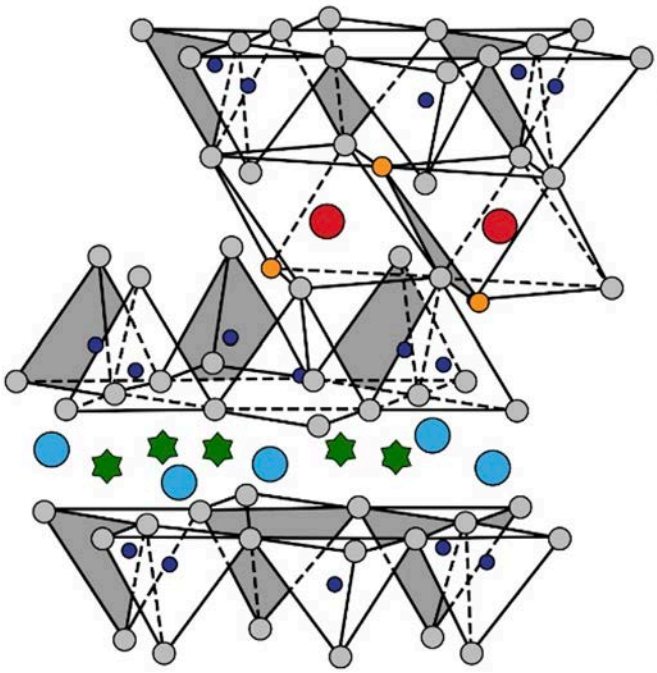
The following research highlights exemplify the most relevant investigations and results in the group over 2021.

Research Highlights 2021

RH1: Development of experimental systems for abiotic polymerization of ribonucleotides

One of the research lines of this group is the investigation of the chemical processes that could led to the establishment of the RNA World, within a prebiotic systems chemistry perspective for the origin of life. We have previously published models for the ligation-based, modular evolution of functional RNAs from oligonucleotides, but until now we had not addressed the origin of the first RNA oligomers themselves.

During 2021, in collaboration with the group of Andrés de la Escosura (UAM), we have developed experimental systems for the abiotic polymerization of RNA oligonucleotides from cyclic phosphate-containing monomers (and their mixtures), using various clay minerals at different pHs and ionic strengths as catalytic substrates. This line of research will produce the first publications in 2022.

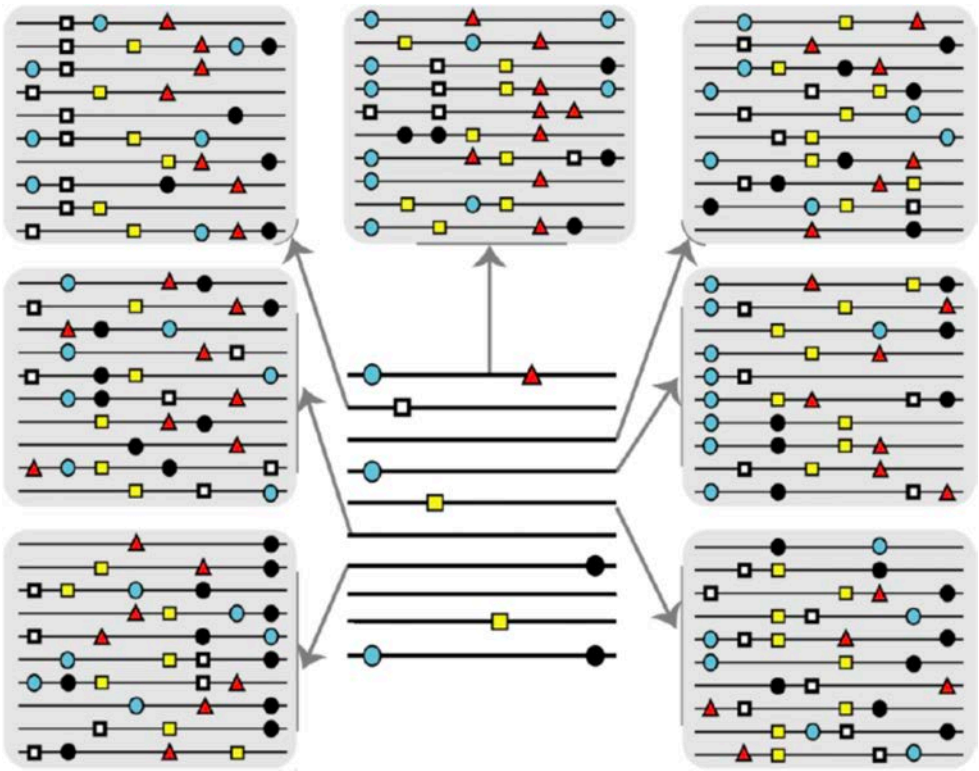


Schematic representation of a montmorillonite-type clay, showing the presence of adsorbed ribonucleotides in the interlayer by green six-pointed stars.

Research Highlights 2021

RH2: Evolution of virus RNA quasispecies under different selective pressures

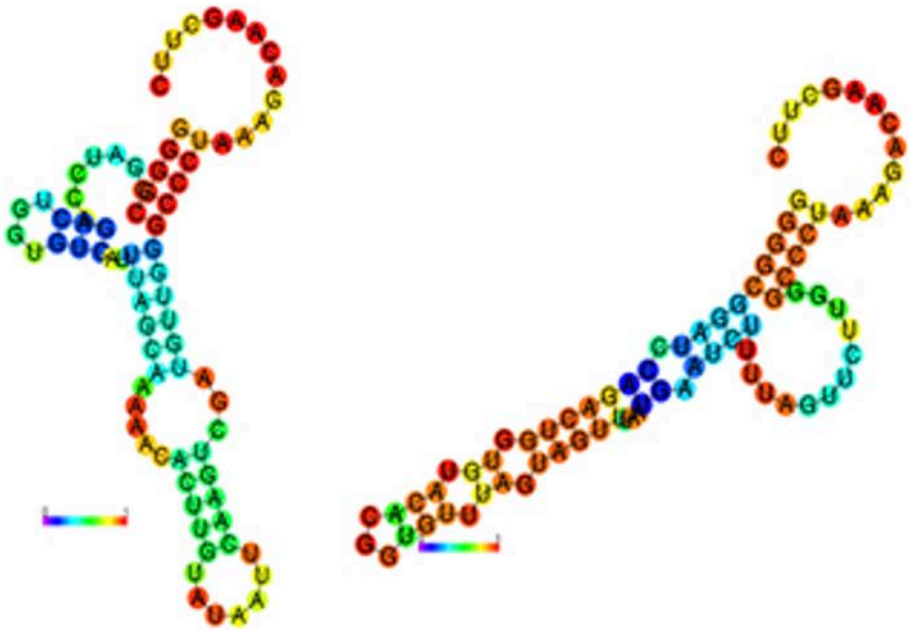
RNA virus quasispecies provide very suitable models for investigating the replication and population dynamics of RNA molecules during the RNA World. Replication of RNA viruses is characterized by exploration of sequence space, which facilitates their adaptation to changing environments mainly in response to positive selection, while further diversification may be boosted by modifications of the population size. In collaboration with the group of Prof. Esteban Domingo (CBMSO, CSIC-UAM), we have investigated quasispecies dynamics for the last years, using different RNA virus as model systems. In 2021, our research with hepatitis C virus (HCV) have shown that the expansion in sequence space of a viral clone continues despite prolonged replication in a stable environment. Characterization of the quasispecies expansion was based on the quantification of diversity indices, the occurrence of intra-population mutational waves (variations in mutant frequencies), and individual residue variations in mutant spectra. We hypothesize that these observations have as a common origin a permanent state of HCV population disequilibrium, even upon extensive viral replication in the absence of external selective constraints or changes in population size. Such a persistent disequilibrium may facilitate finding alternative mutational pathways for quasispecies dynamics and adaptation.



Evolution of RNA quasispecies under different selective pressures (García-Crespo et al., 2021).

RH3: In vitro selection of RNA and DNA aptamers against molecular targets relevant in biotechnology and astrobiology

In our research group, we have set up and optimized different systems for the *in vitro* selection and evolution of nucleic acids, focused on the production of aptamers against various kinds of molecules of interest in biotechnology and astrobiology. During 2021 we have completed the selection and functional characterization of RNA and DNA aptamers against the HCV core protein (article published in 2022). In collaboration with research groups from the International Iberian Nanotechnology Laboratory (INL, Braga, Portugal), Institute of Physics (Czech Academy of Sciences, Prague, Czech Republic) and Institute of Materials Science of Madrid (ICMM, CSIC), the anti-HCVcore aptamer showing the highest affinity and specificity for its target has been used as a molecular probe for the fabrication of ultrasensitive graphene-based aptasensors (article currently in preparation). This research line has produced two international patents, filed in 2021. In parallel, during 2021 we have developed and characterized DNA aptamers against various conserved peptides in metal-binding proteins, which will be used to build biosensors for biomarker detection in planetary exploration (manuscript in preparation).



Examples of RNA aptamers obtained in the group by means of *in vitro* evolution against different kinds of ligands.

Publications

Rivilla VM, Jiménez-Serra I, Martín-Pintado J, Briones C, Rodríguez-Almeida LF, Rico-Villas F, Tercero B, Zeng S, Colzi L, de Vicente P, Martín S, Requena-Torres MA (2021). Discovery in space of ethanolamine, the simplest phospholipid head group. *Proc. Natl. Acad. Sci. USA*: 118: e2101314118.

García-Crespo C, Gallego I, Soria ME, de Ávila AI, Martínez-González B, Vazquez-Sirvent L, Lobo-Vega R, Moreno E, Gómez J, Briones C, Gregori J, Quer J, Domingo E, Perales C (2021). Population disequilibrium as promoter of adaptive explorations in hepatitis C virus. *Viruses* 13: 616.

Patents in 2021

'Biosensor for the detection of hepatitis C virus'. Asignee: CSIC, INTA, International Iberian Nanotechnology Laboratory (INL), Universidade do Minho (UMinho). Inventors: L.F. Vázquez, I. Palacio, J.A. Martín-Gago, M.F. López-Fagúndez, M.M. García-Hernández, C. Briones, M. Moreno, A. Náñez, B. Torres-Vázquez, P. Alpuim, T. Domingues, P. Cabral. Application no. (priority date): EP21382711, European (29.07.2021). Status: pending.

'Aptamers against the hepatitis C virus core protein'. Asignee: CSIC, INTA, Fundación para la Investigación Biomédica del Hospital Universitario Ramón y Cajal (FIBioHRC), Aptus Biotech, S.L. Inventors: C. Briones, A.M. de Lucas, A. Fragoso, M. Moreno, M. Fernández-Algar, A. García-Sacristán, V.M. González, E. Marín, B. Torres-Vázquez. Application no. (priority date): EP21382710, European (29.07.2021). Status: pending.

Funded projects in 2021

'Graphene aptasensor bioelectronics: a neural interface for neurotransmission probing in neurological disorders'. PI Consortium (3 subprojects): Pedro Alpuim (International Iberian Nanotechnology Laboratory, INL, Braga, Portugal); PI Subproject CAB: C. Briones. Funding entity: 'La Caixa' Foundation, Health Research 2021 Call (Ref.: HR21-00410). Budget: 908.539,19 € (total Project); 130.000 € (Subproject CAB). Duration: 01/11/2021-31/10/2024.

Main science outreach activities in 2021

C. Briones and I. Jiménez-Serra, coordinators of the chapter entitled 'The origins of life: from chemistry to biology' in the book 'Origins, (co)evolution, diversity and synthesis of life'. CSIC White Books 2030. Ed. CSIC, Madrid, 2021. Pages 21-52. URL: *http://libros.csic.es/product_info.php?cPath=164&products_id=1459&PHPSESSID=e08ea1eb1e6a68d59424fd7b6d081bc3*. C. Briones, founding member of the CSIC initiative 'LifeHUB.CSIC'.

C. Briones, author of the chapter entitled 'En busca del ADN: un viaje en el tiempo y el espacio' in the book 'Genes. Escribiendo el guion de la vida'. Ed. Almuzara (Colección Guadalmazán), Córdoba, 2021. Pages 335-353. URL: *https://almuzaralibros.com/fichalibro.php?edi=5&libro=5709&nuevo=5709*.

J.A. Rodríguez-Manfredi and C. Briones, Article '*Perseverance*: el *rover* con el que la NASA buscará vida en Marte', Magazine 'Astronomía', February 2021. URL: https://www.globalastronomia.com/producto/astronomia-febrero-2021-no260-pdf/.

C. Briones, video 'Tres historias de la exploración espacial y un mensaje para la humanidad' in the Project 'Aprendemos Juntos' (El País – BBVA). April 2021. URL: https://www.youtube.com/watch?v=8JZxoHTPYgY (5:40 min) and https://www.youtube.com/watch?v=_QBsezgXD9g&t=2s (54:18 min).

C. Briones, 'Microorganismos en la evolución del Cosmos', closing lecture of the cycle 'Microbiología en la era del Antropoceno' to commemorate the 75th anniversary of the Spanish Society of Microbiology (SEM). Museo Nacional de Ciencias Naturales, Madrid, December 2, 2021. URL: https://www.mncn.csic.es/es/sociedad-de-amigos-del-museo/microorganismos-en-la-evolucion-del-cosmos.

Molecular mechanisms of biological adaptation

Coordinator: José Eduardo González-Pastor

Senior Researchers

Salvador Mirete Castañeda

Posdoctorals

Patricia de Francisco Martínez

Patricia Pérez Arnáiz

Predoctorals

Macarena Benguigui de la Cámara

Sara Gómez de Frutos

Jorge Díaz-Rullo Aroco

Felipe Ruymán Alonso Ravelo

Technicians

Carolina González de Figueras PhD

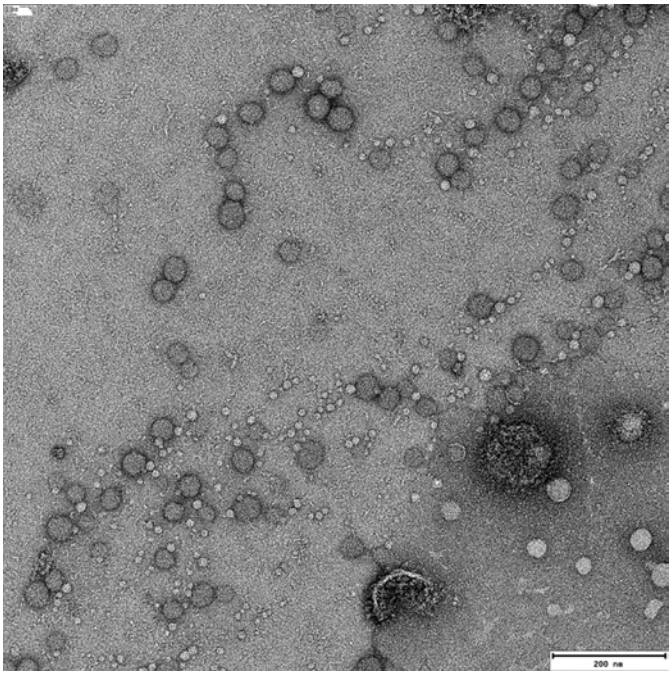
Students (Master, TFG, others)

Agustina Bourg (Master student)

Javier Nebot Labrado (TFG)

Alessia Cassaro (Erasmus student)

Gloria López Morales (internship student)



DNA-containing extracellular vesicles produced by the extreme halophilic archaea *Haloquadratum walsbyi*

Summary

Microorganisms that inhabit extreme environments (extremophiles), have developed complex molecular mechanisms that allow them to survive in these conditions. The research in this group is focused on the discovery and characterization of new molecular adaptation mechanisms from extremophiles, more specifically those that thrive in hypersaline environments considered analogous to Mars and icy satellites such as Europa (Jupiter) and Enceladus (Saturn) (contribution to objectives O3.2 and O5.6 of CAB Strategic Plan). A major problem is that a high percentage of environmental microorganisms cannot be cultivated or there are no molecular tools for their genetic manipulation, and therefore their study is impossible. Thus, this group is using culture independent techniques, such as metagenomic sequencing, functional metagenomics and metatranscriptomics, which allow access to the genetic information of all the microorganisms present in a certain environmental sample, and then be able to study their adaptation strategies to extreme conditions. In addition, they are also exploring the design of microorganisms and plants that are more resistant to the conditions of space or other planetary bodies, by expressing in them resistance genes isolated from extremophiles (contribution to O5.7 of the Strategic Plan).

Currently, this group is researching in: i) molecular mechanisms of adaptation to perchlorate, UV radiation and day/night cycles in microorganisms that inhabit hypersaline environments; ii) gene transfer mechanisms in extreme halophilic microorganisms, such as the square archaea *Haloquadratum walsbyi*; iii) expression of UV and acid resistance genes in the plant *Arabidopsis thaliana*. The following research highlights exemplify the most relevant investigations and results in the group.

Research Highlights 2021

RH1: Queuosine regulates adhesion, biofilm formation and virulence in Bacteria by translational modulation of genes enriched in NAU codons

In previous studies, we reported the identification of genes from extremophiles that conferred resistance to perchlorate, UV-radiation, and acidic pH, some of them related to queuosine (Q) biosynthesis. Q is a hypermodified nucleoside present at the wobble position of tRNAs containing GUN anticodon. Although its physiological role remains elusive, evidence supports that Q-tRNAs regulates NAU codons translational speed. Therefore, Q would affect especially the translation of genes enriched in NAU codons (Q-genes), and the function of these genes could predict the role of Q. We showed that Q can regulate in bacteria the translational efficiency of genes containing NAU codons *in vivo*. A bioinformatical analysis was developed for identifying the Q-genes of different bacteria and studying the physiological processes in which they were involved. Q-genes were predicted to regulate adhesion, biofilm formation or virulence in most of analyzed bacteria. Experimental data confirmed the predicted Q-related phenotypes: Q modulated adhesion and cell aggregation in *Escherichia coli*, sporulation and biofilm formation in *Bacillus subtilis* (Figure 1), contact-dependent growth inhibition in *Pseudomonas putida* and virulence in human pathogens. Therefore, our work shows that Q may modulate those processes in which Q-genes are especially involved, such as resistance to extreme conditions, and may open the door to the development of novel treatments for bacterial diseases.

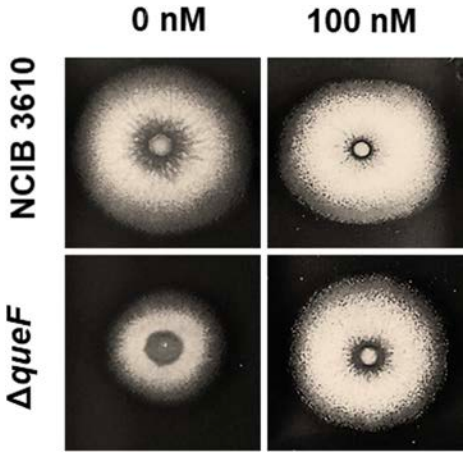


Fig. 1. Biofilm formation capacity depends on Q. *B. subtilis* NCIB 3610 and NCIB 3610 Δ*queF* mutant (Δ*queF*) strains were grown on MSgg-agar medium supplemented with 0 or 100 nM $preQ_1$ (Q precursor) for 16 h at 30°C, and colony sizes were analyzed.

RH2: Insights on the evolution of metabolic networks of extreme halophilic microorganisms by dominating codon bias.

This work was developed in collaboration with the Laboratory of Computational and Quantitative Biology of Alessandra Carbone in Sorbonne University of Paris (France). The main objective was to reconstruct and compare the metabolic pathways dominated by codon bias of the two predominant microorganisms of different hypersaline environments: the bacteria *Salinibacter ruber* and the archaea *Haloquadratum walsbyi*. For this purpose, domains from all proteins of each genome were annotated and used to define a group of coding sequences that is representative of dominating codon bias (CAI values). CAI analysis is useful to reconstruct biochemical and regulatory pathways in biased organisms. Genes with high codon bias describe important metabolic pathways for the lifestyle of an organism that involve especially biased genes. The most representative and biased functions for each microorganism were studied with a 3D representation of COG Groups in relation to their CAI values (Figure 2). Other approaches, such as comparative KEGG pathways, were obtained (data not shown). Future analyses should be done in order to correlate these results with metatranscriptomics data previously obtained from day/night cycles of these microorganisms. This correlation could help to confirm and explain the hypothesis of a possible partitioning temporal niche event that we previously described between these dominating species in hypersaline environments.

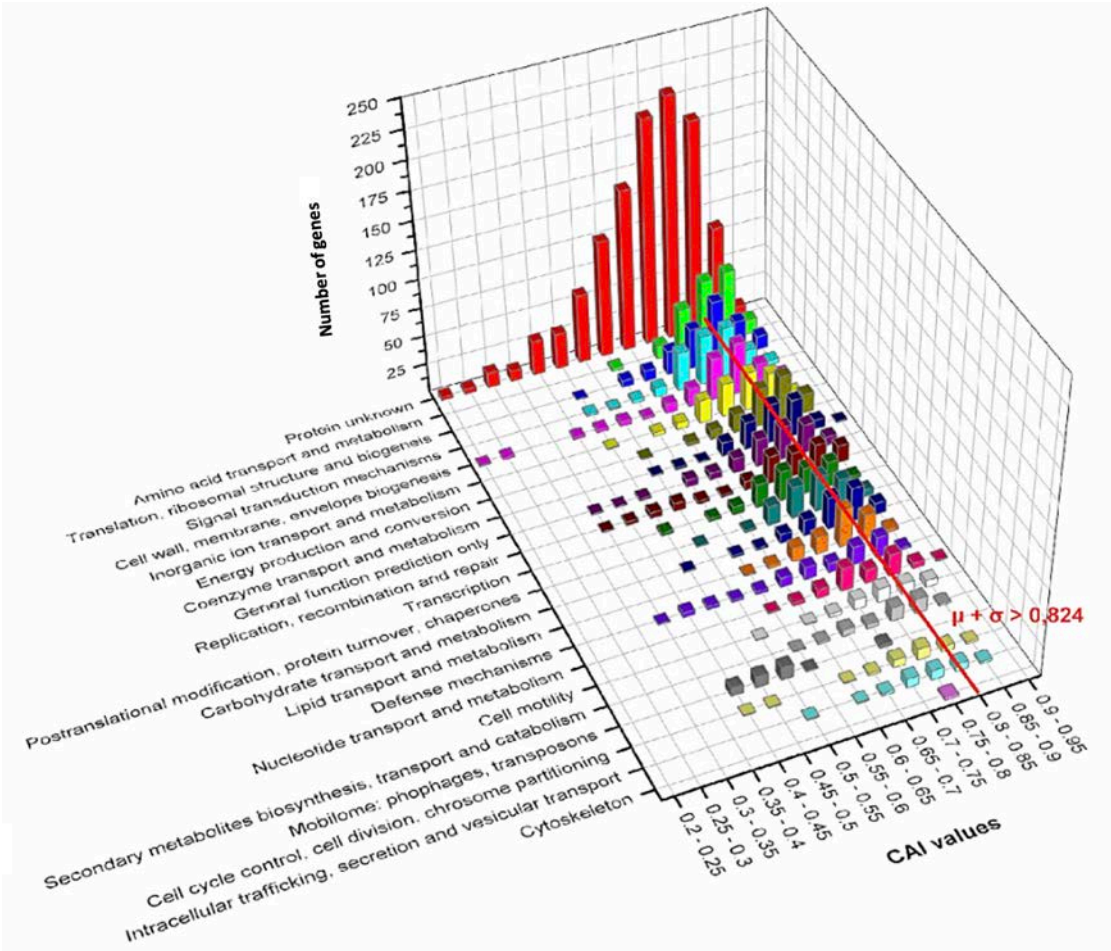


Fig. 2. **Example of COG categories distribution by CAI values in 3D dimensions for *Salinibacter ruber*.** Reference set, codon weights and CAI values were calculated with the program CAIJAVA. Genes with CAI value close to 1 are made by highly frequent codons and represent the most biased ones, while genes ranking lowest are less affected by selective bias.

RH3: Characterization of extracellular vesicles produced by the extreme halophile archaea Haloquadratum walsbyi

Haloquadratum walsbyi is an extreme halophile archaea first discovered in the early 1980s in a coastal brine of the Sinai Peninsula (Egypt). It has been reported as the most abundant microorganism in hypersaline habitats and its square cell shape is really characteristic. Analyzing cultures of *H. walsbyi* grown at 42°C under light-dark cycles (12h/12h), we have detected, at specific cell densities (A_{600nm}: 0.16-0.26), the production of extracellular vesicles (EVs) that contain DNA. We have detected this phenomenon, undescribed until now for *Hqr. walsbyi*, in both a natural strain isolated from Santa Pola salterns and in a collection strain (DSM 16790). Transmission electron microscopy has shown that EVs have a diameter of around 50 nm.

We have extracted and sequenced the DNA content of the EVs and it corresponds to all the genomic and PL47 plasmid DNA of Hqr. walsbyi. The proteome of these vesicles was also analyzed and nearly 900 proteins were identified. Preliminary analyses showed that there is an apparent enrichment in proteins involved in translation and post-translational modifications, and protein turnover (including chaperones), energy generation and conversion (including ATPases, bacteriorhodopsins and proteins of the electron transport chain). Also abundant are proteins such as FtsZ, and homologues of *Sulfolobus* Vps4 protein, which are also present and thought to be key in the production of extracellular vesicles by other Euryarchaeota (such as *Thermococcus*).

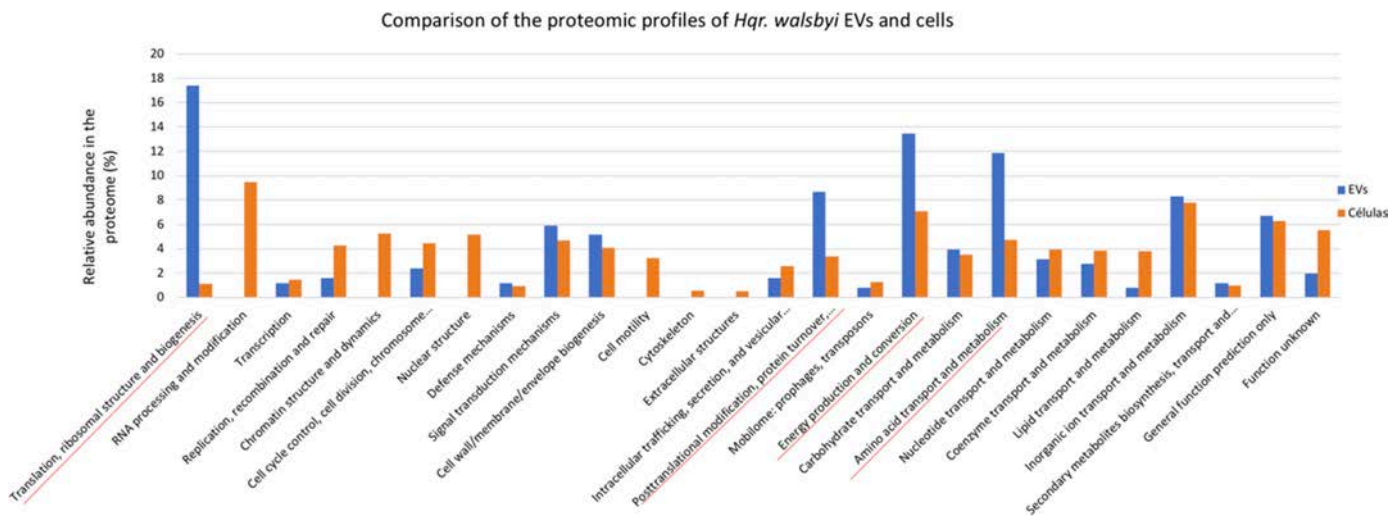


Figure 3. Comparison of the proteomes of extracellular vesicles (EVs) (orange bars) and the global proteome (blue bars) of *Hqr. walsbyi* based on COGs analysis.

RH4: Construction of plants expressing an acid resistance gene

In a previous work of our group, genes that confer resistance to acid pH were isolated from samples of microorganisms from the Rio Tinto by means of functional metagenomics. One of these recovered genes was *clpP*, which encodes the ATP-dependent protease ClpP (proteolytic subunit ClpP). This gene was cloned and expressed in the laboratory model plant *Arabidopsis thaliana* (using the flower dip method) to determine if the resulting transgenic plants improved their resistance to more acidic pH. For this purpose, different plant lines expressing the *clpP* gene were grown in liquid MS medium with different pHs (Figure 4A). The measurement of the dry weight of the different lines of plants modified with *clpP* indicated that at the tested pHs they grew more efficiently than the unmodified plants (Figure 4B), which suggests that the *clpP* gene could contribute to a greater resistance to acidic pH in *A .thaliana*.

Our group also demonstrated that the *clpP* gene confers resistance to the toxic compound perchlorate (identified on Mars) and the possible cross-resistance of this transgenic plant to this compound and to other types of stress such as UV radiation are currently being tested.

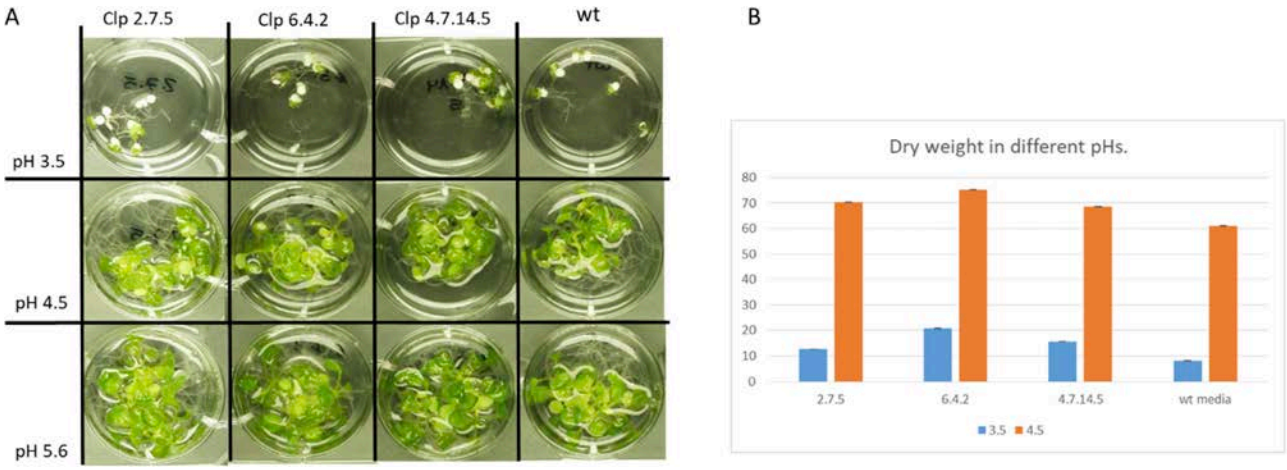


Figure 4. A) Growth of wt and three independent lines of clpP-modified plants in liquid MS medium with acid pHs (3.5 and 4.5) and the control pH (5.6). B) Comparison of the dry weight of each plant with respect to the dry weight of the same plant in the control medium (pH 5.6)

Publications

Díaz-Rullo J, Rodríguez-Valdecantos G, Torres-Rojas F, Cid L, Vargas IT, González B, González-Pastor JE. 2021. Mining for Perchlorate Resistance Genes in Microorganisms From Sediments of a Hypersaline Pond in Atacama Desert, Chile. Front Microbiol. Jul 23;12:723874. doi: 10.3389/fmicb.2021.723874.

Donoso RA, Ruiz D, Gárate-Castro C, Villegas P, González-Pastor JE, de Lorenzo V, González B, Pérez-Pantoja D. 2021. Identification of a self-sufficient cytochrome P450 monooxygenase from Cupriavidus pinatubonensis JMP134 involved in 2-hydroxyphenylacetic acid catabolism, via homogentisate pathway. Microb Biotechnol. Sep;14(5):1944-1960. doi: 10.1111/1751-7915.13865. Epub 2021 Jun 22.

Viver T, Conrad RE, Orellana LH, Urdiain M, González-Pastor JE, Hatt JK, Amann R, Antón J, Konstantinidis KT, Rosselló-Móra R. 2021. Distinct ecotypes within a natural haloarchaeal population enable adaptation to changing environmental conditions without causing population sweeps. ISME J. Apr;15(4):1178-1191. doi: 10.1038/s41396-020-00842-5. Epub 2020 Dec 20.

Funded projects in 2021

TITLE: Developing -Omics strategies to unveil species pangenomes, viral coevolution and adaptation at the salt concentration edges SP3. *PI:* **J.E. González Pastor** (CSIC). Coordinated project with: Ramon Rosselló-Móra –IMEDEA- (coordinator), Josefa Antón Botella –Universidad de Alicante- (coordinadora) and Francesc Rosselló Llompart (Universidad de las Islas Baleares). *FUNDING SOURCE:* Ministerio de Ciencia e Innovación (Spanish Government). *CODE:* PGC2018-096956-B-C42. *DURATION: From* 01/01/2019 to 31/12/2021 *PARTICIPATING RESEARCHERS:* 4 (4 subprojects). *FUNDING:* 156.090 €.

Outreach (most relevant contributions)

"**Concurso Patata Marciana**". Sep/2021. José Eduardo González-Pastor, member of the scientific-technical jury.

Collaboration in the project "**divulga-AQUIS**" (FCT-20-16399, PI: Marisa Rua, University of Vigo), aimed at high school students. Oct/2021-Feb/2022. José Eduardo González-Pastor is responsible of the section about "Origin of Life and Extreme Environments". Participation in interviews conducted by students.

Conference: "Exploring new mechanisms of resistance to extreme conditions in microorganisms and their use in biotechnology". **Seminars of the Department of Microbiology & Molecular Genetics, Michigan State University**. 23/11/2021. José Eduardo González-Pastor

Collaboration with the "**Program Iberdrola Innova I+D+i**" developed by "Fundación San Patricio". This is a contest for high school students in which they have to write a bibliographic and research work on different scientific topics. July/2021-May/2022. José Eduardo González-Pastor is responsible for the topic "Spatial Agriculture", he prepared a document that serves as a basis for the students' work and participated in forums with the students to solve problems. (https://www.programainvestiga.org/presentacion.php)

Microbial Biodiversity

Coordinator: Ángeles Aguilera Bazán

Senior Researchers
Cristina Cid Sánchez
Elena González-Toril

Predoctorals
Jesús Javier Rey Samper

Technicians
Eva García López
Graciela de Diego Castilla

Students TFM
Guillem Tomás Tenes UCM

Students TFGs
Susana Moñino Ramos, UAM
Sara Pasquale El Bobakry, UAM
Carlota Fernández González, UAH
Javier López Gramage, UAM
Agustín Carbajo Usano, UAM
Manuel Fernández Cuesta, UAH
Fátima Ruiz Blas UAH
Silvia Sánchez Casanova
Sonia Peña Pérez
María Luisa Martin Cerezo

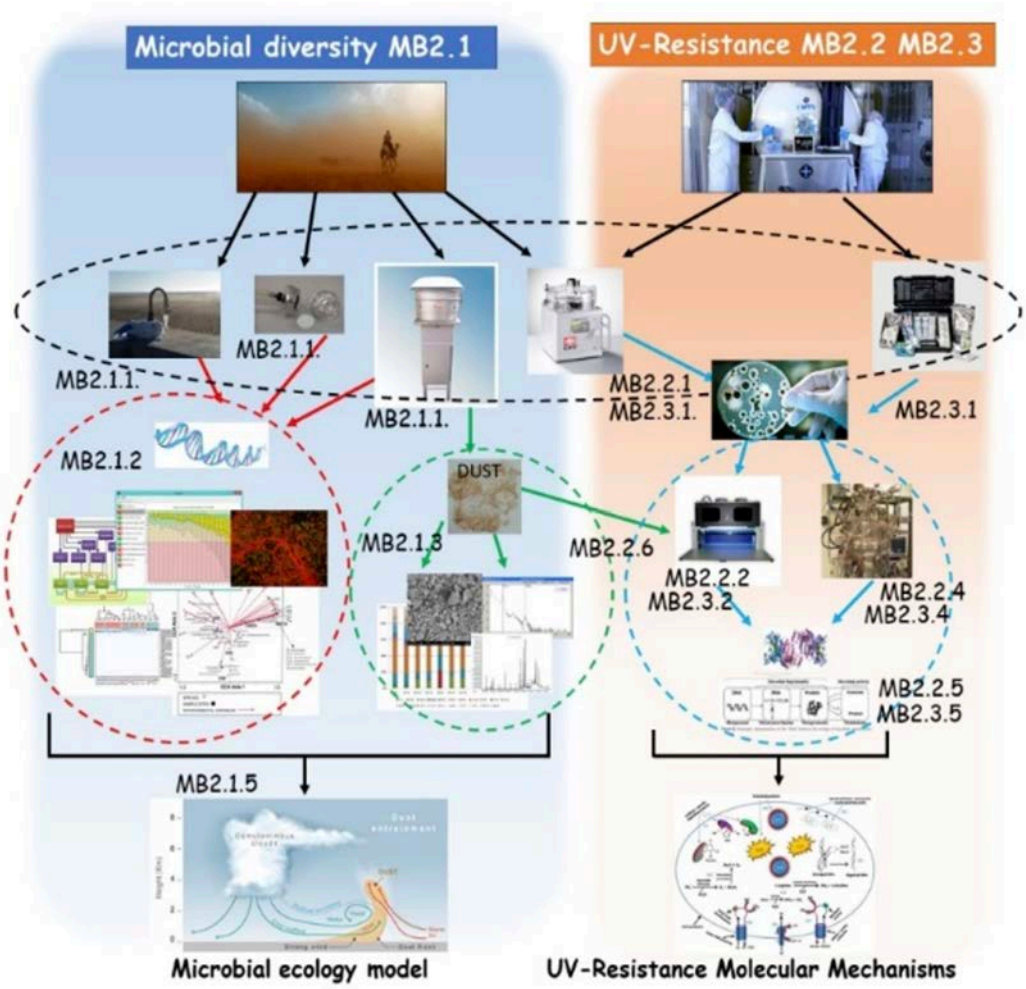
Summary

This group contributes to objective O5. To understand the basic principles of life in planetary environments, its early evolution and adaptability to diverse and often extreme conditions, of Center Strategic Plan by addressing the question of how metabolic diversity has occurred as well as its molecular adaptations to the extreme environmental physicochemical parameters. The following research highlights exemplify the most relevant investigations and results in the group.

Research Highlights 2021

RH1: The cycle of aerosols on Mars and Earth, a comparative study. Implications for life and planetary protection (CAMELIA_MICRO)

The purpose of this project is to investigate the atmospheric dispersal of mineral aerosols, organics and bioburden through the atmosphere of Mars, and then also on the atmosphere and surface of Earth, to provide an analogy case. Specific goals are: a) Study of the biodiversity and microbial dispersion associated to Saharan dust intrusions, b) Molecular mechanisms of resistance to ultraviolet radiation. Analysis of the potential protective role of dust. Molecular mechanisms activated when exposed to Martian conditions on Mars and space environment Simulation Chambers, c) Isolation of microorganisms from clean rooms of spacecraft assembly. Molecular mechanisms activated when exposed to Martian conditions on Mars and space environment Simulation Chambers. We already produce a database of the atmospheric microbial diversity obtained from sampling in different meteorological situations, and seasons of Saharan intrusion and non-intrusion. In addition, we have a culture collection of microorganisms isolated during Saharan intrusions, isolates from clean rooms and isolates from the stratosphere. The resistance of the microorganisms to different extreme conditions, including those of the Martian atmosphere, are being carried out.



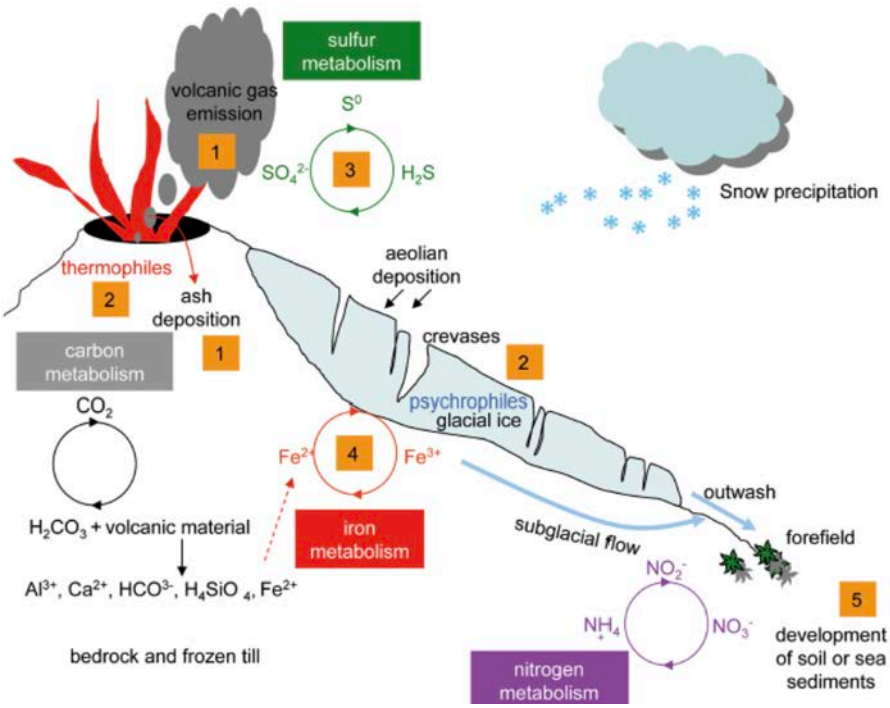
Workflow in the analysis of atmospheric ecology.

RH2: Comparative Proteomic Analysis of Psychrophilic vs. Mesophilic Bacterial Species Reveals Different Strategies to Achieve Temperature Adaptation (POLAR_BIOSENSOR)

The old debate of nature (genes) versus nurture (environmental variables) is topical concerning the effect of climate change on environmental microorganisms. Specifically, the Polar Regions are experiencing a drastic increase in temperature caused by the rise in greenhouse gas emissions. This study, in an attempt to mimic the molecular adaptation of polar microorganisms, combines proteomic approaches with a classical microbiological analysis in three bacterial species *Shewanella oneidensis*, *S. frigidimarina*, and *Psychrobacter frigidicola*. Both Shewanellas are members of the same genus but they live in different environments. Besides, *S. frigidimarina* and *P. frigidicola* share the same natural environment, but belong to a different genus. The comparison of the strategies employed by each bacterial species estimates the contribution of genome versus environmental variables in the adaptation to temperature. The results show a greater versatility of acclimatization for the genus *Shewanella* with respect to *Psychrobacter*. Besides, *S. frigidimarina* was the bestadapted specie to thermal variations in the temperature range 4ºC-30ºC and displayed several adaptation mechanisms common with the other two species. Regarding the molecular machinery used by these bacteria to face the consequences of temperature changes, chaperones have a pivoting role. They form complexes with other proteins in the response to the environment, establishing cooperation with transmembrane proteins, elongation factors and proteins for protection against oxidative damage.

RH3: Microbial communities in volcanic glacier ecosystems (PALEO_ICE)

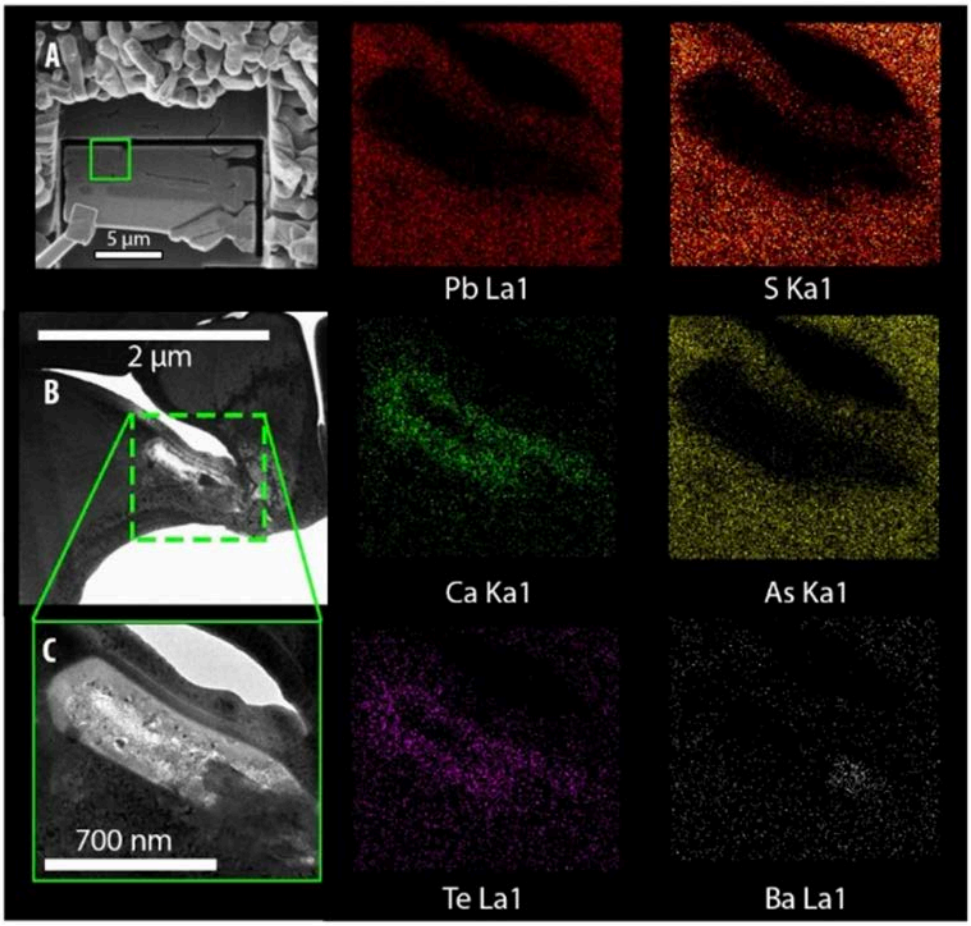
Glaciers constitute a polyextremophilic environment characterized by low temperatures, high solar radiation, a lack of nutrients and low water availability. However, glaciers located in volcanic regions have special characteristics, since the volcanic foci provide them with heat and nutrients that allow the growth of microbial communities highly adapted to this environment. To better know the microbial diversity of the underexplored glacial ecosystems, and to check what their specific characteristics were, we studied the structure of bacterial communities living in volcanic glaciers. In addition to geographic coordinates, many other glacier environmental factors (like volcanic activity, altitude, temperature, pH or ice chemical composition) that can influence the diversity and distribution of microbial communities were considered in this study. Finally, using their taxonomic assignments, an attempt was made to compare how different or similar are the biogeochemical cycles in which these microbiomes are involved.



Biogeochemical cycles in volcanic glaciers.

RH4: Microbiological Control in the Formation of Mineral Deposits (MINLIFE)

The study of the Deep Biosphere is one of the most novel and promising unexplored topics of research due to its relevant implications on studies regarding the origin of life, life in extreme environments, its control over surface lithologies, the formation of low temperature mineral deposits and for the search for life in other planets. In this regard, MINLIFE proposes the study of one of the most interesting mineral deposits from the metallogenic and geomicrobiological point of view, Las Cruces (SW, Spain), in an attempt to know how microorganisms can control the processes of mineral formation and the dissolution and precipitation of metals. The project is aimed at studying mineralogy, isotope geochemistry and the microbial ecology of the deposit as well as the role of the microorganisms in the mineralizing processes. Given the biological origin of the rock, we expected the presence of preserved molecular biosignatures. Indeed, mass spectrometric analysis of the organic extracts of the rocks showed a number of biomarkers consistent with biogenic origin, indicating an anaerobic bacterial ecosystem and strongly reducing conditions, compatible with high sulfatoreduction, explaining the high sulfidization of the rock. Las Cruces showed a unique case of biologically controlled Pb(Ag) mineralization, covered at the roof by a biogenic carbonate layer (13 C ≈ -40 to -20‰). As a consequence of microbial metabolism, there is a gradual reduction of Fe(III), sulfate and Cu(II) to Fe(II), H2S and Cu(I). In the cementation zone, this fact is accompanied by methanogenic CH_4 production, consumed in the overlying biogenic rocks, generating CO2 and producing siderite and calcite.



NanoSIMS analysis of internal structures in fossil bacteria

Publications

Souza-Egipsy, V, et al. 2021. Biofilm mechanics in an extreme acidic environment: Microbiological significance. Soft Matter. DOI: 10.1039/D0SM01975E

González-Martín C. et al. 2021. Airborne bacterial community composition according to their origin in Tenerife, Canary Islands. Frontiers in Microbiology 12:732961.

García-López, E., et al. 2021. Microbial Community Structure Driven by a Volcanic Gradient in Glaciers of the Antarctic Archipelago South Shetland. Microorganisms. 9, 392.

Moreno, A., et al. 2021. The case of a southern European glacier which survived Roman and Medieval warm periods but is disappearing under recent warming. The Cryosphere. https://doi.org/10.5194/tc-15-1157-2021.

Garcia-Lopez, E., et al. 2021. Identification of Biomolecules Involved in the Adaptation to the Environment of Cold-Loving Microorganisms and Metabolic Pathways for Their Production. Biomolecules. 11: 1155.

Garcia-Lopez, E., et al. 2021. Glacial Ice Age Shapes Microbiome Composition in a Receding Southern European Glacier. Front. Microbiol. 12: 714537.

Barbosa A, et al 2021. Ecosistemas polares terrestres, in: Observando los polos. Editorial CSIC. ISBN: 978-84-00-10865-6.

Una mirada polar. Fundación General CSIC. 2021. e-ISBN: 978-84-00-10859-5.

Funded projects in 2021

The cycle of aerosols on Mars and Earth, a comparative study. Implications for life and planetary protection. IPs: M Paz Zorzano, Elena González-Toril. MINECO. PID2019-104205GB-C22. 2020/23. 160.000 €.

Desarrollo e implementación de captadores biológicos atmosféricos de altitud: precipitadores electrostáticos de paso único embarcables en plataformas aéreas de investigación. MINECO. CGL2017-92086-EXP. IP. Ángeles Aguilera. 2018/21. 48.400 €

Microbiological Control in the Formation of Mineral Deposits. MINECO. RTI2018-094867-B-I00. IP: Ángeles Aguilera. 2019/2022. 133.100 €

Red Nacional de Microorganismos Extremófilos (REDEX). MINECO. RED2018-102734-T. 2020/22. IP: Juan Miguel González Grau. IRNASE.13.000 €

Red Temática de Micro y Nanoplásticos en el Medio Ambiente (EnviroPlaNet). MINECO. RED2018-102734-T. 2020/22. IP: Roberto Rosal García. Universidad de Alcalá. 33.000 €

Biomolecules in Planetary Exploration (BPE)

Group leader: Victor Parro García

Senior Researchers

Mercedes Moreno-Paz

Posdoctorals

Laura Sánchez García

David Ruano Gallego

María Ángeles Lezcano Vega

Posdoctoral trainees (1-3 years since PhD thesis):

Predoctorals

Rita Sofía dos Santos Severino

Pedro Mustieles del Ser

Eduardo Alonso Pintado

Pablo de Lucía Finkel

Technicians

Miriam García Villadangos

Miguel Ángel Lominchar

Juan Manuel Manchado Ortega

Students (Master, TFG, others):

Valentine Megevand (TFM, Ecole Normale Supérieure de Lyon, France)

Carolina Diaz Ibánez (TFG, Universidad Autónoma de Madrid)

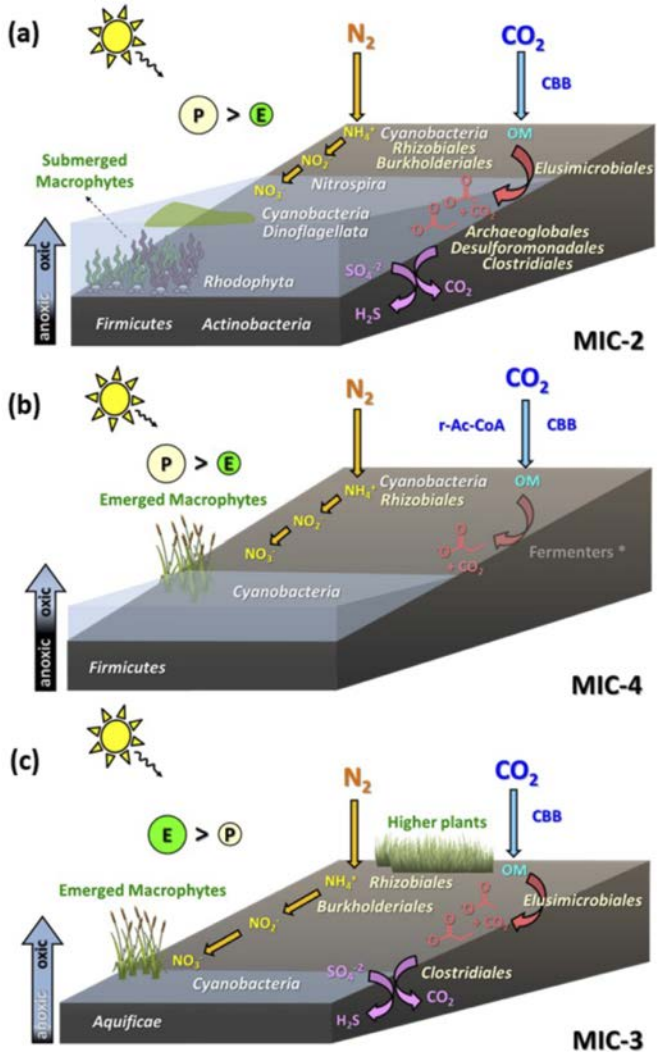
Summary

Multidisciplinary group with biologists, chemists, engineers, technicians and students of different levels (training, Ph.D., degree) whose goal is to investigate the microbial metabolic potential and the preservation of molecular biomarkers (in space and time) in terrestrial analog environments to others found in different planetary bodies. The experimental approach is based on the study of the biological material and the information it provides *in situ* (through field campaigns) and in the laboratory, its preservation and interaction with the physical environment, the identification of molecular biomarkers and the development of methodologies and instrumentation for *in situ* detection. The objective is to infer how life could be in other planets and to design methods and strategies for detecting molecular biomarkers in planetary exploration missions. Over 2021 the group has contributed to objectives O4, O5 and O6 of Center's Strategic Plan with investigations such as: Identifying molecular biomarkers associated with ancient Earth environments and their potential analogies with other worlds (O4.1), deciphering the microbial diversity and adaptation to extreme physicochemical parameters in Antarctic nunataks, as potential analogues of cold and wet early Mars (O5.4) or the implementation of sensors for in situ molecular biomarker detection in planetary exploration and potential terrestrial applications (O6.4).

Research Highlights 2021

RH1: Searching for life signs in the geological record by using lipid biomarkers

The search for life in the Universe greatly depends on our understanding of modern and ancient life-forms on Earth as well as the extent to which we comprehend past and present factors that affect the distribution of life and its interaction with the planetary environment. The analysis of cell membrane-derived lipid compounds bearing recognized resistance to degradation offers great potential to reconstruct the paleobiology of extreme environments in the billion-year time frame. Here, we searched for molecular and carbon isotopic fingerprints of present and past life in extreme environments from Antarctica (recently exposed soils and 3200 years old lacustrine sediments) and the Atacama Desert (Triassic-Jurassic carbonate deposits) to identify biological sources, trace environmental changes and unveil the structure and function of present and past ecosystems. In the Atacama Desert, the analysis of lipid biomarkers was merged with that of other biopolymers of different perdurability and source-diagnosis potential to achieve a way around individual limitations and fosters a kind of synergy in facilitating environmental, biosources and metabolic reconstructions. The multianalytical platform combined lipid-derived biomarkers, metaproteomics and a life detector chip (LDChip) to provide a comprehensive detection of signs of past and recent life in the ca. 200 Ma-old carbonate rocks to reconstruct past life and constraining methodologies and protocols for astrobiological life detection.



Paleoenvironmental reconstruction of the three marine transgression environments in the Triassic-Jurassic Atacama, ordered from the greatest to the lowest marine influence, (a) MIC-2, (b) MIC-4, and (c) MIC-3, according to the combined analysis of lipids, proteins and immunological biomarkers. The relative abundance of aqueous-vs-terrestrial vegetal sources (green), the proportion of prokaryotes (P) over eukaryotes (E), and the prevailing oxic-vs-anoxic conditions were deduced from diagnostic ratios of lipid biomarkers, and the carbon metabolisms on their compound-specific isotopic analysis and proteins results (CBB is Calvin-Benson-Bassham cycle and r-Ac-CoA for reductive acetyl-CoA pathway). Microbial communities were built on the taxonomic annotation of protein sequences and the microbial positive detections by the LDChip (names of phyla in white, of orders in pale yellow).

This work deserved the cover of the November issue of the journal Astrobiology.

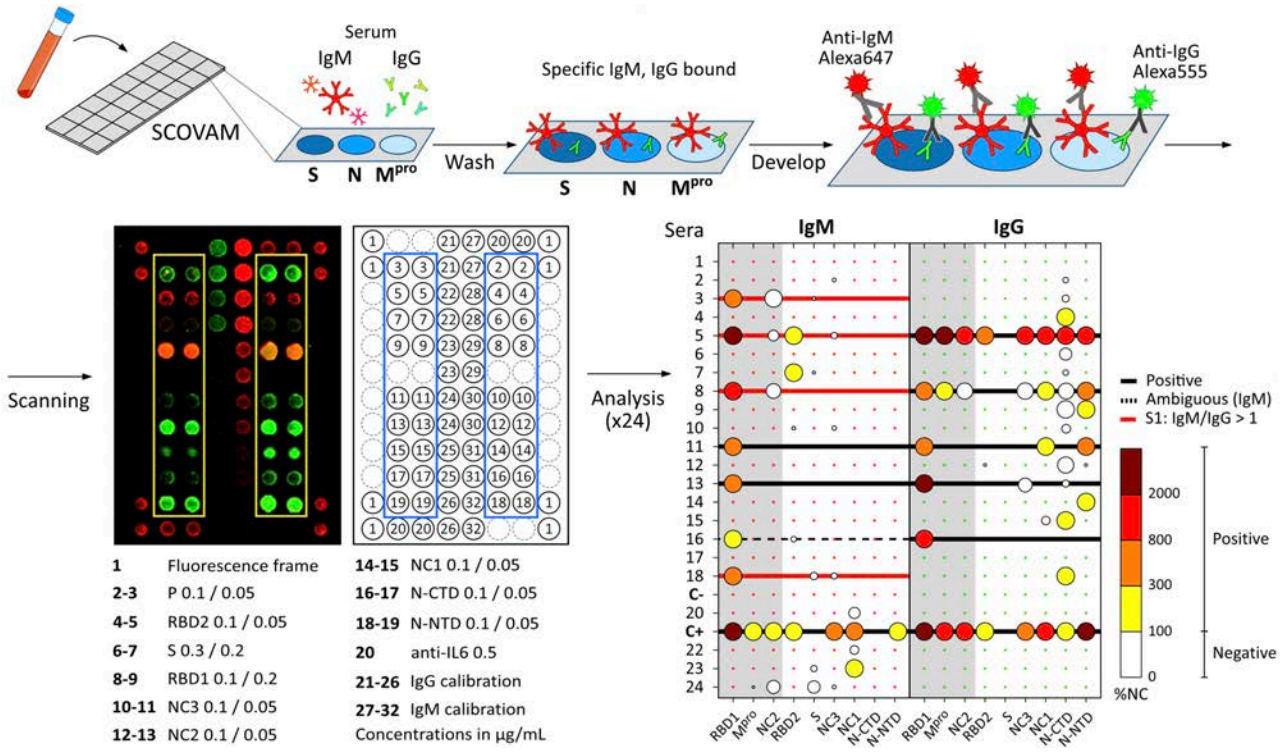
RH2: Characterizing life and searching for biomarkers in extreme terrestrial analogs of Mars

One of the main challenges in Mars exploration is to determine if life ever arose on Mars. In this context, the exploration of terrestrial analogs of Mars is useful to understand their past and present habitability conditions. Nunataks can be considered as potential early Mars analogs, due to the high UV radiation, strong winds and cold temperatures that influence on the lithic substrates and their inhabiting microbial communities. Here, we have investigated the geomicrobiology of the permanently exposed lithic substrates of nunataks from Livingston Island (South Shetlands, Antarctic Peninsula), with focus on prokaryotic community structure and their main metabolic traits. By using a multianalytical approach mainly based on DNA sequencing analysis and a fluorescent sandwich microarray immunoassay (LDChip, Life detector Chip), we have created a biomarker profile that has contributed understanding the metabolic features and biomarker profiles of a potential Martian microbiota. Contrarily to what was hypothesized, the above mentioned conditions create different microhabitats differentially colonized by diverse microbial communities, overlapping differences found in altitude, orientation or location. Bedrock and soil substrates showed a community well-adapted to cold and starvation conditions, and endospore-forming microbial taxa, while loose rocks presented a highly diverse community with a better balance between nutrient accumulation, sheltering and stability. Proteins involved in key metabolisms suggest that microbial primary production has a pivotal role in nutrient cycling in exposed areas with limited deposition of nutrients.

Environmental conditions and main findings of the nunataks form Hurd peninsula, Livingston Island.

RH3: A multiplex antigen microarray for simultaneous IgG and IgM detection against SARS-CoV-2 reveals higher seroprevalence than reported

The surge of SARS-CoV-2 has challenged health systems worldwide and efficient tests to detect viral particles, as well as antibodies generated against them, are needed. Specificity, sensitivity, promptness or scalability are the main parameters to estimate the final performance, but rarely all of them match in a single test. We have developed SCOVAM, a protein microarray with several viral antigens (spike, nucleocapsid, main protease Nsp5) as capturing probes in a fluorescence immunoassay for COVID-19 serological testing. SCOVAM depicts IgG and IgM antibody responses against each of these proteins of 22 individuals in a single microscope slide. It detects specific IgM (0.094 µg ml^{-1}) and IgG (~0.017 µg ml^{-1}) and is scalable and cost-effective. We validated SCOVAM by comparing with a widely used chemiluminescent commercial serological test (n = 742). SCOVAM showed twice the sensitivity and allowed following seroconversion in a single assay. By analysing the prevalence 4 months later in a subset of 76 positive sera, we still detected 93.42% of positives, almost doubling the detection of the commercial assay. The higher sensitivity of SCOVAM is especially relevant to screen sera for convalescent plasma-based treatments, high-throughput antibody response monitoring after vaccination or evaluation of vaccine efficiency.



Legend: Key viral proteins are printed on SCOVAM for the incubation with patient sera. Secondary antibodies detect both specific IgG and IgM antibodies. Fluorescence emission is determined after scanning and images bioinformatically processed for the determination of positive sera.

Publications

Sánchez-García L, Carrizo D, Lezcano MÁ, Moreno-Paz M, Aeppli C, García-Villadangos M, Prieto-Ballesteros O, Demergasso C, Chong G, Parro V. (2021) Time-Integrative Multibiomarker Detection in Triassic-Jurassic Rocks from the Atacama Desert: Relevance to the Search for Basic Life Beyond Earth. Astrobiology 21(11):1421-1437. doi: 10.1089/ast.2020.2339. Epub 2021 Sep 22

Fernández-Martínez MÁ, García-Villadangos M, Moreno-Paz M, Gangloff V, Carrizo D, Blanco Y, González S, Sánchez-García L, Prieto-Ballesteros O, Altshuler I, Whyte LG, Parro V, Fairén AG. Geomicrobiological Heterogeneity of Lithic Habitats in the Extreme Environment of Antarctic Nunataks: A Potential Early Mars Analog. *Front Microbiol*. 2021 Jul 2;12:670982. doi: 10.3389/fmicb.2021.670982. eCollection 2021

Ruano-Gallego D, García-Villadangos M, Moreno-Paz M, Gómez-Elvira J, Postigo M, Simón-Sacristán M, Reyburn HT, Carolis C, Rodrigo N, Codeseira YB, Rueda P, Zúñiga S, Enjuanes L, Parro V. (2021) A multiplex antigen microarray for simultaneous IgG and IgM detection against SARS-CoV-2 reveals higher seroprevalence than reported. *Microb Biotechnol*. 2021 May;14(3):1228-1236. doi: 10.1111/1751-7915.13801.

Glass B. J.; C. Stoker; D. Bergman; B. Asher; J. Eigenbrode; T. Stucky; C. McKay; V. Parro; and S. J. Seitz (2021) The Icebreaker Sample Acquisition System (SAS) 17th Biennial International Conference on Engineering, Science, Construction, and Operations in Challenging Environments

Funded projects in 2021

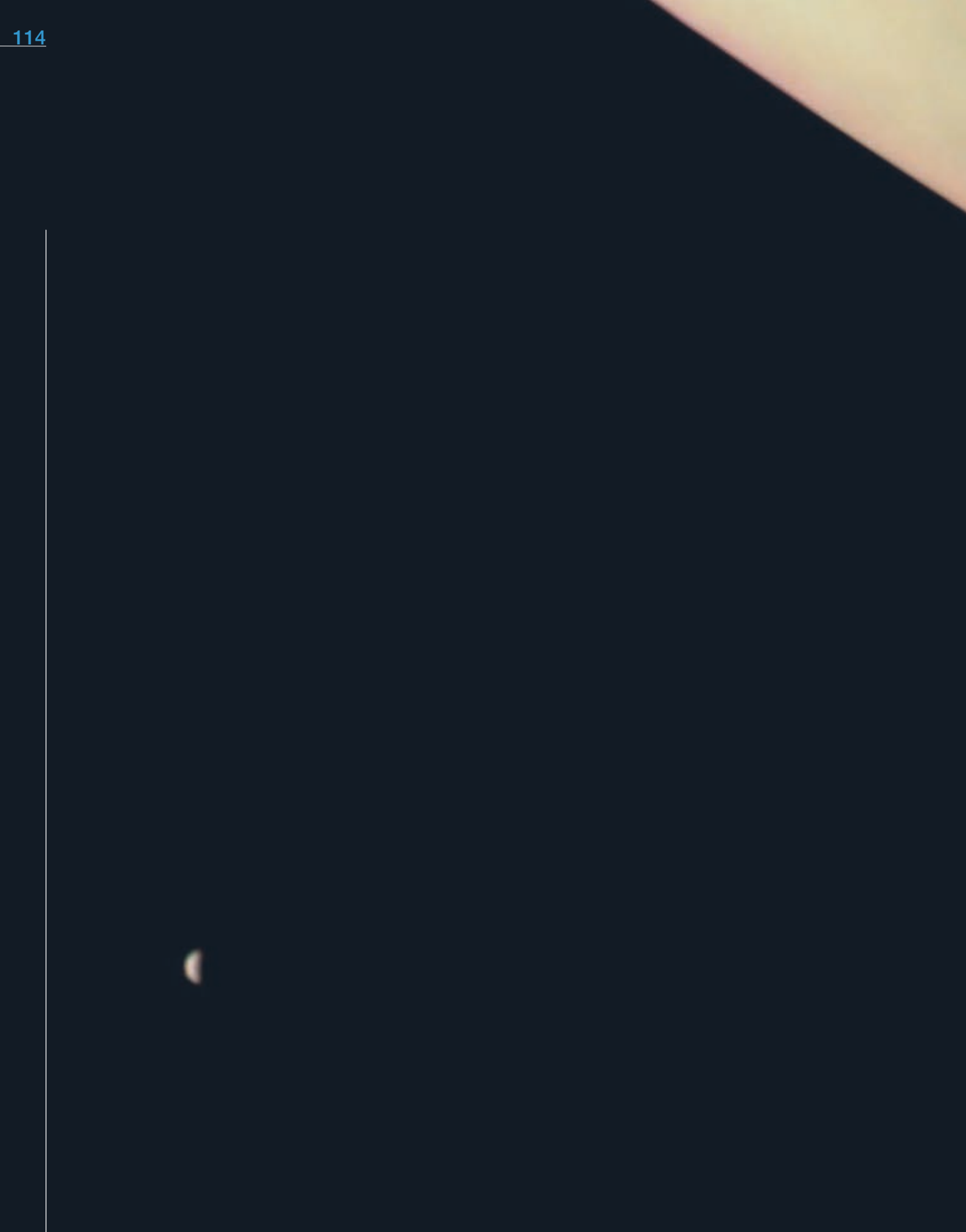
Title: SOLID: *Detección de Señales de Vida en Exploración Planetaria*.

Funding Agency: Agencia Estatal de Investigación (AEI, MICINN) Nº: RTI2018-094368-B-I00

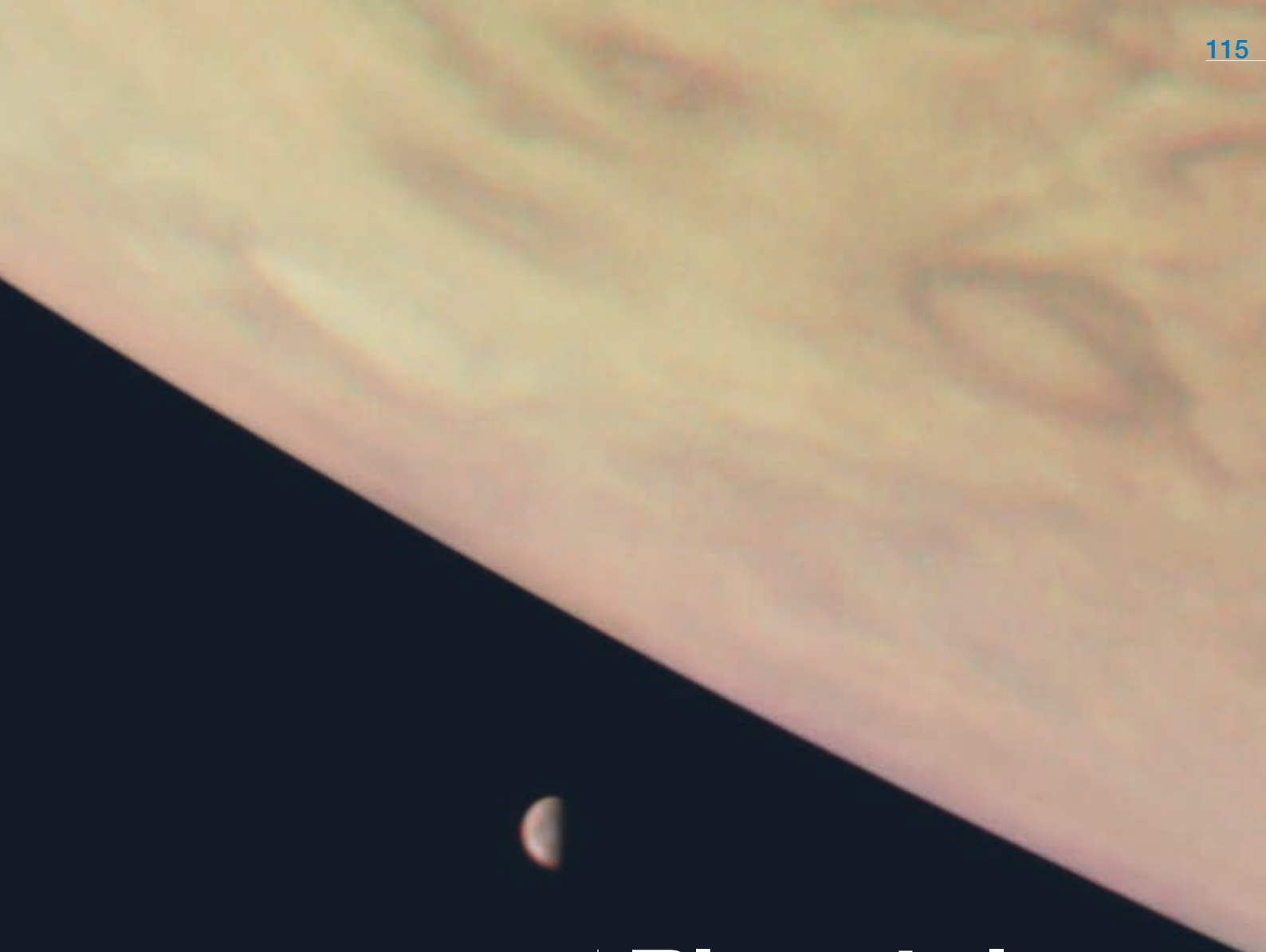
Duration: **01-09-2019 to 31-08-2021**.

PI1, **Victorino Parro**; PI2, Mercedes Moreno-Paz, (CAB, CSIC-INTA) **482.000,00 €**

La bahía Sur en la isla Doumer, cerca de la costa oriental de la península antártica, fue uno de los lugares visitados en busca de sulfuros ácidos. **Crédito: Elena González Toril**



Juno Observes Jupiter, Io y Europa **Crédito: NASA/JPL-Caltech/SwRI/MSSS/Roman Tkachenko**



Planetology and Habitability department of

Heads of Department:

Felipe Gómez Gómez

The Department of Planetology and Habitability has developed a transdisciplinary activity since its creation, a reflection of this is that it is made up of 2 Research Groups:

- Planetary Geology and Atmospheres (PGA)
- Habitability and Extreme environments (HEE)

Summary

Participation in space missions and international panels

The Department of Planetary Geology and Habitability has two representatives on the Planetary Protection Panel (PPP) of COSPAR (SPAce Research Committee): Scientific Commissions B - Space Studies of the Earth-Moon System, Planets and Small Bodies of Solar Systems. This year, the panel launched discussions on the Moon's planetary protection categorization. The Department also has a representative within the Mars Sample Return Scientific Management Group 2 (MSPG-2), an international panel that defines the plan to maximize the scientific return of the first samples to be brought to Earth from Mars. This plan will be an addendum to the ESA-NASA agreement for the Mars Sample Return campaign. The group also has a representative in Perseverance, as a Return Sample Science Participating Scientist (RSS-PS). As part of Perseverance operations, there are a total of 10 representatives who have been selected by NASA and 5 selected by ESA, to document procedures, select samples and provide the required on-site observations and cache samples. that the future ESA-NASA mission will bring back to Earth.

Participation in the ExoMars TGO and Curiosity science teams continues as a science team. Due to programmatic issues, the launch of the rover and the ExoMars platform was delayed from 2020 to 2022. The group has participated in the Rover Scientific Operations Working Group (RSOWG): mapping quads for new landing ellipses at Oxia Planum , and in the rover and surface platform integration test activities with Thales Alenia (France and Italy) and Lavochkin. We have joined the team of the Raman RLS / Exomars and RAX / MMX instruments in which we have tasks related to the future scientific exploitation of the mission.

Regarding the future of the exploration of Mars, the members of this group have also been involved in the generation of several white papers of the MEPAG 2020 community as contributions to the next Decadal Study of Planetary Sciences, such as: "Towards the prediction of the climate and Martian dust storms "; "Deep Trek: Science of habitability and subsurface life on Mars" and "Deep Trek: Mission concepts to explore habitability and subsurface life on Mars"; "Knowledge gaps on planetary protection and enabling science for human missions on Mars".

We participate in two research projects associated with planetary missions financed by MINECO: "Technical operations and scientific exploitation of ExoMars RLS data, and contribution to MMX RAX" and "Science and instrumentation for the study of biogeochemical processes on Mars". In addition, we received funding from ESA through a contract to carry out the study "Measurements of thermal and dielectric properties of ice in support of future radar measurements of Jovian icy moons".

Planetary Geology and Atmospheres (PGA)

Group leader: Olga Prieto Ballesteros

Senior Researchers
Daniel Carrizo Gallardo
M. Isabel Herreros Cid
Antonio Molina
Jens Ormö
Maria Paz Zorzano Mier
Alberto Olof Ormo
Olga Prieto Ballesteros
Antonio Molina Jurado
Postdoctorals
Victoria Muñoz Iglesias
Predoctorals
Ana de Dios Cubillas
Óscar Ercilla
Federico Mansilla
Cristina Robas.
Technicians
Maria Paz Martín Redondo
Paloma Martínez Sarmiento
María Teresa Fernández Sampedro
Teresa Martínez Pérez
Sonia Maria Vega Garcia
Students (Master, TFG, others):
Teresa Martínez Pérez
Belén Gómez Cifuentes
Alba Pereira Cebrian
Marcos Mora Rueda
Alejandro Suárez Gordo

Summary

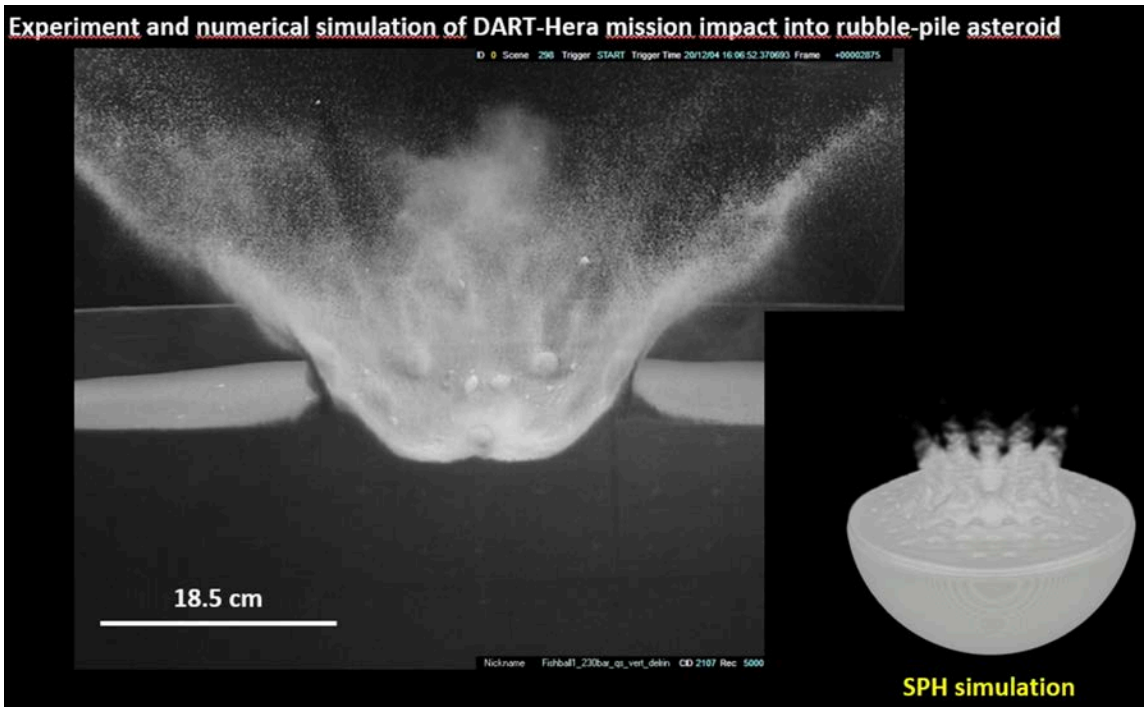
This group contributes to the objectives O3, O4 and O6 of the Strategic plan by participating in: 1) planetary exploration missions to Mars and its moons (ExoMars2022, Trace Gas Orbiter, MMX, Curiosity and in Perseverance as Returned Sample Scientists and in science operations), asteroids (DART, Hera), Mercury (Bepi-Colombo) and the Jovian system (JUICE). We scientifically supported the development of instruments like the Raman spectrometers for the habitability characterization of Mars (RLS) and Phobos (RAX); 2) international panels such as the COSPAR Planetary Protection Panel, and in the international group that has designed the plan for Mars Sample Return, from sampling to analysis on Earth; 3) particular laboratory and modeling investigations and terrestrial analog studies for answering planetary science questions such as: a) the transport of aerosols on the atmosphere of Earth as an analogue of the dust transport on Mars, b) the deflection of asteroids using kinetic impactors, c) the thermal and electrical properties of ice mixtures for future radar signal interpretation, d) how lipids biomarkers and their stable isotopic composition can give us unequivocal information about the presence of life (extinct or extant) in the Solar System and exoplanets or e) the deltas formation processes on Mars.

The following research highlights exemplify the most relevant investigations and results in the group.

Research Highlights 2021

RH1. Projectile impact experiments in support of the DART (NASA) and Hera (ESA) space missions to evaluate the use of kinetic impactor for the deflection of Earth-threatening asteroids

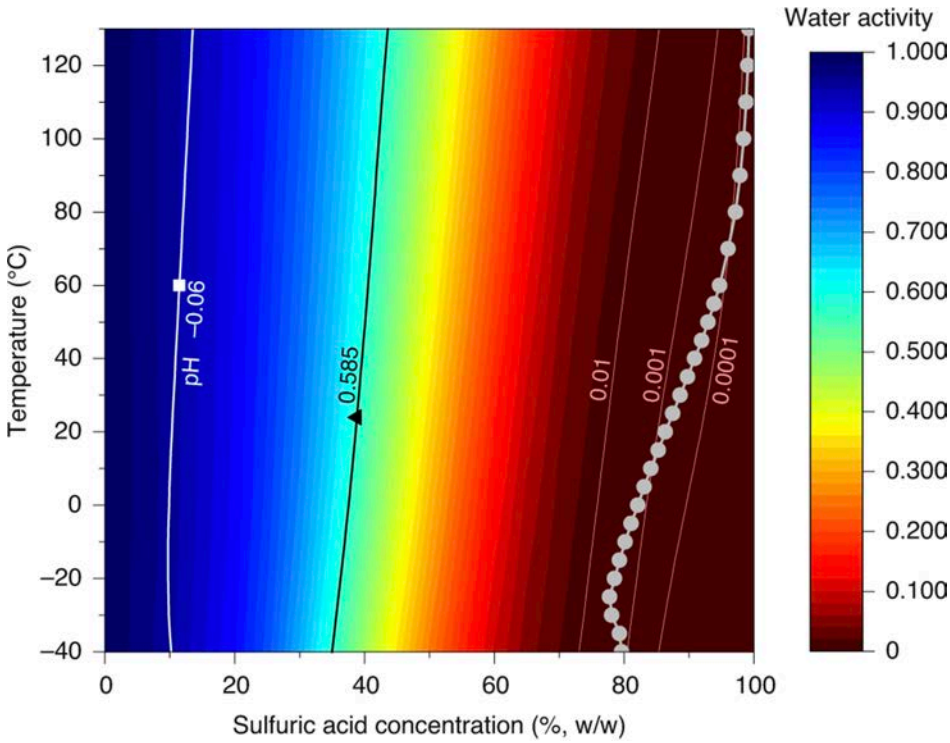
NASA's Double Asteroid Redirection Test (DART) will impact the smaller component of the 65803 Didymos asteroid system, Dimorphos, and alter its orbital period around the primary, thus demonstrating the controlled deflection capabilities of near-Earth asteroids by a kinetic impactor. ESA's Hera mission will arrive at Dimorphos several years after the DART impact and provide a detailed characterization of the impact outcome, including the morphometry and morphology of the crater. Recent impact experiments and numerical studies have shown that the kinetic impact efficiency depends strongly on the target properties. Therefore, for a successful interpretation of the DART impact outcome it is important to understand the influence of asteroid properties on the cratering process. Moreover, the DART impact outcome analysis will be based on numerical models, which require extensive and accurate prior validation. Here we perform impact experiments and numerical simulations specifically designed to mimic asteroid surface materials and structures (e.g., layered targets, rubble piles). The experiments are performed at the Experimental Projectile Impact Chamber (EPIC) at Centro de Astrobiología CSIC-INTA, Spain. In the international collaboration we use the iSALE-2D and the Bern's SPH shock physics codes to simulate the laboratory experiments.



Comparison between EPIC impact experiment performed at CAB CSIC-INTA and SPH simulation performed at University of Bern, Switzerland.

RH2. Venus clouds are not habitable because of their extremely low water activity

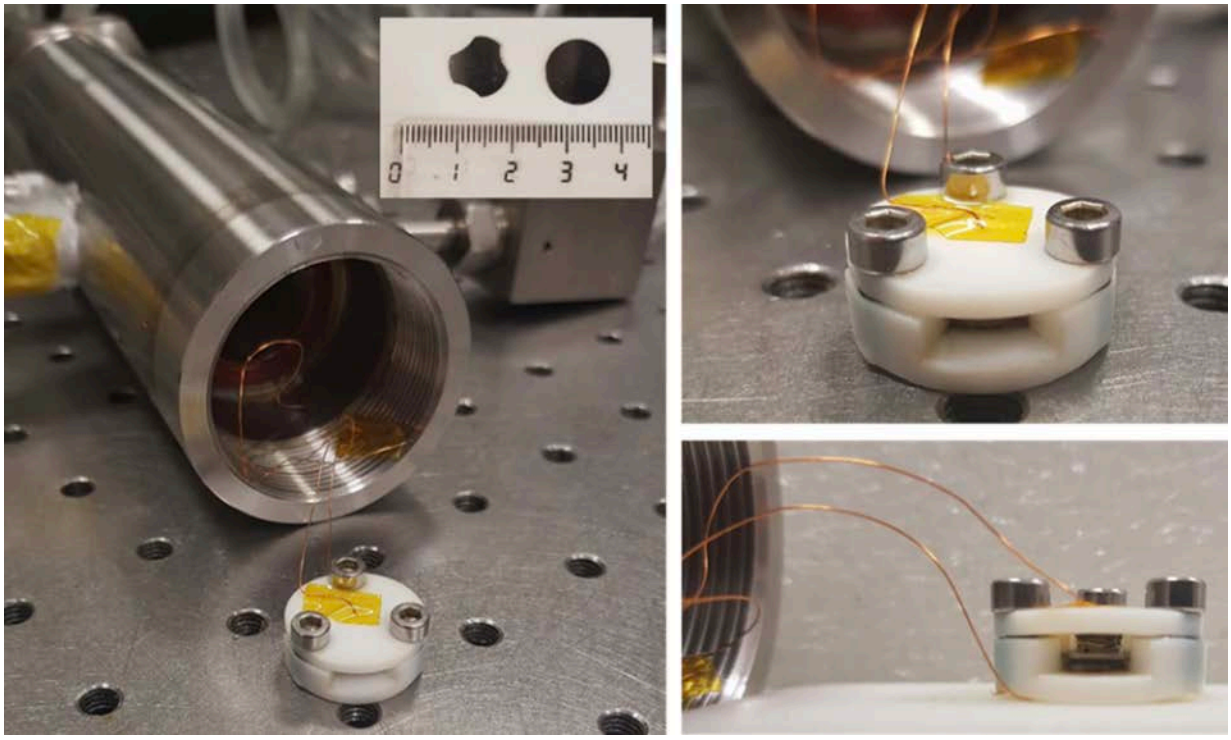
The recent suggestion of phosphine in Venus's atmosphere has regenerated interest in the idea of life in clouds. Calculations of water activity reveal that this parameter can be a substantial barrier to habitability for clouds of Solar System planets. In particular, water activity within droplets of Venus's clouds is more than 100-fold below the threshold for biotic activity of known extremophiles. Here we compute the water activity within the clouds of Venus and other Solar System planets from observations of temperature and water-vapour abundance. We find water-activity values of sulfuric acid droplets, which constitute the bulk of Venus's clouds, of <= 0.004, two orders of magnitude below the 0.585 limit for known extremophiles. Considering other planets, ice formation on Mars imposes a water activity of <= 0.537, slightly below the habitable range, whereas conditions are biologically permissive (>0.585) at Jupiter's clouds (although other factors such as their composition may play a role in limiting their habitability). By way of comparison, Earth's troposphere conditions are, in general, biologically permissive, whereas the atmosphere becomes too dry for active life above the middle stratosphere. The approach used in the current study can also be applied to extrasolar planets.



Map of water activity of liquid H2SO4–H2O mixtures as a function of temperature and sulfuric acid concentration over the temperature range pertinent to active life (between −40 °C and 130 °C).

RH3. Thermal properties of ice mixtures in support to JUICE radar measurements

Experimental information is necessary for modelling planetary features as well as interpret the space mission data in terms of geodynamical, geochemical petrological activity and habitability. Thermal and electrical properties, for example the results we found from the study of mixtures of ices in extreme conditions relevant to the Galilean moons, which was funded by an ESA contract. They confirmed measurable differences on the solid and liquid phases at systems with different chemical composition This information will be crucial for the correct interpretation of the radar instruments on board coming missions to the Galilean satellites concerning their structure and composition: Radar for Icy Moon Exploration (RIME) at JUICE, and Radar for Europa Assessment and Sounding Ocean to Near-surface (REASON) at Europa Clipper.



Images of the high pressure cell for the electric measurements (from the final report to ESA)

RH4. Investigating molecular and isotopic fingerprints of life on Greenland Ice Sheet (GIS) cryoecosystems with astrobiological interest for icy worlds and Mars

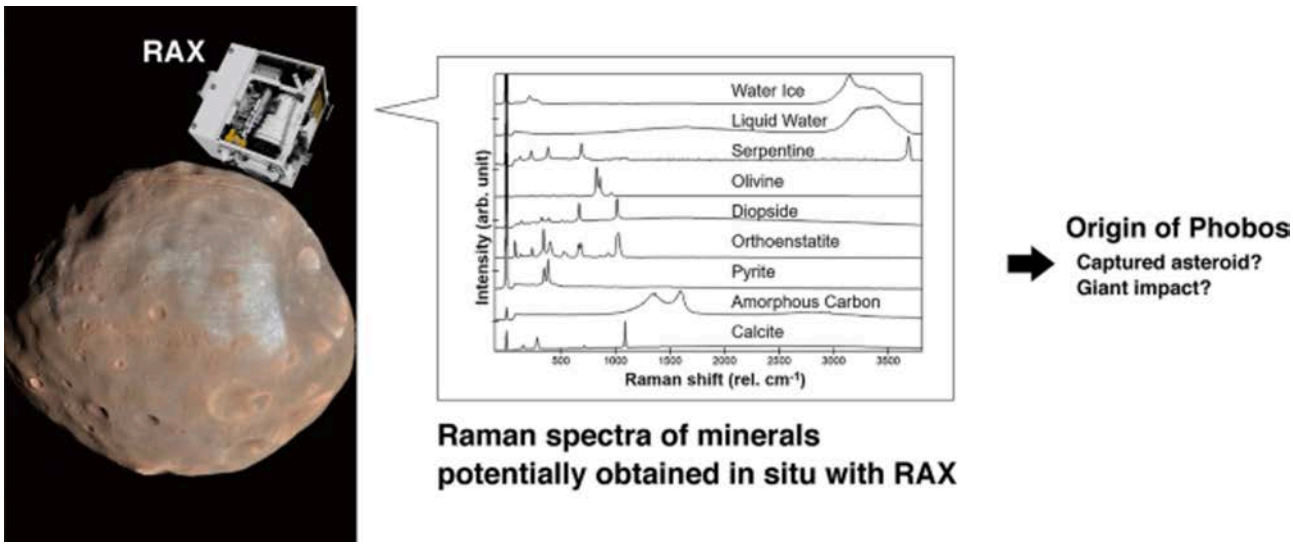
Glaciers and ice sheets are extreme environments where indigenous microorganisms must survive prolonged exposure to subzero temperatures and background radiation for geological time scales. The development of functional microbial ecosystems in permafrost environments may have implications in the search for past or extant life in icy worlds beyond the Earth. In the Solar System, Europa and Enceladus have been recognized as the icy worlds with highest likelihood to harbor life, largely because liquid water could be in contact with rocks. Both satellites are believed to contain a global ocean of salty water under a rigid icy crust that would provide the scenario for an interaction between briny water and rocks, and the conditions for life to arise. The permanent Greenland Ice Sheet (GIS) represents a possible analog of such icy worlds, constituting an important long-term repository of psychrophilic microorganisms. In 2021 we visited GIS for investigating molecular and isotopic lipid biomarkers of microorganisms inhabiting different cryo-ecosystems (subglacial, englacial and supraglacial) in its glacial environment as a simplification of analogous icy-world compartments to obtain clues of a potential life development on analogous extraterrestrial cold environments.

Image of the field campaign at Greenland developed in 2021

RH5: RLS and RAX Raman spectrometers onboard ExoMars2022 and MMX missions, respectively

Exomars 2022 was planned to be launched in September 2022 to target an ancient location interpreted to have strong potential for past habitability and for preserving physical and chemical biosignatures (Oxia Planum, a clay-bearing plain located on the eastern border of Chryse Planitia). Rosalind Franklin main goal is searching for signs of extinct life, and for that it has the Analytical Laboratory Drawer (ALD), which includes RLS and a drilling system. Among the activities of the science team during 2021 were: 1) the selection of some representative samples (natural or synthetic) for the cooperative characterization by the rover payload instruments;2) the ExoMars rover Simulation Operation Training campaign to rehearse the science operations processes, as in the Science Operations Plan with the focus on the strategic plan. Science team activities simulated during planning included decision-making, journaling, etc. in order to account for different operational scenarios and planning time horizons.

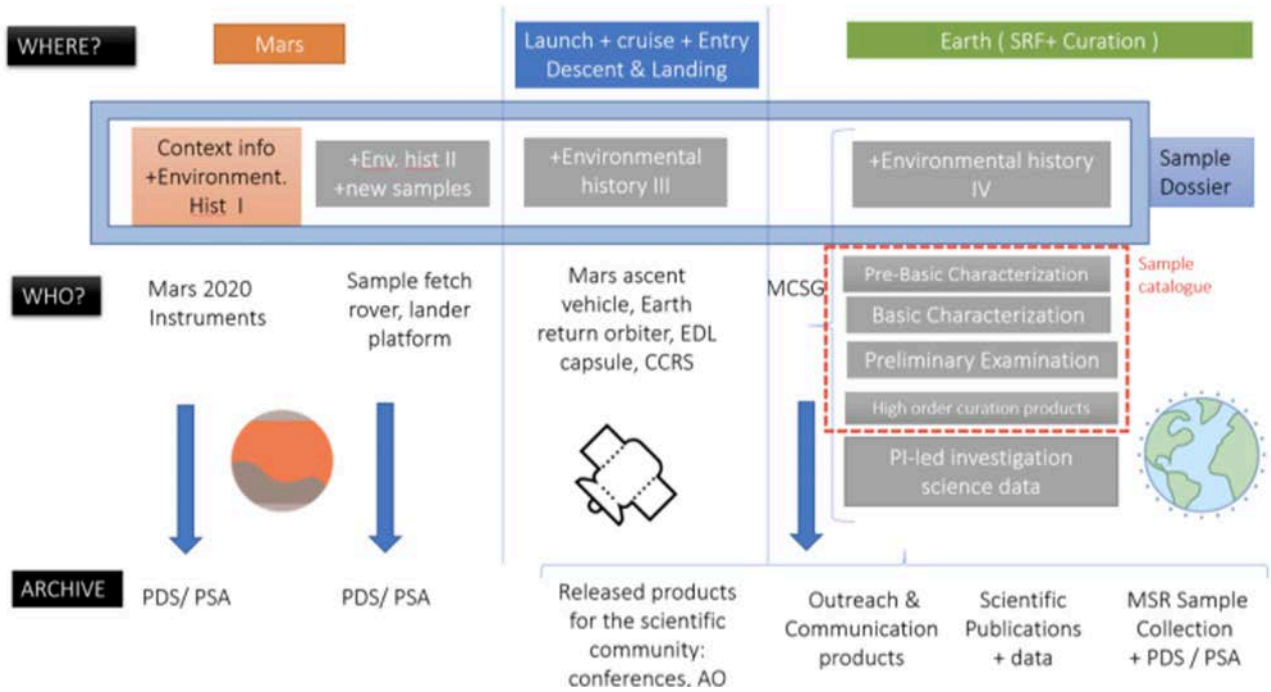
The MMX mission will be launched in 2024 to conduct orbital sensing observations of the two Mars moons, Phobos and Deimos, and will also perform *in situ* observations on, and return samples from Phobos. Main motivation for MMX is to understand the origin, evolution and formation of the Solar System bodies and to observe processes, which have effects on the evolution of the Mars system from the new vantage point and to advance our understanding of Mars surface environmental transition. RAX will perform spectroscopic measurements on Phobos' surface, which will be used both to identify its mineralogy and to support the characterization of a potential landing site for MMX mission sample return. And so, at the end, the RAX measurements will be directly compared with Raman measurements obtained from the RLS instrument during the ExoMars 2022 mission.



RAX Raman spectrometer for studying Phobos' mineralogy (from Cho et al. 2021)

RH6: Sampling as part of the Returned Sample Scientists (RSS) team, with Perseverance: 6 rock samples and 1 atmospheric sample

Perseverance rover landed at Jezero crater on Mars. The rover is equipped with 43 canisters in which it will deposit geological samples from Mars, to be retrieved and returned to Earth in a future mission called Mars Sample Return. The Return Sample Science Participating Scientists (RSS-PS) (10 from the US and 5 European), form a group that focuses on promoting the identification, collection, documentation, and interpretation of Jezero samples. The RSS participate in operations and collect the critical information that shapes the Initial Reports of the samples and the bundles of data that will be used in the future by other scientists once they are returned to Earth and analyzed. The analysis of the abraded patches that belong to the same rocks where the first 6 samples have been acquired, reveal that the present day Jezero crater floor consists of igneous rocks, rich in olivine, which have been exposed to different aqueous episodes. These patches contain organics and salts which suggests that biological organic material could also be preserved within the sample rock cores. One of the sample tubes was sealed with a sample of ambient atmospheric and one of the tubes was sealed as witness probe for contamination control.



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Funded projects in 2021

OPERACION TECNICA Y EXPLOTACION CIENTIFICA DE DATOS EN RLS DE EXOMARS, Y CONTRIBUCION AL RAX DE MMX (PID2019-107442RB-C32). MICINN. PIs: Olga Prieto Ballesteros and Daniel Carrizo. 01/01/2020-31/12/2022. 665.379 EUR

THE CYCLE OF AEROSOLS ON MARS AND EARTH, A COMPARATIVE STUDY. IMPLICATIONS FOR LIFE AND PLANETARY PROTECTION (CAMELIA). PI: Maria-Paz Zorzano. Julio 2020-Junio 2023. 165.200 EUR.

DEVELOPMENT OF A COMBINED CAPACITY OF NUMERICAL AND EXPERIMENTAL SIMULATION OF COSMIC IMPACTS WITH SPECIAL FOCUS ON EFFECTS OF MARINE TARGETS, 01/01/2020 until 31/12/2021. Spanish Research Council (CSIC) support for international cooperation: I-LINK project LINKA20203. Total funding: 23001,24 EUR P.I: Jens Ormo

MEASUREMENTS OF THERMAL AND DIELECTRIC PROPERTIES OF ICES IN SUPPORT TO FUTURE RADAR MEASUREMENTS OF JOVIAN ICY MOONS. ESA, Contract No. 4000126441/19/ES/CM with CSIC. Period: 2019-2021; Funding: 100.000 euros. PI: Olga Prieto Ballesteros and Guillermo Muñoz Caro

Publications

EXTREME ENVIRONMENTS IN PLANETARY EXPLORATION: GEOLIPIDS, STABLE ISOTOPES AND MINERALS IN KING GORGE ISLAND, ANTARCTICA. 2019-2023. Funding: IAU (Uruguayan Antarctic Institute), 20000 EUR. Participation: PI: D. Carrizo

TÉCNICAS TRANSVERSALES PARA LA VISUALIZACIÓN Y ANÁLISIS DE DATOS COMPLEJOS Y MULTIMODALES (PID2020-113013RB-C21), PI: Luis Ignacio Pastor Pérez and Susana Mata Fernández; MICINN, Sep 2021 – Sep 2024, (Research Team members: Isabel Herreros, Antonio Molina)

CARACTERIZACIÓN GEOFÍSICA DE LA GEOMETRÍA ESTRUCTURAL PROFUNDA DEL RELLENO SEDIMENTARIO EN LA CUENCA NEÓGENA DE TABERNAS (ALMERÍA SE ESPAÑA): MEDIDAS Y ESTUDIO DEL PERFIL GRAVIMÉTRICO, MAGNÉTICO Y SÍSMICO, PARA DETERMINAR LAS ANOMALÍAS GEOFÍSICAS PRODUCIDAS POR UN POSIBLE EVENTO CATASTRÓFICO DURANTE EL MIOCENO, 01/12/2021-31/11/2023. Proyectos de I+D en el marco del Programa Operativo FEDER Andalucía 2014-2020 Proyectos de Fomento y Generación de Conocimiento "Frontera" UAL2020-RNM-B1980.P.I Antonio Garcia Jerez, Univ. Almería. Total funding: 30.000E. (Research Team members: Isabel Herreros, Antonio Molina)

SCIENCE AND INSTRUMENTATION FOR THE STUDY OF (BIO)-GEOCHEMICAL PROCESSES IN MARS. 2020-2021. Funding: MINECO. (20000 €). Coordinator: Juan Manuel Madariaga. (Research Team members: Daniel Carrizo, Olga Prieto Ballesteros)

Public Outreach Activities, TFG and TFM

*Student name: TERESA MARTÍNEZ PÉREZ
Beca de Introducción a la Investigación para Estudiantes Universitarios "JAE Intro ICU" (JAEIntro-2020-CAB-03). Title: Estudio mediante modelización numérica de los procesos dinámicos que pudieron dar lugar a ciertas morfologías observadas en Marte
Person/s in charge: M. Isabel Herreros Cid y Antonio Molina Jurado
Duration: 01/01/2021 to 31/05/2021 (6 months)

*Student name: BELÉN GÓMEZ CIFUENTES
Prácticas externas: Title: Modelización de procesos hidrogeológicos en Marte
Person/s in charge: M. Isabel Herreros and Antonio Molina
Duration: 01/02/2021 to 31/05/2021 (5 months); 15 horas semanales (17 semanas)

TFM: Title: Reconstrucción mediante modelización numérica de la formación de un depósito deltaico en la región de Coprates-Catena, Valles Marineris, Marte
Máster Universitario en Ciencia y Tecnología desde el Espacio, Universidad de Alcalá (UAH)
Tutors: Antonio Molina, M. Isabel Herreros, and Miguel Ángel de Pablo (UAH)
Defense date: 30/09/2021
Grade: Sobresaliente (10/10)

*Student name: ALBA PEREIRA CEBRIAN
TFG: Title: MEDIDAS DE PROPIEDADES TÉRMICAS DE MUESTRAS DE ANÁLOGOS TERRESTRES CON APLICACIÓN A MARTE, PARA EL CÁLCULO DE LA INERCIA TÉRMICA EN FUNCIÓN DE LA COMPOSICIÓN QUÍMICA Y EL ESTADO DE AGREGACIÓN DE LOS SUELOS
Máster Universitario en Ciencia y Tecnología desde el Espacio, Universidad Rey Juan Carlos
Tutors: Victoria Muñoz Iglesias
Defense date: 30/09/2021
Grade: Sobresaliente (10/10)

*Student name: MARCOS MORA RUEDA
TFM: Title: Estudio de la formación de cráteres de impacto en el marco de las misiones espaciales DART-Hera.
Máster Universitario en Ingeniería Industrial, Universidad Carlos III de Madrid.
Tutors: M. Isabel Herreros and Jens Ormö
Defense date: 14/07/2021
Grade: Sobresaliente (9.8/10)

*Student name: ALEJANDRO SUÁREZ GORDO
Prácticas externas: Title: Modelos numéricos para el estudio hidrodinámico del sistema de acuíferos subterráneos del Río Tinto (Huelva).
Person/s in charge: M. Isabel Herreros and Cristina Escudero
Duration: 22/02/2021 to 31/07/2021 (5 months - 360 hours)

Outreach (most relevant contributions)

V Ciclo de Conferencias de Cassiopeia. Universidad de la Laguna. “Destino: Europa”. 14 de Abril. Olga Prieto Ballesteros

VII Curso de Astrofísica: Astrobiología y Sistemas Planetarios. Universidad de Teruel. 8-10septiembre 2021. Búsqueda de ambientes habitables en el sistema solar exterior. Olga Prieto Ballesteros

Madrid ama la Química 2021. REAL SOCIEDAD ESPAÑOLA DE QUÍMICA. Estudiando las lunas heladas en el laboratorio 17 de Noviembre. Olga Prieto Ballesteros

Quadrivium Ciclo de Conferencias. ExoEstrato - Sociedad Andaluza de Astrogeología. OCÉANOS EXTRATERRESTRES. Olga Prieto Ballesteros

Ciclo de conferencias en la Residencia de Estudiantes CSIC. El origen de la Vida. El Sistema Solar: la diversidad de escenarios posibles. Olga Prieto Ballesteros

Ciclo de conferencias en la Residencia de Estudiantes CSIC. El origen de la Vida. Mesa redonda: Modera: María Paz Zorzano Mier

Press release. Investigadores del CAB estudian en laboratorio minerales de gran importancia en planetología tras ser descubiertos en Ceres. Muñoz-Iglesias V. et al.

Press release. CAB (CSIC-INTA) participa en la primera misión espacial defensiva de la historia: la misión DART de la NASA, cuyo lanzamiento está previsto el 24 de noviembre. Jens Ormö and M. Isabel Herreros.

Cursos de formación continua. ESCUELA ESPAÑOLA DE ALTAS PRESIONES 2021. Universidad de Valencia. “La presión en la Astrobiología”. Victoria Muñoz Iglesias

PechaKucha Centro de Astrobiología CSIC INTA. “A methane in Titan”. Victoria Muñoz Iglesias.

Awards

Outstanding Paper award 2021. European Astrobiology Network Association (EANA). The Complex Molecules Detector (CMOLD): A fluidic-based instrument suite to search for biochemical complexity on Mars and icy moons by Fairén et al. (including O. Prieto-Ballesteros) (2020).

Accesit 2 in the 5th PhDay of EDUCM, Escuela de Doctorado de la UCM: “Explorando la geología interna de los mundos helados: más allá de la corteza de hielo”. Oscar Ercilla.

Habitability and Extreme Environments (HEE)

Head: Dr. Felipe Gómez

Senior Researchers

Ricardo Amils Pibernat

Alberto Gonzalez Fairén

Postdoctorals

Armando Javier Azua Bustos

Laura Garcia Descalzo

Cristina Escudero Parada

Alicia Lopez Jimenez

Francesco Salese

Fuencisla Cañadas Blasco

PhD

Marcos Mora

Cristina Robas García

Technicians

Nuria Rodriguez Gonzalez

Summary

This group contributes mainly to objective 5 of our strategic plan, namely, to study the habitability of extreme environments on Earth as terrestrial analogues of other planetary settings, as well as to study the adaptability of life to extreme physico-chemical parameters. Additionally, this group explore the fingerprints that life can leave in the medium and its tight contact with mineral world. Members of the group are part of the REMS and MEDA instrument to characterize the martian near ground atmosphere as part of the NASA`s MSL and Mars2020 missions. Over 2021 we have been working on the habitability and microbial metabolic traits of the polyextremophilic environment of the Dallol area in Ethiopia, as well as daily participation in the REMS and MEDA operations and scientific discussions.

Research Highlights 2021

RH1. Methanogenesis at High Temperature, High Ionic Strength and Low pH in the Volcanic Area of Dallol, Ethiopia

The Dallol geothermal area originated as a result of seismic activity and the presence of a shallow underground volcano, both due to the divergence of two tectonic plates. In its ascent, hot water dissolves and drags away the subsurface salts. The temperature of the water that comes out of the chimneys is higher than 100 C, with a pH close to zero and high mineral concentration. These factors make Dallol a polyextreme environment. So far, nanohaloarchaeas, present in the salts that form the walls of the chimneys, have been the only living beings reported in this extreme environment. Through the use of complementary techniques: culture in microcosms, methane stable isotope signature and hybridization with specific probes, the methanogenic activity in the Dallol area has been assessed. Methane production in microcosms, positive hybridization with the Methanosarcinales probe and the 13CCH4-values measured, show the existence of extensive methanogenic activity in the hydrogeothermic Dallol system. A methylotrophic pathway, carried out by Methanohalobium and Methanosarcina-like genera, could be the dominant pathway for methane production in this environment.

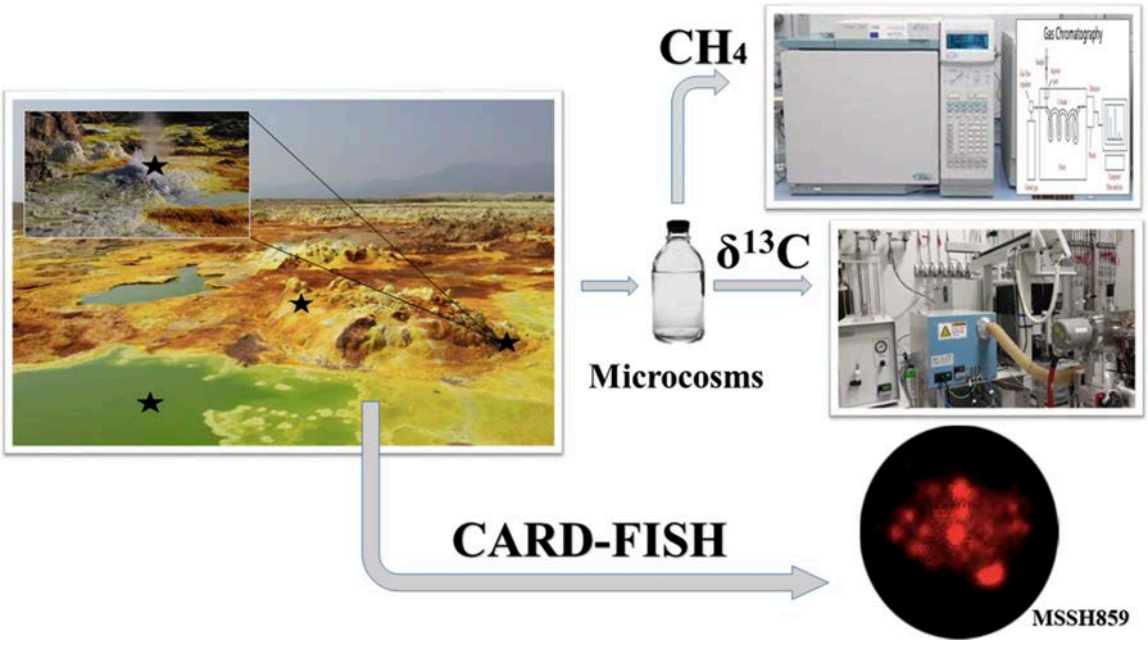
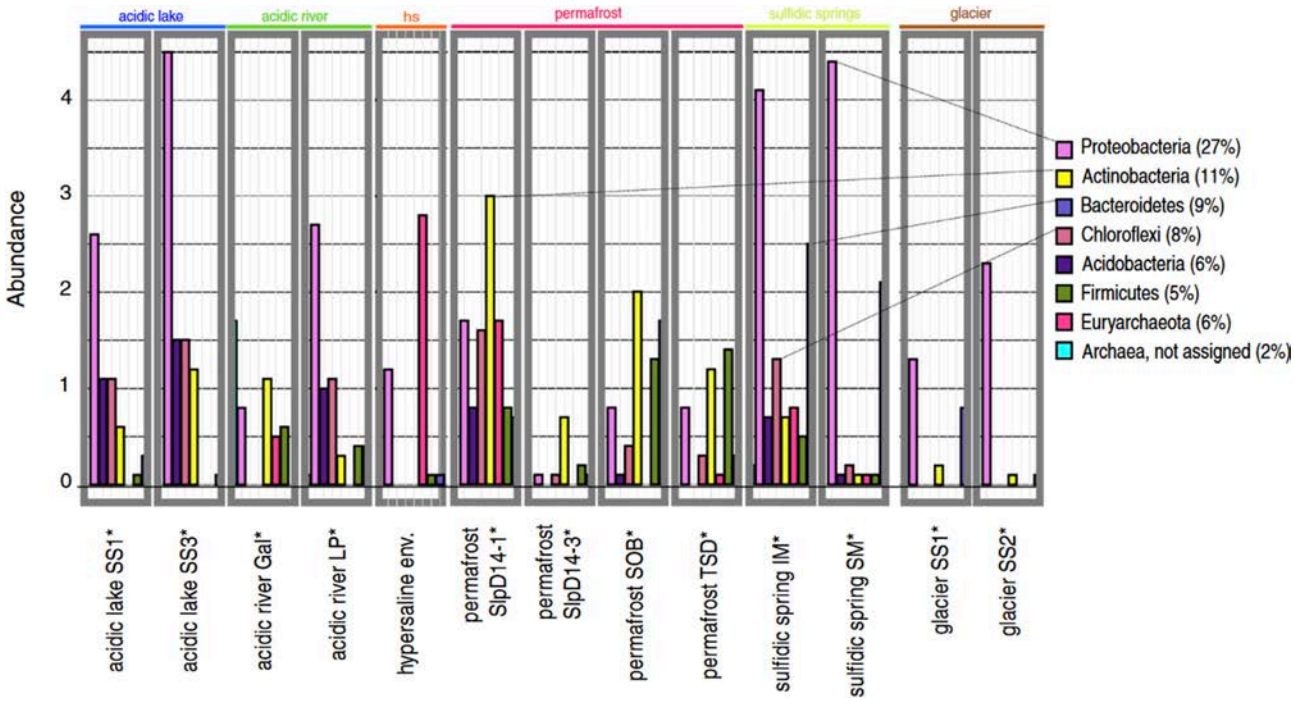


Diagram presenting a brief summary of the sampling location (Dallol) and the methodology and results obtained in this work where we reported the presence of methanogenic metabolism in the very extreme conditions of the geothermal area of Dallol (Ethiopia)

Research Highlights 2021

RH2. Taxonomic and functional analyses of intact microbial communities thriving in extreme, astrobiology-relevant, anoxic sites

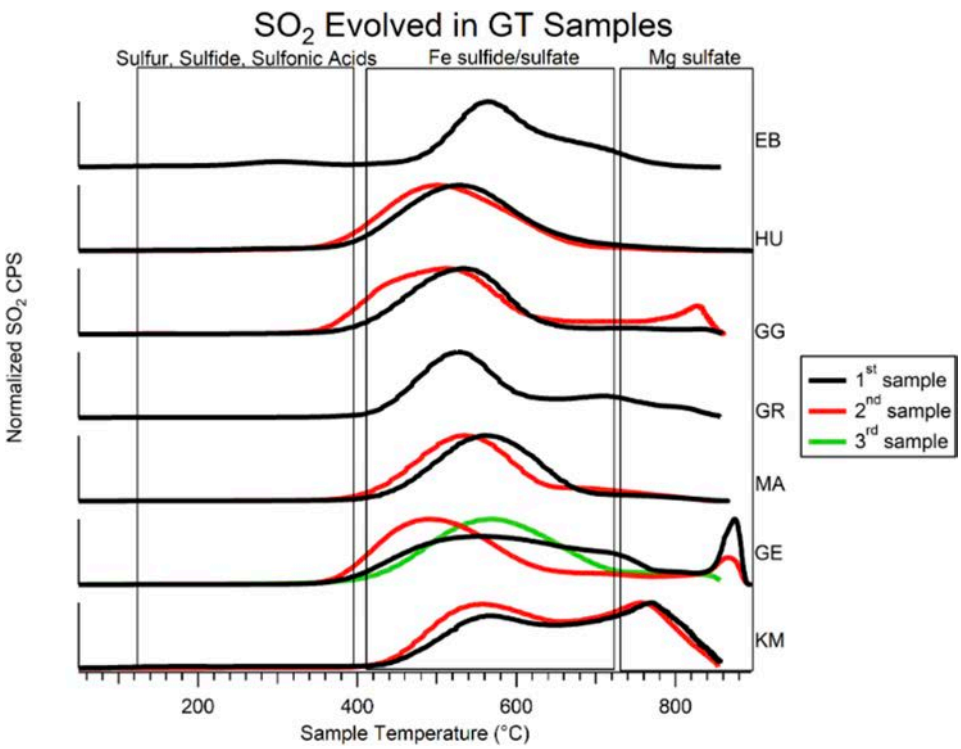
Extreme terrestrial, analogue environments are widely used models to study the limits of life and to infer habitability of extraterrestrial settings. In contrast to Earth's ecosystems, potential extraterrestrial biotopes are usually characterized by a lack of oxygen. In the MASE project (Mars Analogues for Space Exploration), we selected representative anoxic analogue environments (permafrost, salt-mine, acidic lake and river, sulfur springs) for the comprehensive analysis of their microbial communities. We assessed the microbiome profile of intact cells by propidium monoazide-based amplicon and shotgun metagenome sequencing, supplemented with an extensive cultivation effort. The information retrieved from microbiome analyses on the intact microbial community thriving in the MASE sites, together with the isolation of 31 model microorganisms and successful binning of 15 high-quality genomes allowed us to observe principle pathways, which pinpoint specific microbial functions in the MASE sites compared to moderate environments. The microorganisms were characterized by an impressive machinery to withstand physical and chemical pressures. All levels of our analyses revealed the strong and omnipresent dependency of the microbial communities on complex organic matter. Moreover, we identified an extremotolerant cosmopolitan group of 34 poly-extremophiles thriving in all sites. As conclusion we can say that our results reveal the presence of a core microbiome and microbial taxonomic similarities between saline and acidic anoxic environments. Our work further emphasizes the importance of the environmental, terrestrial parameters for the functionality of a microbial community, but also reveals a high proportion of living microorganisms in extreme environments with a high adaptation potential within habitability borders.



Most abundant phyla of the microbial community (based on "universal" primer set, "microbiome"). The relative abundance of each taxon is shown on the y-axis. The total relative abundance, summed up for all samples, is given in brackets behind the taxa names in the legends.

RH3. Oxidized and reduced sulfur observed by the Sample Analysis at Mars (SAM) instrument suite on the Curiosity rover within the Glen Torridon region at Gale crater, Mars

In this work published in JGR journal we report the presence of both sulfide and sulfate (oxideze and reduced sulfur) with its important astrobiological implications. The Mars Science Laboratory (MSL) Curiosity rover has been assessing the habitability and geologic history of Gale crater, Mars since landing in 2012. One of the primary objectives of the mission was to investigate a clay-bearing unit identified using orbital spectral data, designated the Glen Torridon (GT) region. This region was of particular interest because of its elevated abundance of clay minerals that may have preserved geochemical evidence of ancient habitable environments. The Curiosity rover explored the GT region for ~750 sols and analyzed eight drilled samples with the Sample Analysis at Mars (SAM) instrument suite using evolved gas analysis-mass spectrometry. Evolved sulfur-bearing gases provided insight about the composition of sulfur-containing compounds in Martian samples. Evolved gases were analyzed by three methods to understand the oxidation state of sulfur in the samples: (1) SO_2 evolution temperature, (2) quadratic discriminant analysis comparing SAM data to SAM-like laboratory investigations, and (3) sulfur isotope values from evolved $^{34}SO_2/^{32}SO_2$. The results of these three methods were consistent with the majority of sulfur in the GT region being in an oxidized state, but two of the eight samples analyzed by SAM were consistent with the presence of small amounts of reduced sulfur. The oxidized and reduced sulfur could have a variety of sources and represents a nonequilibrium assemblage that could have supported putative ancient chemolithotrophic metabolisms.

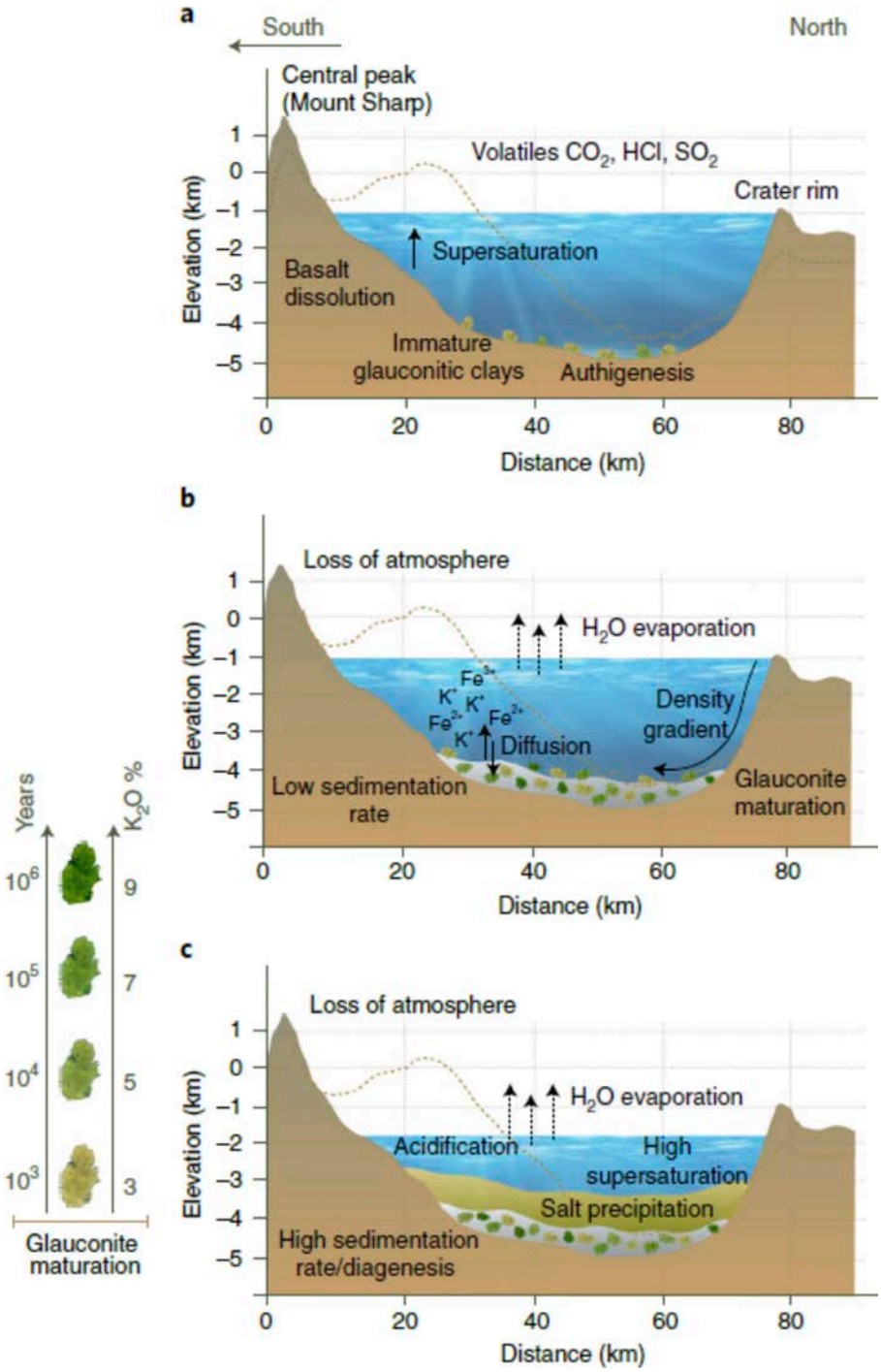


Possible sequence of precipitation of glauconitic clays in the Murray formation and main steps of the physico-chemical evolution of the water column.

Research Highlights 2021

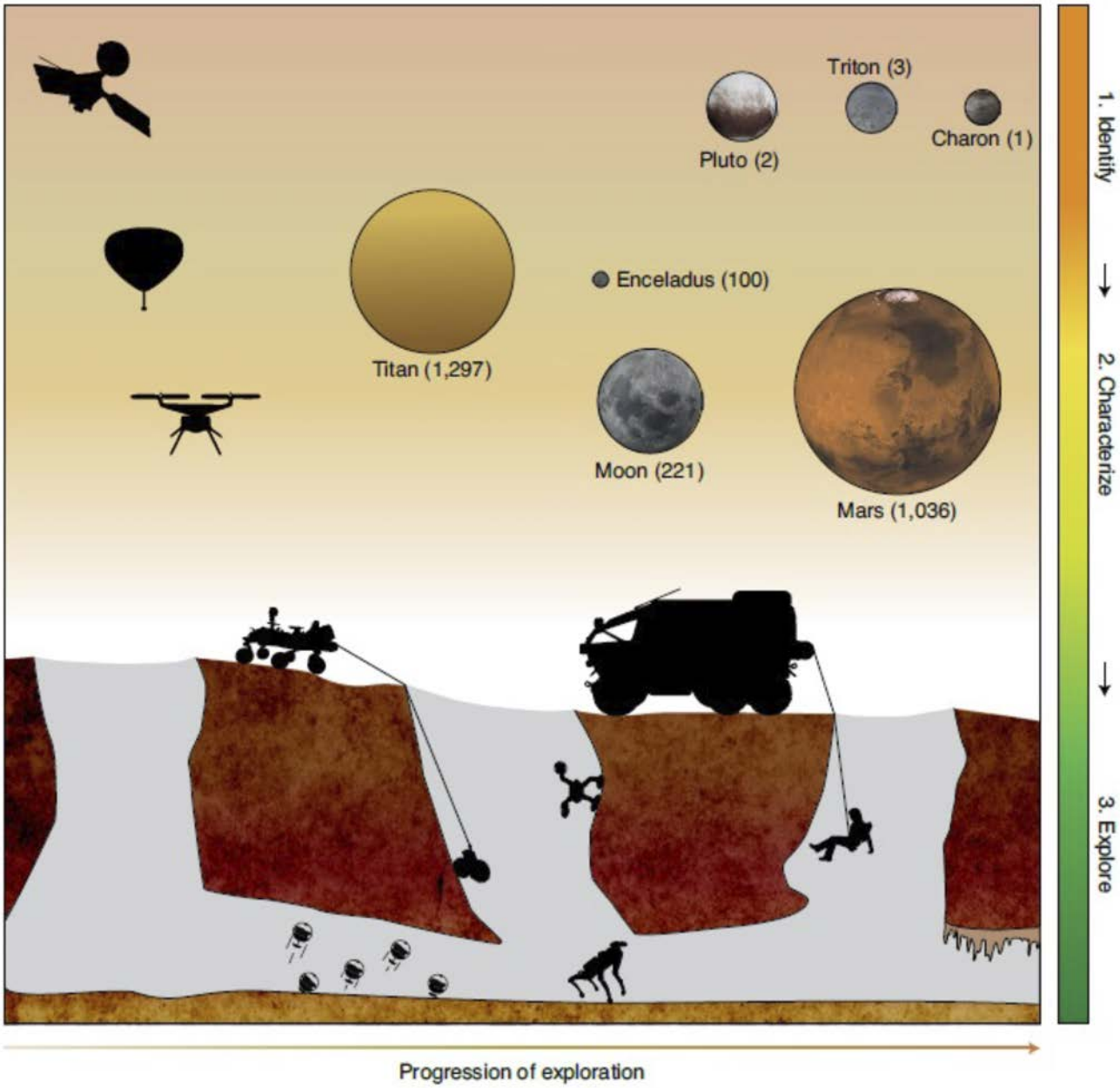
RH4. Long-lasting habitable periods in Gale crater constrained by glauconitic clays

This paper presents the first identification on Mars of a particular type of clay, called glauconite, whose presence makes it possible to describe in detail the sedimentation conditions in oceans or lakes over long periods of time. To identify glauconites in Gale, we used X-ray diffraction (XRD) data obtained with the Chemistry and Mineralogy (CheMin) instrument on Curiosity. CheMin analyzed sediments extracted from several of Curiosity's drill holes in the Gale sediments. This work provides strong evidence that Gale Crater Lake was present for long periods of time, characterized by extremely slow sedimentation processes, and in a regime of stagnant waters and slow evaporation at low temperatures. That is, it met the necessary conditions to substantiate biological processes.



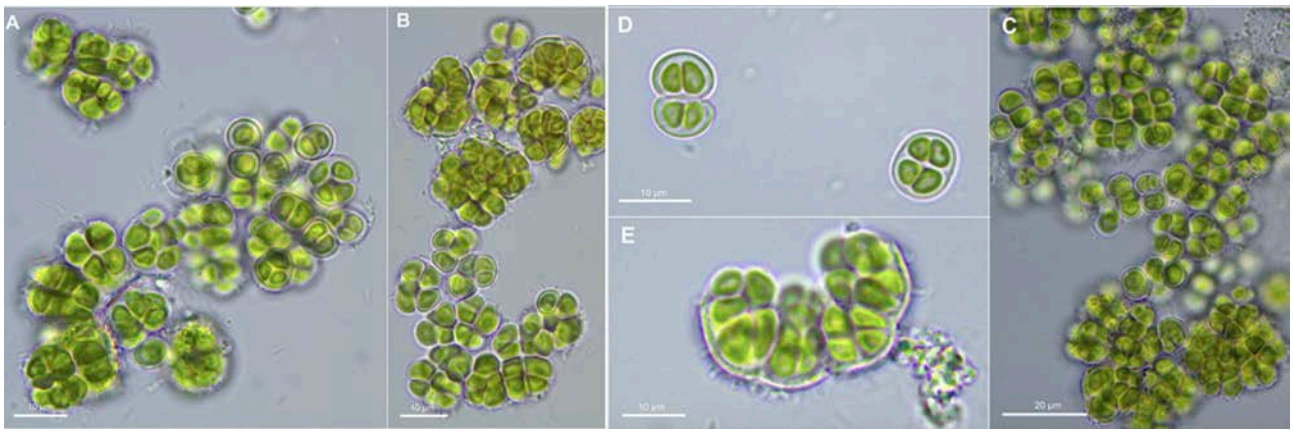
RH5. A roadmap for planetary caves science and exploration

2021 is the International Year of Caves and Karst. To honour this occasion, we wish to emphasize the vast potential embodied in planetary subsurfaces. While researchers have pondered the possibility of extraterrestrial caves for more than 50 years, we have now entered the incipient phase of planetary caves exploration. Caves are important because they provide records of a planetary body's geological, meteorological and environmental history. On Mars, this may include evidence of past or even present microbial life. For the Moon and Mars, caves could protect human explorers from the harmful and inhospitable surface environment. In this work we emphasized on the need to explore planetary caves on Mars and the Moon, as caves provide records of a planetary body's geological, meteorological and environmental history, and in the case of Mars, may include evidences of past or even present microbial life.



RH6. Emendation of the Coccoid Cyanobacterial Genus *Gloeocapsopsis* and Description of the New Species *Gloeocapsopsis diffluens* sp. nov. and Gloeocapsopsis dulcis sp. nov. Isolated From the Coastal Range of the Atacama Desert, Chile

We also continued understanding the extremophiles of the Atacama. We formally introduced one of the dessication-tolerance cyanobacteria we found in the Atacama, a microorganism we are further studying to understand not only the molecular mechanisms involved in extreme desiccation tolerance, but also radiation tolerance. The taxonomy of coccoid cyanobacteria, such as Chroococcidiopsis, Pleurocapsa, Chroococcus, Gloeothece, Gloeocapsa, Gloeocapsopsis, and the related recent genera Sinocapsa and Aliterella, can easily be intermixed when solely compared on a morphological basis. There is still little support on the taxonomic position of some of the addressed genera, as genetic information is available only for a fraction of species that have been described solely on morphology. Modern polyphasic approaches that combine classic morphological investigations with DNA-based molecular analyses and the evaluation of ecological properties can disentangle these easily confusable unicellular genera. By using such an approach, we present here the formal description of two novel unicellular cyanobacterial species that inhabit the Coastal Range of the Atacama Desert, Gloeocapsopsis dulcis (first reported as Gloeocapsopsis AAB1) and Gloeocapsopsis diffluens. Both species could be clearly separated from previously reported species by 16S rRNA and 16S–23S ITS gene sequencing, the resulting secondary structures, p-distance analyses of the 16S–23S ITS, and morphology. For avoiding further confusions emendation of the genus Gloeocapsopsis as well as epitypification of the type species Gloeocapsopsis crepidinum based on the strain LEGE06123 were conducted.



Morphological characteristics of G. crepidinum strain LEGE06123. (A-C) show single cells and macrocolonies with thick, limited, and hyaline sheaths. (D) shows a pair of double cells (upper left corner), each surrounded by a sheath and tetrad of cells (lower right corner). (E) shows the rupture of macrocolony.

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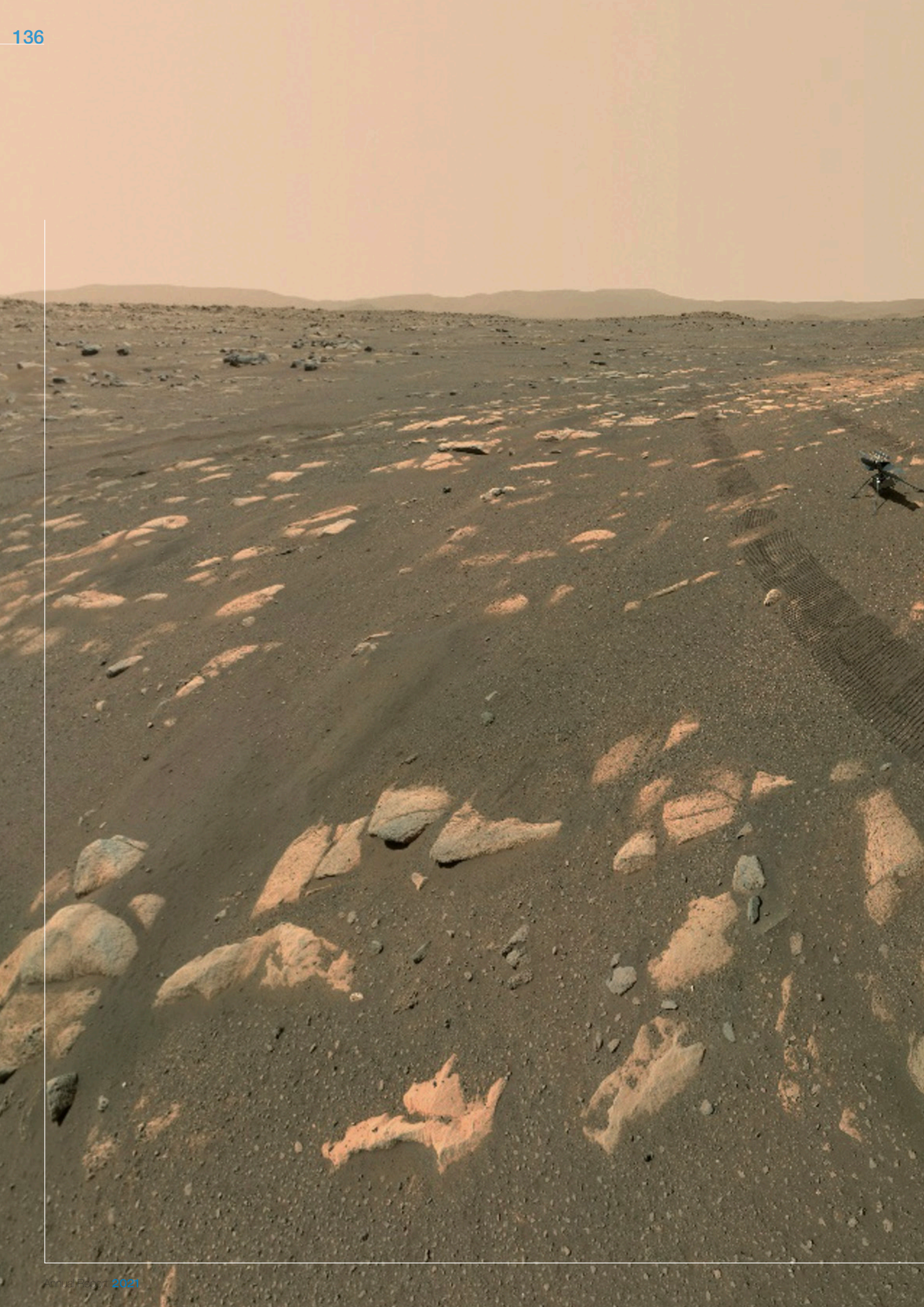

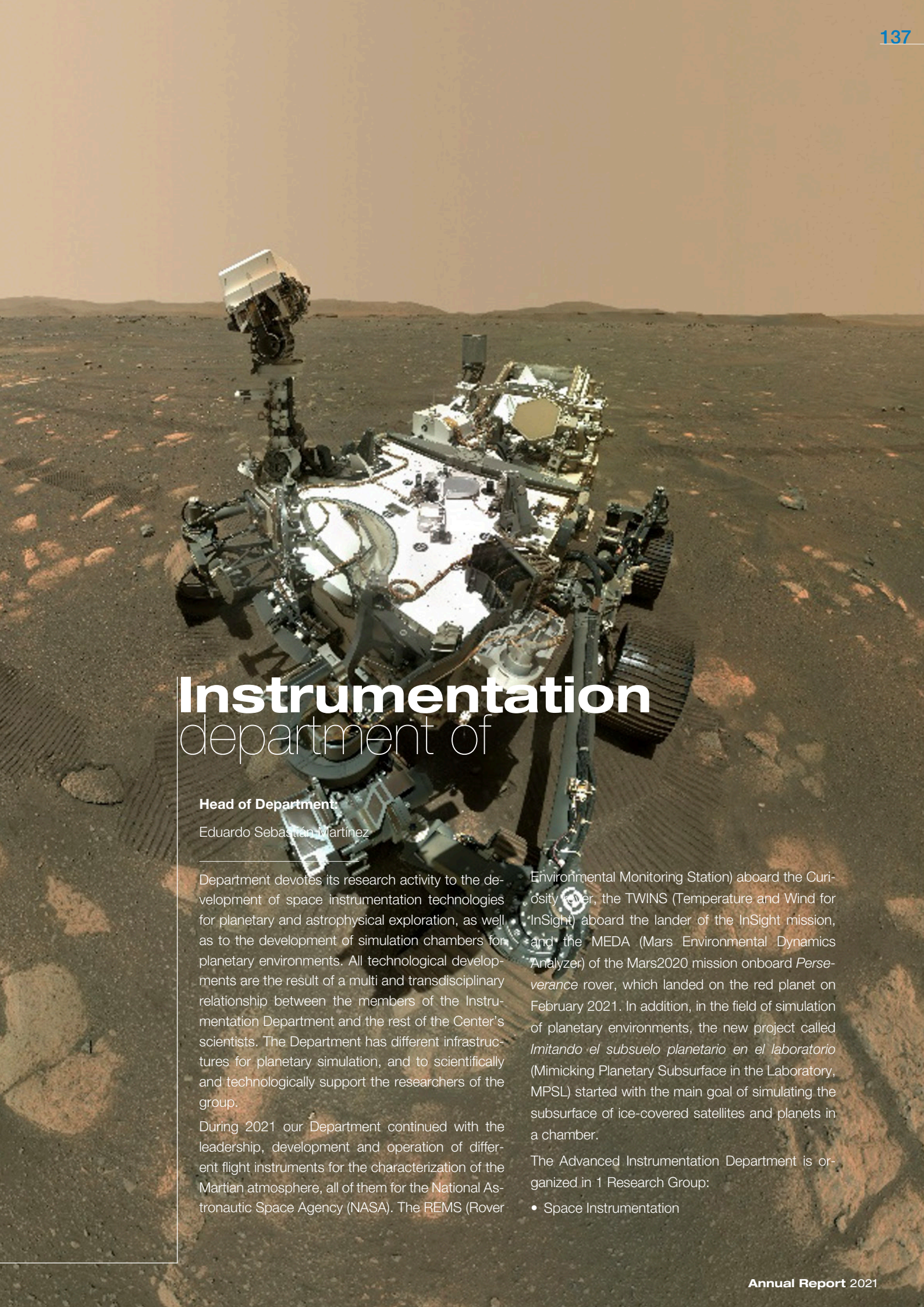

Instrumentation department of

Head of Department:

Eduardo Sebastián Martínez

Department devotes its research activity to the development of space instrumentation technologies for planetary and astrophysical exploration, as well as to the development of simulation chambers for planetary environments. All technological developments are the result of a multi and transdisciplinary relationship between the members of the Instrumentation Department and the rest of the Center's scientists. The Department has different infrastructures for planetary simulation, and to scientifically and technologically support the researchers of the group.

During 2021 our Department continued with the leadership, development and operation of different flight instruments for the characterization of the Martian atmosphere, all of them for the National Astronautic Space Agency (NASA). The REMS (Rover Environmental Monitoring Station) aboard the Curiosity rover, the TWINS (Temperature and Wind for InSight) aboard the lander of the InSight mission, and the MEDA (Mars Environmental Dynamics Analyzer) of the Mars2020 mission onboard *Perseverance* rover, which landed on the red planet on February 2021. In addition, in the field of simulation of planetary environments, the new project called *Imitando el subsuelo planetario en el laboratorio* (Mimicking Planetary Subsurface in the Laboratory, MPSL) started with the main goal of simulating the subsurface of ice-covered satellites and planets in a chamber.

The Advanced Instrumentation Department is organized in 1 Research Group:

- Space Instrumentation

Space Instrumentation (SI)

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Jesus Manuel Sobrado Vallecillo
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Javier Martin Soler
Julio José Romeral Planelló
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María de las Mercedes Marín Jiménez
Maria Rosario Urqui O'callaghan
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Students (Master, TFG, others):
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Eduardo Blanco Sarabia
Estela Barroso Sánchez
Gema Martínez Esteve
Leire Salamero Lorea
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Lucia Gómez Miguel
María Marco Navarro
Olga Balsalobre Ruza
Santiago Virtus Rubio
Victoria Renieblas Ariño

Summary

Experimentation and simulation play a fundamental role in the accomplishment of objectives the Centro de Astrobiología. In many cases, experiments are carried out in the laboratory, in others during field campaigns by studying natural processes, and in other cases in space, either by remote observation or by in situ analysis and measurements on the surface of planetary bodies. This group covers the all the technological aspects of these developments, from the conception of prototypes and instruments, the design and supervision of the industry specialized in the manufacture of flight models, to the execution of testing campaigns for the validation and maturation of the instrumentation and technologies, either in simulation chambers or in representative environments (the so-called terrestrial analogues). Also, in the scientific field, it carries out the exploitation of the data, through analysis, hypothetization, modeling and validation of results, as far as the study of the environment of other planets is concerned.

The group thus contributes to objectives Ob3.2, Ob3.5, Ob4.2, Ob6.3 and Ob6.6 of the Center Strategic Plan by studying the habitability of subsurface of other planetary environments and the effect of extreme physicochemical parameters in the laboratory. It also addresses the understanding of past and present Martian habitability through the dynamics of the Martian atmosphere. Finally, the group is also leading the development of environmental sensors for *insitu* planetary atmospheric characterization and habitability assessment, and is contributing to the definition of the future ESA and NASA missions with Astrobiological objectives and including environmental sensors.

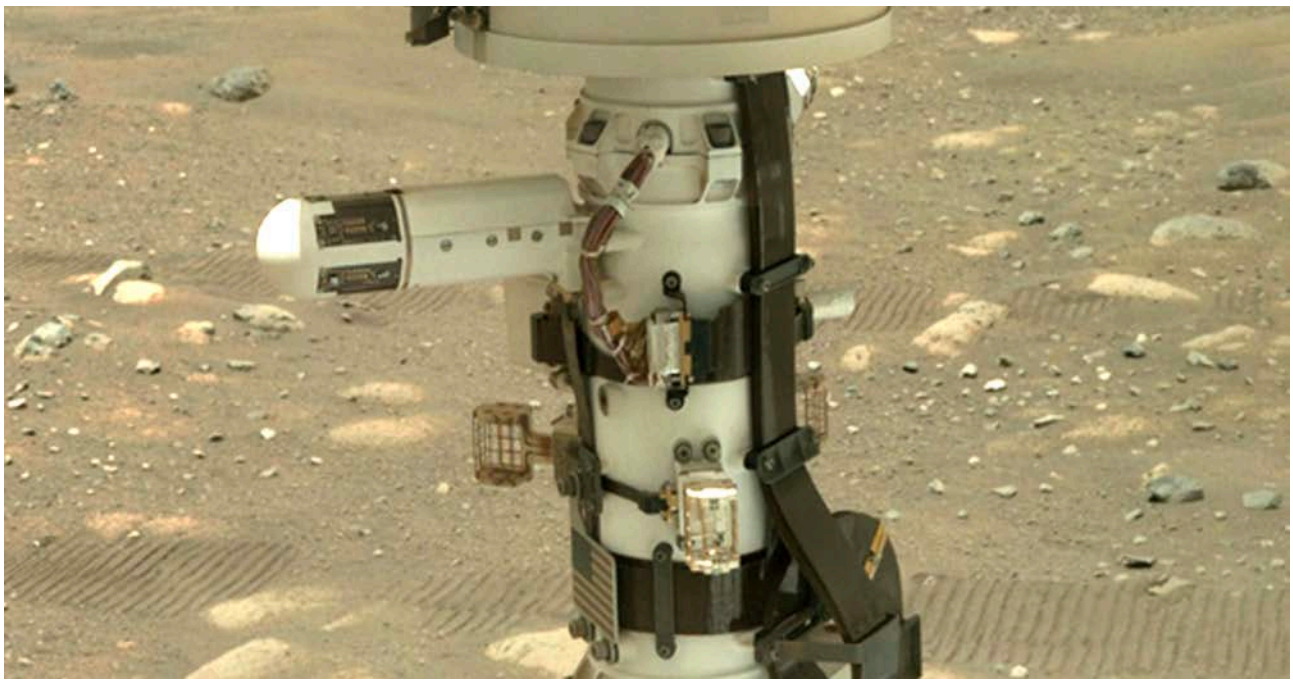
Research Highlights 2021

RA1. Development and operation of REMS, TWINS and MEDA instruments for the study of planetary atmospheres

The Space Instrumentation group is leading the development and operation of three space instruments dedicated to environmental characterization of the Martian atmosphere and the study of the physical properties of its dust. MEDA (Mars Environmental Dynamics Analyzer) for NASA's Perseverance rover, TWINS (Temperatures and Winds for InSight) of NASA's InSight mission and REMS (Rover Environmental Monitoring Station) for the NASA's Curiosity rover. All three are currently in operation.

These instruments and projects have contributed to consolidate Spain as an international reference in the field of the Martian atmospheric characterization. They have combined advances in the frontier of scientific and technological knowledge within our country, uniting and harmonizing a significant part of the scientific and technological community interested in the Martian atmosphere, in a transversal way to different NASA missions. For these projects, the CAB has collaborated with national and international partners as the *Departamento de Cargas Útiles* at the *Instituto Nacional de Técnica Aeroespacial*, CRISA Airbus Defense and Space, AVS Added Value Solutions, ALTER Technology, the University of the Basque Country, the Polytechnic University of Catalonia, the Rocasolano Physics-Chemistry Institute (CSIC) and the *University of Alcalá*, the Finnish Meteorological Institute, the Jet Propulsion Laboratory, the Lunar and Planetary Institute, Aeolis Research, the Space Science Institute, NASA Goddard Space Flight Center, Carnegie Institution and the John Hopkins APL as international partners.

MEDA is conceived as a suit of sensors that record: relative humidity (Relative Humidity Sensor - HS), air temperature (Air Temperature Sensor - ATS), net balance of IR radiation (Thermal IR Sensor - TIRS), speed and direction of the Martian wind (Wind Sensors - WS), radiation and properties of the suspended aerosols (Radiation and Dust Sensor - RDS), and atmospheric pressure (Pressure Sensor - PS). Throughout 2021, as part of the latest phase D activities, the team continued working intensively on completing the calibration of the instrument, fine-tuning the ground segment software, and learning how to interpret the station data from the results of field campaigns. At the same time, the calibration of the various sensors that make up MEDA was completed and the results were published. The international scientific commu-

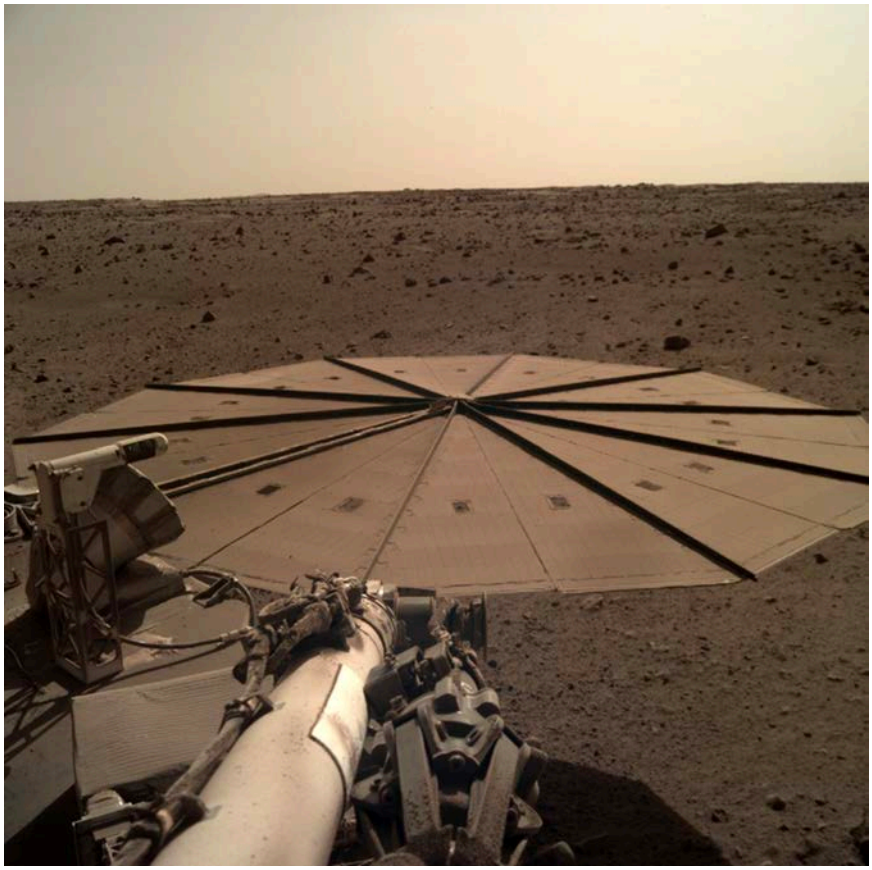


MEDA sensors on the Perseverance rover mast during Martian operations, image taken April 6, 2021.

nity's knowledge of the calibration results is essential for a correct interpretation of the data provided by the environmental station. Without a doubt, the most relevant event was the landing on the surface of Mars of the *Perseverance* rover on February 18, 2021, thus starting phase E of the project. Since then, both the engineering and the scientific teams of the project have led the instrument operation tasks, in close collaboration with NASA personnel and the rest of the mission. This activity has enabled the first MEDA scientific data to be obtained from the surface of Mars, and support the first flights of the Mars helicopter *Ingenuity*. Scientific data have been made available to the international scientific community in the PDS (Planetary Data System).

Throughout 2021, TWINS provided a continuous log of the local winds and temperatures at the landing site (Elysium Planitia). Both InSight and TWINS have performed with great success. However, the accumulation of dust on the surface of the solar panels has reduced the energy available to the spacecraft, forcing measurement times to be reduced. The scientific data provided by TWINS are allowing to rule out false seismic readings caused by the strong winds in the environment, and is of great scientific value given the detailed record that it is carrying out.

REMS is operating on the surface of Mars, in Gale Crater, since August 2012, collecting data on pressure, air and ground temperatures, wind speed and direction, atmospheric relative humidity and incident ultraviolet radiation. During this time, the instrument has collected more than 90 million readings from each of the sensors. Throughout the year 2021, in addition to the daily operation of REMS, the group participated in the analysis of the scientific data obtained by the instrument, also contributing to the discussions and scientific meetings that periodically and frequently bring together all the national and international members of the REMS team.



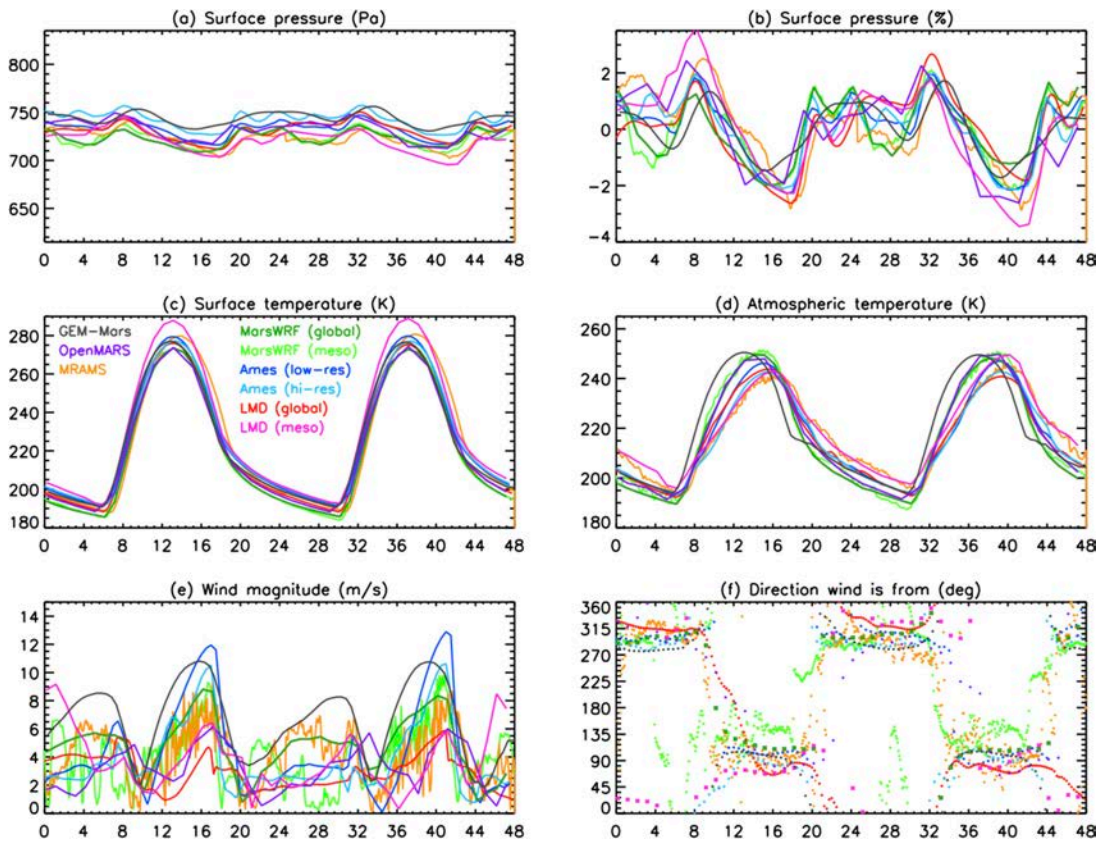
TWINS boom and InSight lander solar panel, image taken November 6, 2021.

Study and modeling of Martian atmospheric dynamics and its main constituents

In addition to the development and the daily operation of MEDA, TWINS and REMS, the group was actively involved in the scientific exploitation of the data and its publication during the year 2021. These are some of the most relevant results:

RH2: Multi-model Meteorological and Aeolian Predictions for Mars 2020 and the Jezero Crater Region

This work summarizes and compares the results of nine simulations used to predict the meteorology and aeolian activity of the Mars 2020 landing site region. Predicted seasonal variations of pressure and surface and atmospheric temperature generally agree. Daily pressure cycles vary more between simulations, possibly due to differences in atmospheric dust distributions. Jezero crater sits inside and close to the NW rim of the huge Isidis basin, whose daytime upslope (~east-southeasterly) and nighttime downslope (~northwesterly) winds are predicted to dominate except around summer solstice, when the global circulation produces more southerly wind directions. Wind predictions vary hugely, with annual maximum speeds varying from 11 to 19 m/s and daily mean wind speeds peaking in the first half of summer for most simulations but in the second half of the year for two. Most simulations predict net annual sand transport toward the WNW, which is generally consistent with aeolian observations, and peak sand fluxes in the first half of summer, with the weakest fluxes around winter solstice due to opposition between the global circulation and daytime upslope winds. Vortex activity is predicted to peak in summer and dip around winter solstice, and to be greater than at InSight and much greater than in Gale crater.

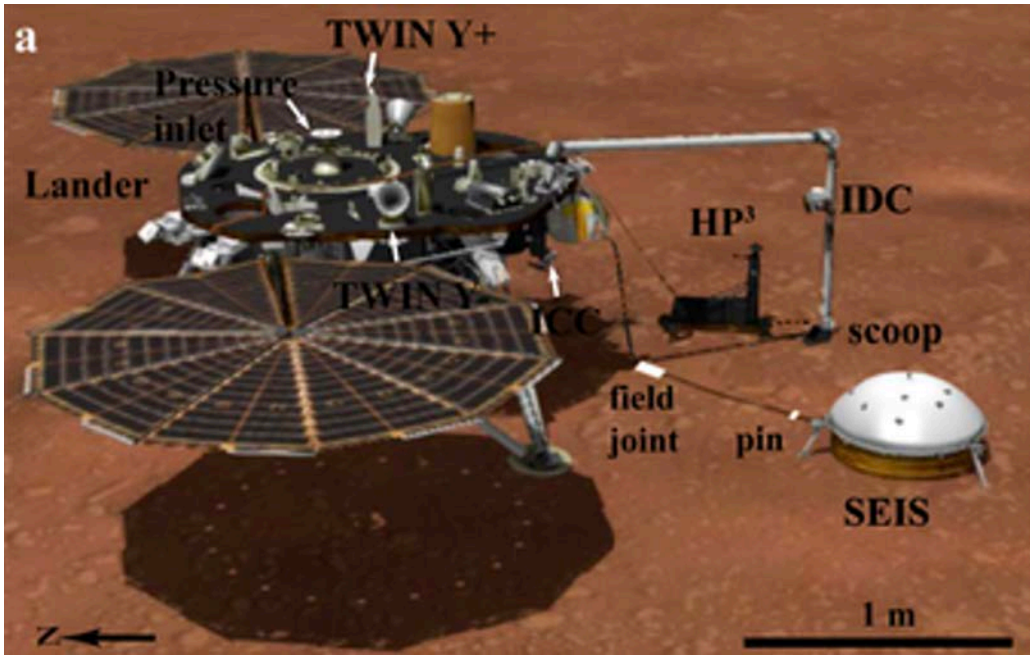


Diurnal cycles of pressure, temperature and wind in all nine model simulations at the Perseverance landing site at the time of landing.

Research Highlights 2021

RH3: Vortex-Dominated Aeolian Activity at InSight's Landing Site, Part 1: Multi-Instrument Observations, Analysis, and Implications

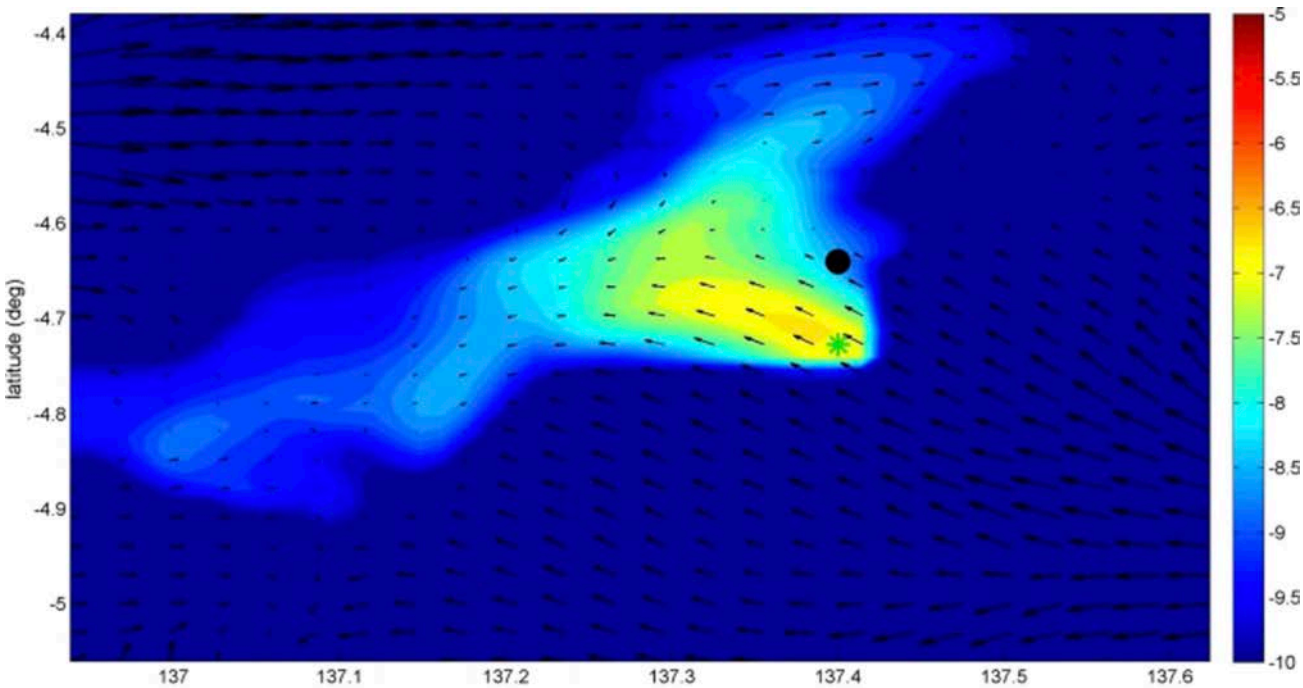
Aeolian activity, the movement of dust and sand by the wind, is common on Earth and has been observed on other planets, including Mars. A new Mars lander, InSight, has for the first time monitored aeolian changes by combining imaging with weather, seismic and magnetic field measurements. Sand grains are seen moving along the ground and dust is lifted from both artificial and natural surfaces. We found these changes were rare, but almost always happened in the early afternoon when tornado-like phenomena, called convective vortices, passed by the lander, sometimes leaving dark surface trails behind. The combination of the background wind speed and the rotational wind speed within a vortex was likely to be high enough to detach particles from the surface and set them into motion. When these vortices passed by the lander, the seismometer detected the ground tilting, and there was a pulse in the magnetic field, indicating charged particles were part of these dust-clearing events.



Virtual 3D view of the InSight lander and its setting in Elysium Planitia.

RH4: A three-dimensional atmospheric dispersion model for Mars

Atmospheric local to regional dispersion models are widely used on Earth to predict and study the effects of chemical species emitted into the atmosphere and to contextualize sparse data acquired at particular locations and/or times. However, to date, no local toregional dispersion models for Mars have been developed; only mesoscale/microscale meteorological models have some dispersion and chemical capabilities, but they do not offer the versatility of a dedicated atmospheric dispersion model when studying the dispersion of chemical species in the atmosphere, as it is performed on Earth. In this study, a new three-dimensional local to regional scale Eulerian atmospheric dispersion model for Mars (DISVERMAR) that can simulate emissions to the Martian atmosphere from particular locations or regions including chemical loss and predefined deposition rates, is presented. The model can deal with topography and non-uniform grids. As a case study, the model is applied to the simulation of methane spikes as detected by NASA's Mars Science Laboratory (MSL); this choice is made given the strong interest in and controversy regarding the detection and variability of this chemical species on Mars.

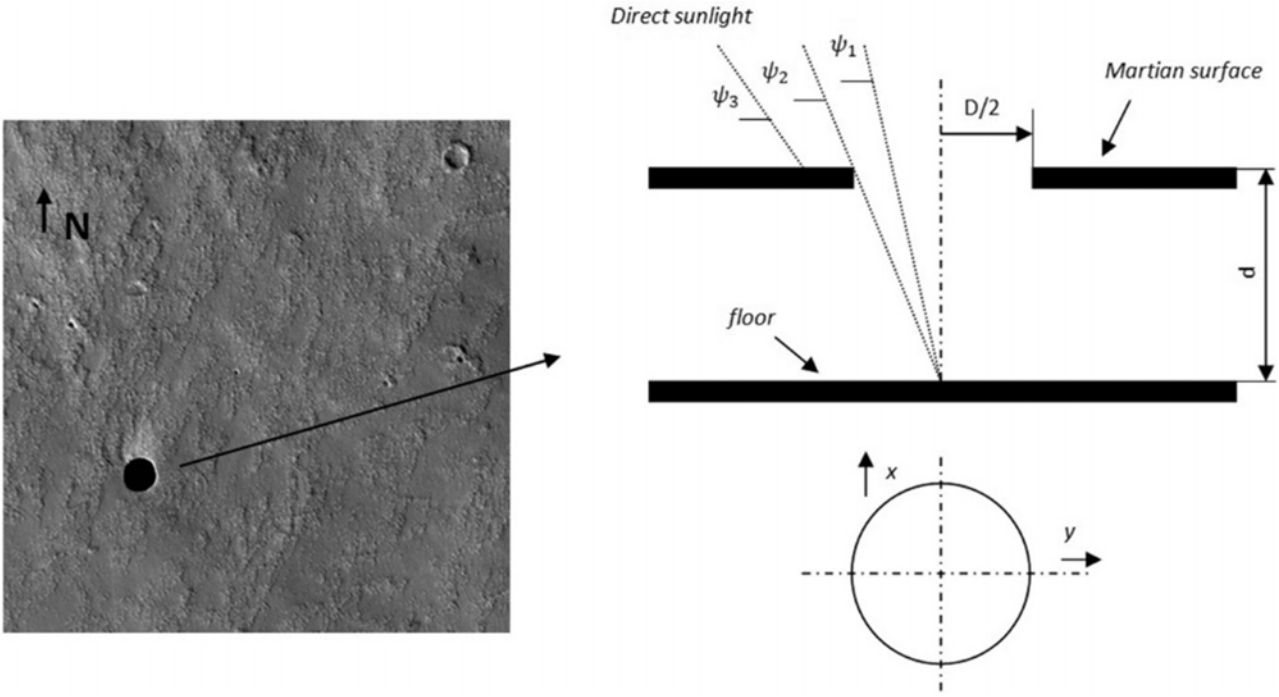


Example of model dispersion results for methane spike in Gale crater.

RH5: The ultraviolet radiation environment and shielding in pit craters and cave skylights on Mars

Martian caves and their entrances have been proposed as habitable environments and regions that could have preserved evidence of life, mostly due to their natural shielding from the damaging ionizing and non-ionizing radiation present on the surface. However, no studies to date have quantitatively determined the shielding offered by these voids on Mars.

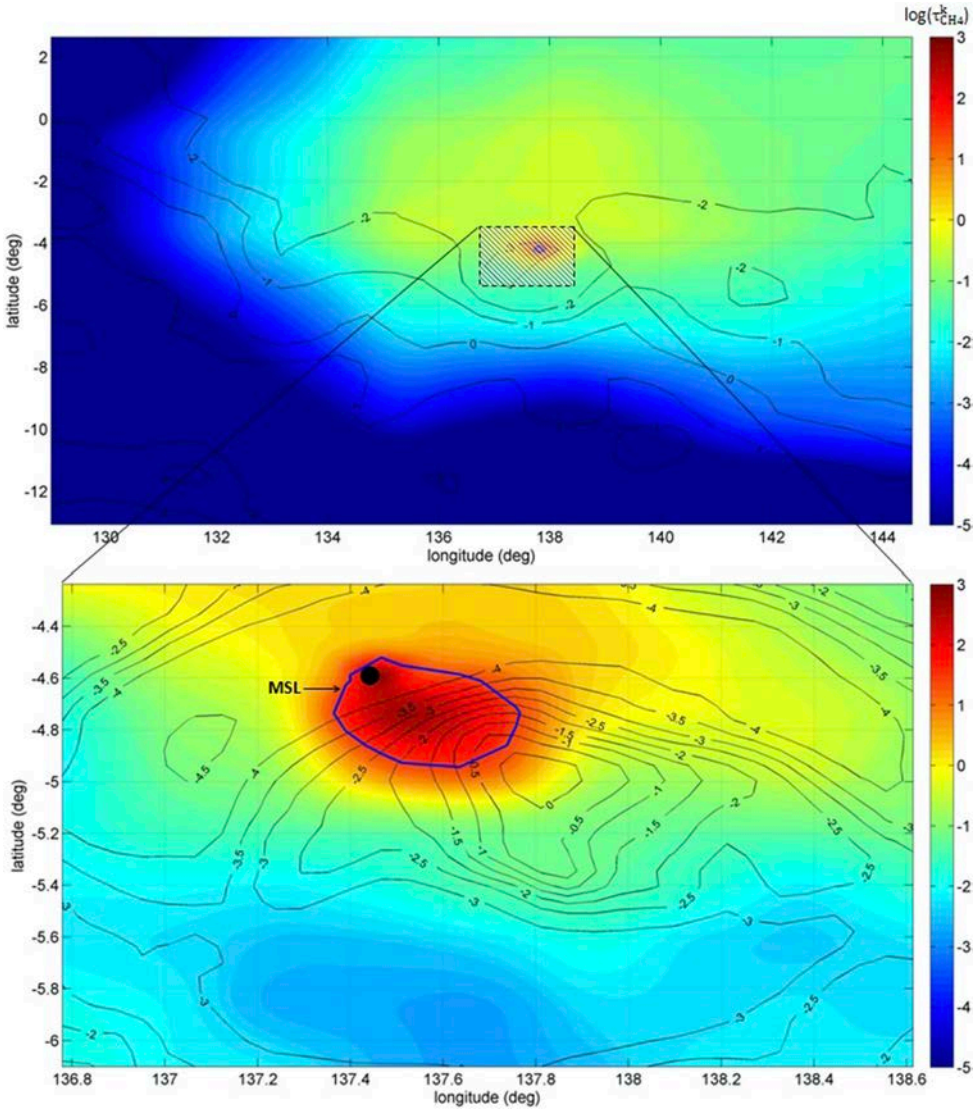
We have studied the ultraviolet (UV) radiation environment in such environments, by means of radiative transfer model simulations applied to representative void geometries on Mars. The results strongly suggest that pit craters and cave skylights are shielded from the damaging UV radiation found on the Martian surface. Numerical simulations of cave entrances show a reduction even more than two orders of magnitude in UV radiation, both in the maximum instantaneous and cumulative doses, throughout the year and at any location of the planet. The attenuated UV irradiance in cavernous spaces remains stable in a 10 Myr timescale, while at the same time the photosynthetically active radiation is higher than the minimum required for Earth-like phototrophs. The intermediate radiation environment between the damaging radiation on the surface and the permanent darkness of a hypothetical cave offered by voids on Mars may represent favorable environments for habitability without constraining the type of energy source for potential as-yet unknown Martian organisms.



Cavernous spaces on Martian surface captured by the Mars Reconnaissance Orbiter's (MRO) HiRISE camera, and its geometrical model.

RH6: Constraints on Emission Source Locations of Methane Detected by Mars Science Laboratory

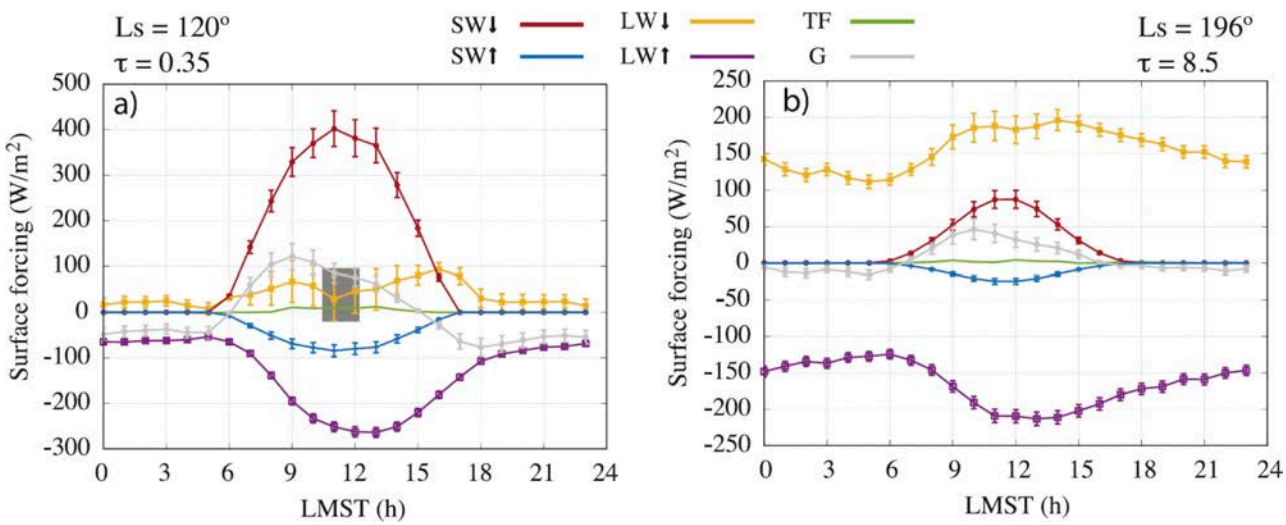
Curiosity rover has detected both a background abundance and transient spikes in methane abundance in recent years in Mars' Gale Crater. These methane spikes were suggested to be produced by a local or regional emission source. On the other hand, the background measurements were originally postulated to be the result of a global methane abundance on Mars. However, recent high accuracy observations by the Trace Gas Orbiter (TGO) have not detected any methane in the Martian atmosphere, apparently contradicting Curiosity measurements. Numerical simulations indicate that both the spikes and the background measurements performed by Curiosity would have the same origin in localized methane emissions close to the rover. These results simultaneously satisfy the constraints imposed by TGO and Curiosity observations, although they are unlikely or problematic: either there exists a strong and unknown loss mechanism in the atmosphere that prevents the accumulation of global methane, or methane emissions are extremely uncommon on Mars and Curiosity rover has fortuitously landed next to one of them.



Model simulation of the required methane chemical loss time constant in the atmosphere (Earth years, in logarithmic scale), as a function of the location of the emission source of methane, based on the MSL's observations to date.

RH7: The Surface Energy Budget at Gale crater during the first 2500 sols of the Mars Science Laboratory mission

The primary energy input at the Martian surface is the solar radiation, which depends on the time of the day and season, geographical location (latitude and altitude) and the abundance of dust and gas in the atmosphere. Another energy input is the atmospheric thermal forcing, which depends on the vertical distribution of dust and water ice aerosols, as well as CO_2 and H_2O molecules. Together with the reflected solar radiation and the thermal radiation emitted by the surface, these four terms make up the net radiative forcing of the surface. In response to it, energy outputs such as turbulent motions and water phase changes emerge to cool down/warm up the ground. The remaining energy is available to control the thermal environment in the surface, and shallow subsurface through conduction into the soil. By using first of their kind measurements from REMS, the energy inputs and outputs across Curiosity's traverse over the first 2500 Martian days of the mission are calculated. Their temporal variations were analyzed, and related to the potential mechanisms that could cause. An accurate determination of the surface energy budget is key to preparing for human exploration of Mars, as it contributes to improve the predictive capabilities of numerical models.

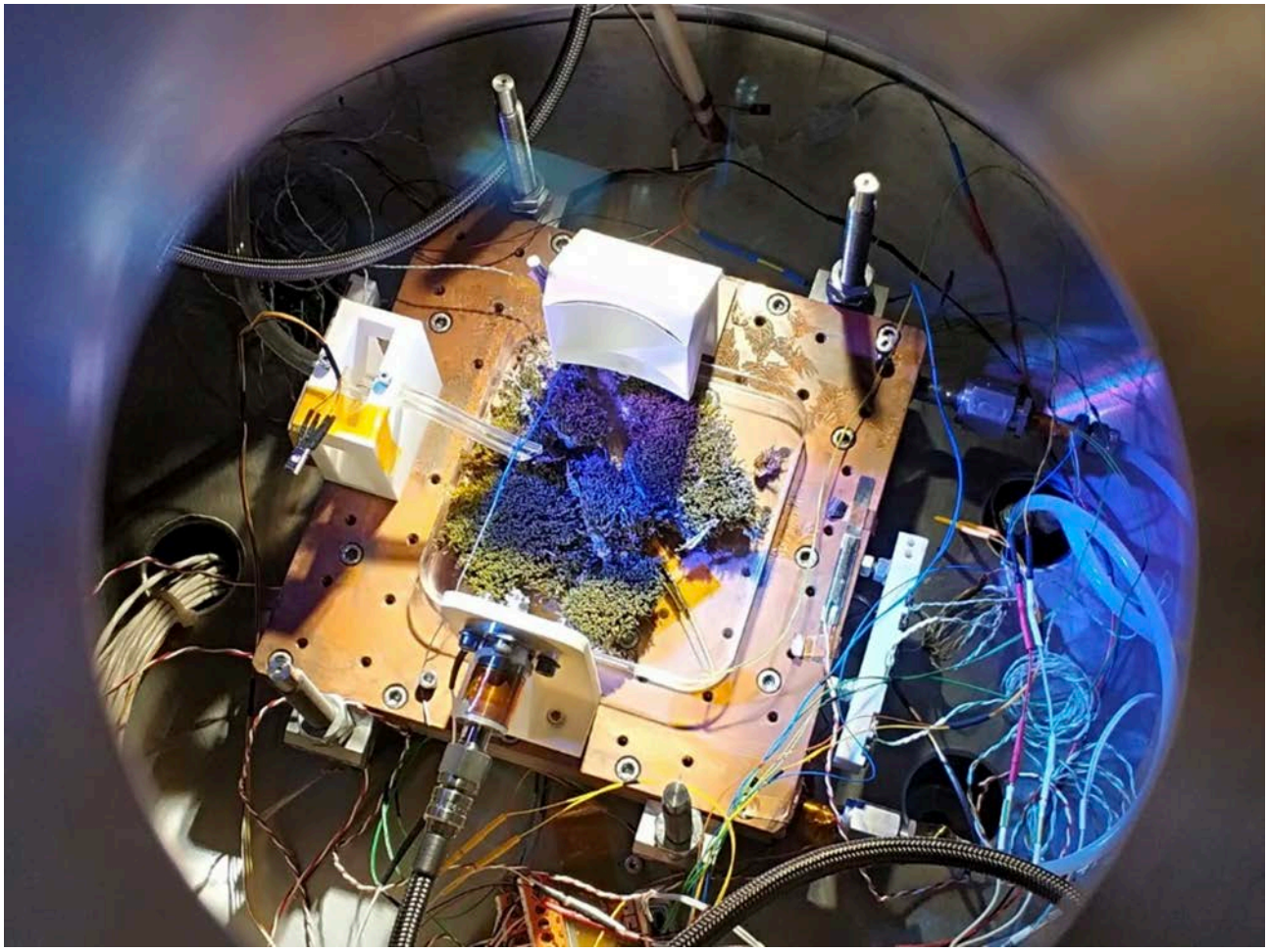


Diurnal variation of the surface energy budget on sols 607 (a) and 2085 (b).

RH8: Replication in simulation chambers of astrobiologically relevant planetary conditions.

It would be possible that a species of moss (Sphagnum) could survive or adapt on the icy and acidic surface and with strong irradiation from the Sun, as occurs on the red planet of our solar system. Engineering makes it possible to recreate extreme environments inside a vacuum chamber, and simulate the atmosphere and environmental conditions of any extraterrestrial environment in order to study in the laboratory what can happen in a space environment. The MARTE chamber simulates the dew and allows the water cycle inside. A whole collection of sensors and devices keep the system self-controlled according to the requirements of the sample to be studied.

From this experiment (WLOM project) we start to recreate the Martian subsurface inside a new reactor that has the possibility to simulate the influence of water ice on different biological samples (MPSL project).



Sphagnum moss inside the MARTE vacuum chamber is a biosignature for monitoring the Mars water cycle.

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(Pérez P, et al. 2021. Tittle. Journal name, vol, pages)

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S. Zurita-Zurita, F. J. Escribano, J. Sáez-Landete and J. A. Rodríguez-Manfredi. 2021 Denoising Atmospheric Temperature Measurements Taken by the Mars Science Laboratory on the Martian Surface, in IEEE Transactions on Instrumentation and Measurement, vol. 70, pp. 1-10, Art no. 9502910, doi: 10.1109/TIM.2020.3034986.

Funded projects in 2021

Project title: Ciencia y tecnología de instrumentos espaciales para la caracterización del ambiente marciano en múltiples misiones de NASA
Principal Investigator: José Antonio Rodríguez Manfredi / Eduardo Sebastián Martínez
Financing entity: PLAN NACIONAL I+D (RTI2018-098728-B-C31)
Participating entities: CAB,UPC y IMSE.
Durations: 1/2019-12/2021
Grant amount: 2.372.205,00€

Project title: Imitando el subsuelo planetario en el laboratorio (MPSL).
Principal Investigator: Jesús Manuel Sobrado Vallecillo
Financing entity: PLAN NACIONAL I+D (PID2020-114047GB-100)
Participating entities: CAB.
Durations: 9/2021-8/2024 **Grant amount:** 96.500,00€

Public Outreach Activities, TFG and TFM

Título: Potenciostato de baja potencia para control y monitorización remota de sensores ambientales
Alumno: Estela Barroso Sánchez
Universidad: Universidad de Alcalá
Facultad / Escuela: Máster en Ingeniería de Telecomunicación
Fecha: Septiembre-2021

Título: Mass Production Process Design of the Green Moon Project Encapsulated Habitats for Future Space Agriculture and Habitability
Alumno: Jose María Ortega-Hernández
Universidad: Wrexham Glyndwr University, UK
Facultad / Escuela: MS Mechanical Manufacturin Engineeering
Fecha: Mayo-2021

Publications

Outreach (most relevant contributions)

Acto con motivo del aterrizaje de Mars2020-Perseverence, Centro de Astrobiología 18 de Febrero de 2021

RTVE ciencia, febrero 2021, ¿Por qué es importante la llegada del Perseverance a Marte?

LaSexta Noticias, septiembre de 2021, Las cuevas en Marte podrían servir de refugio para la vida.

RTVE Órbita Laika, octubre de 2021, Rover perseverancve y MEDA: Próxima parada Marte.

RTVE El Cazador de Cerebros, abril 2021, Exploración de Marte.

RTVE Documental La última frontera. Episodio 3, noviembre 2021, Marte nos espera.

La Estación de Monitoreo Ambiental Rover (REMS) en el rover Curiosity Mars de la NASA incluye sensores de temperatura y humedad montados en el mástil del rover. Una de las botavaras REMS se extiende hacia la izquierda desde el mástil en esta vista.

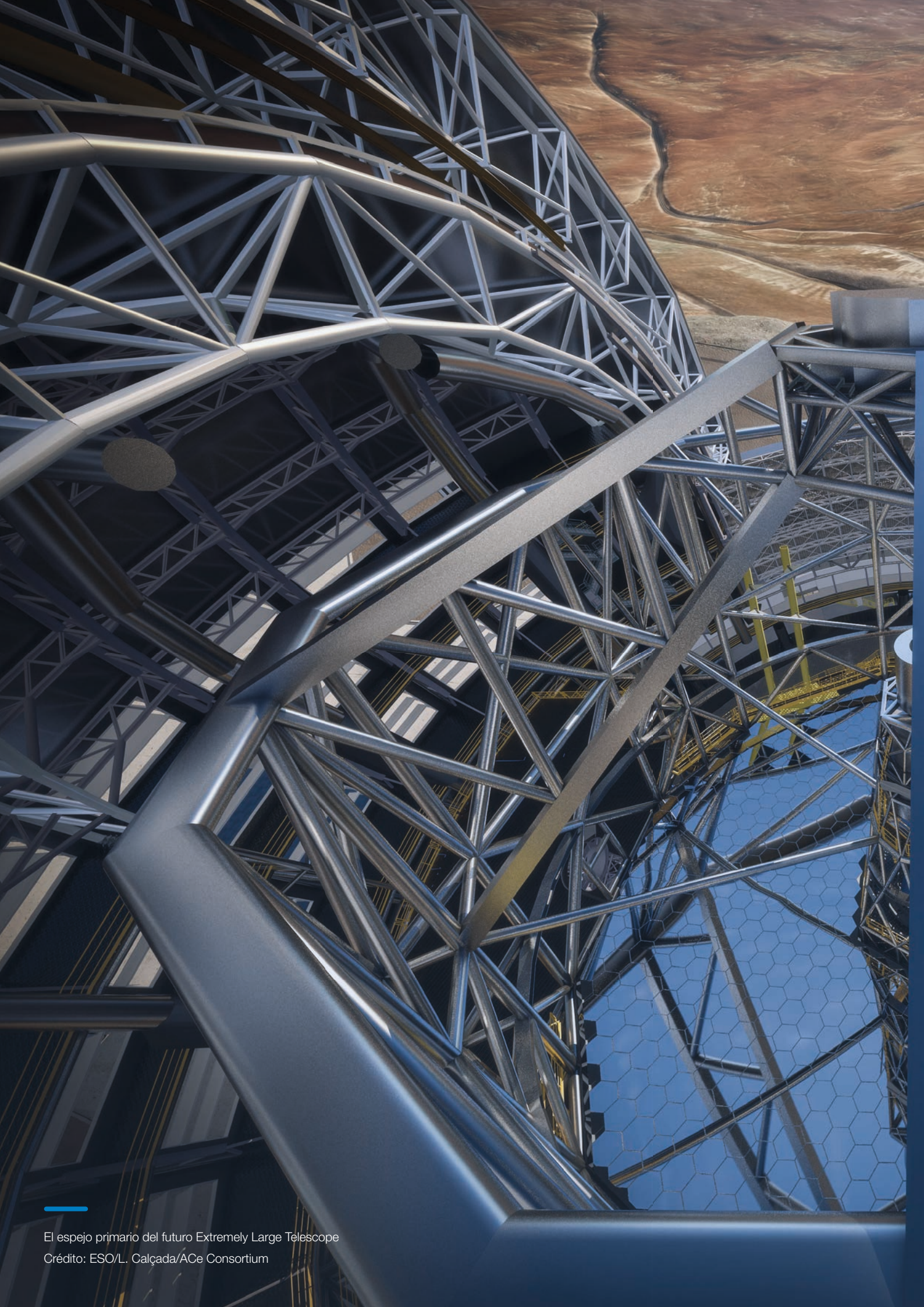
España proporcionó REMS al Proyecto del Laboratorio de Ciencias de Marte de la NASA. La estación de seguimiento ha proporcionado información sobre la presión del aire, la humedad relativa, la temperatura del aire, la temperatura del suelo, el viento y la radiación ultravioleta en todas las estaciones marcianas y en todo momento del día o de la noche.

Credit: NASA/JPL-Caltech/MSSS

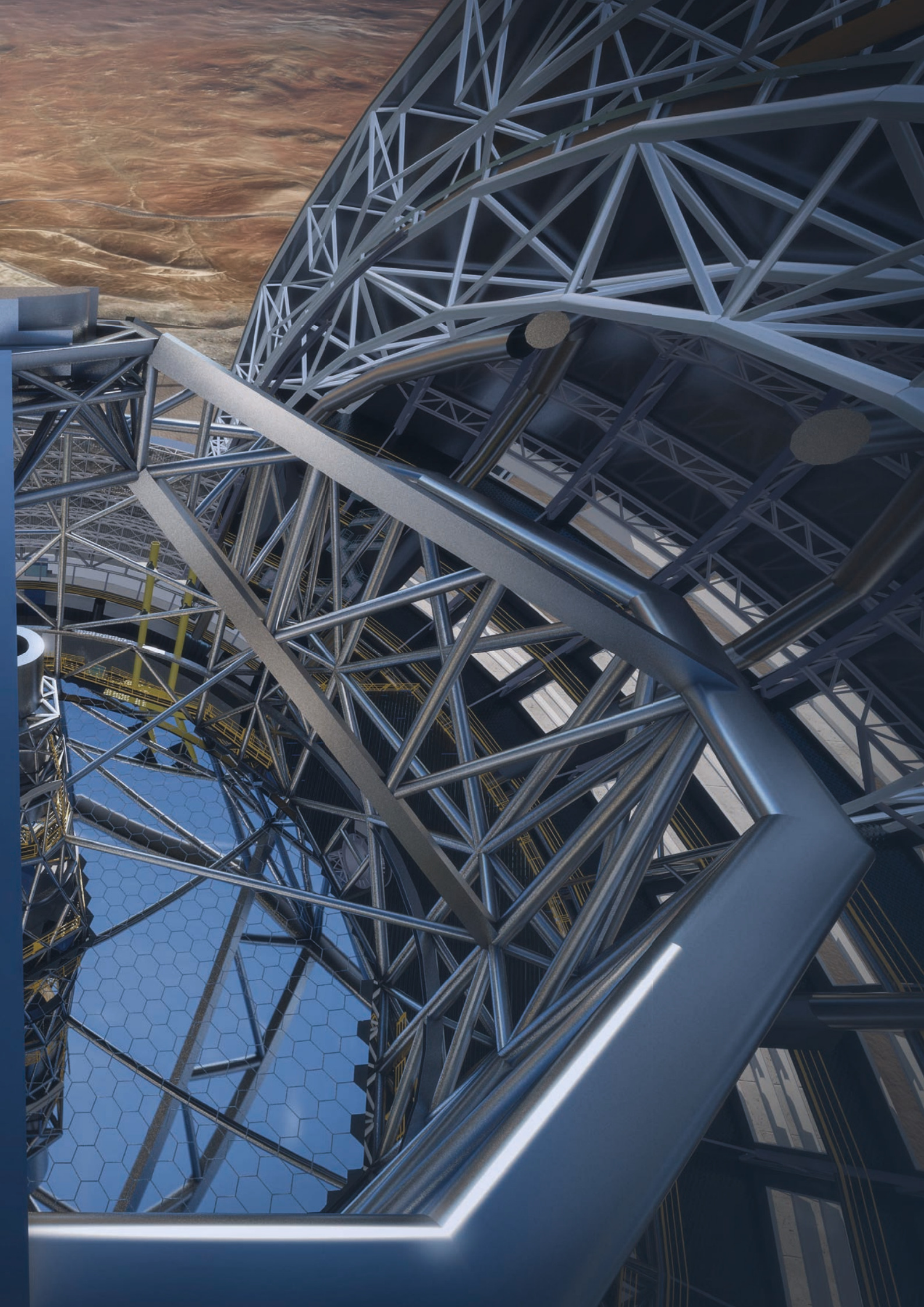
Detalle en proximidad de una de las chimeneas surgidas por precipitación de las sales arrastradas por el agua hirviendo procedente del volcán subterráneo en Dallol.

Crédito: Felipe Gómez

La Mina de las Cruces es la mayor mina a cielo abierto activa en Europa y la segunda mayor productora de cobre a nivel europeo. Es uno de los sitios del mundo donde es más evidente la interacción entre la actividad biológica y los depósitos minerales.



El espejo primario del futuro Extremely Large Telescope
Crédito: ESO/L. Calçada/ACe Consortium



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MEDA wind sensor. Créditos: NASA/JPL-Caltech