AstroPAH

A Newsletter on Astronomical PAHs

Issue 60 • July 2019

Dragonfly

Editorial

Dear Colleagues,

We are glad to share with you our July issue, before our annual August break. We will be back with new AstroPAH science to share in September!

NASA recently announced the selection of the next New Frontiers mission, *Dragonfly*, which will arrive in the Saturn's moon Titan within the next 15 years. This mission will constitute an important milestone in the study of prebiotic chemical processes in the Solar System, on a moon with complex organic chemistry. Our In Focus, contributed by Dr. Sarah Hörst and Dr. Ella Sciamma-O'Brien presents the *Dragonfly* mission, where you can read more about the project, scientific objectives and science team involved.

New publications on the catalysis of hydrogenation reactions by H_nPAHs in the interstellar medium, the properties of iron pseudocarbynes, and the interactions of H and H_2 with diamond-like carbon surfaces are advertised in the Abstracts section.

In the AGU 2019 fall meeting a Session on Atmospheric Processes, Particles and Chemistry is being organized; see the full call for abstract in the Meetings section. We also wish to report the recent announcement of the European Conference on Laboratory Astrophysics ECLA 2020 - Linking Dust, Ice and Gas in Space, which will be held from 19 to 24 of April 2020, in Italy. Save the dates!

We hope you enjoy reading our newsletter and wish you a wonderful summer break. In the meantime, do not hesitate to send us your contributions. See you in September!

Enjoy reading our newsletter!

The Editorial Team

Next issue: 19 September 2019.
Submission deadline: 6 September 2019.

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PAH Picture of the Month

An artist's impression of Dragonfly mission concept of entry, descent, landing, surface operations, and flight at Titan. Dragonfly has been selected as NASA's next New Frontiers mission. For more information visit http://dragonfly.jhuapl.edu/index.php.

Credits: Johns Hopkins APL. Reproduced with permission.

In Focus

DRAGONFLY:
NASA's next New Frontiers Mission to explore Titan

by Sarah Hörst and Ella Sciamma-O'Brien

(Information and graphics presented here come from the official website for the Dragonfly mission)

NASA has announced that the next New Frontiers mission to explore our solar system will be Dragonfly, a dual quadcopter that will fly to multiple sites on Titan, exploring a variety of locations looking for prebiotic chemical processes on Titan that could provide clues to the chemical interactions that occurred before life developed on Earth. Dragonfly will take advantage of Titan's dense atmosphere to become the first vehicle ever to fly its entire science payload to new places for repeatable and targeted access to surface materials. Dragonfly is planned to launch in 2026 and arrive in 2034.

TITAN

Titan is an ocean world, possessing both a subsurface liquid water ocean as well as lakes and seas of hydrocarbons on its surface, and it is the only moon in our solar system with a dense atmosphere. The Cassini-Huygens mission, a joint project between NASA and ESA, revealed that Titan is an incredibly complex world with numerous interesting planetary processes. The Cassini Orbiter, which explored the Saturnian system from July 2004 to September 2017, used radar and imaging at near-infrared wavelengths to map much of Titan's surface and make detailed studies of its atmosphere. The Huygens Probe descended through Titan's atmosphere in January 2015 providing in-situ measurements from deep in Titan's atmosphere and its surface. Cassini-

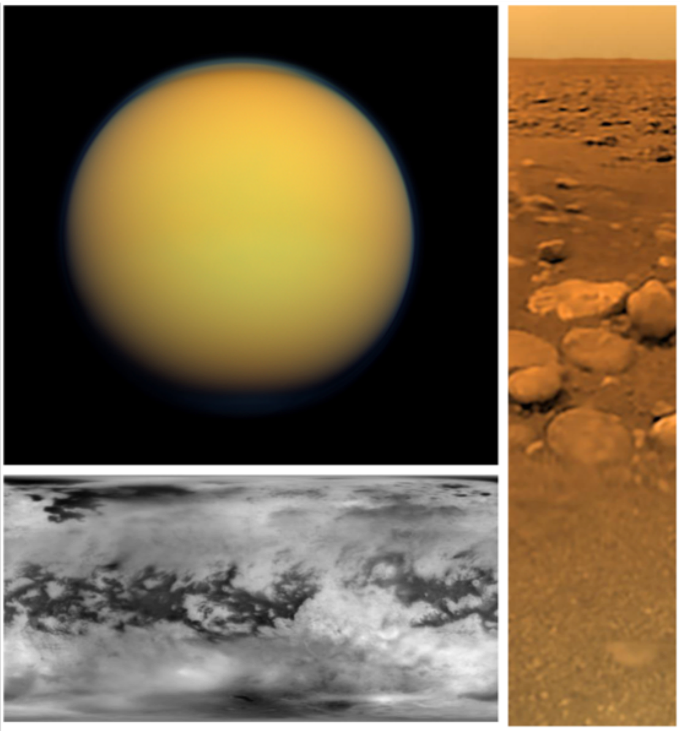

IMAGE CREDIT: (Top Left) NASA/JPL-Caltech/SSI, (Bottom Left) NASA/JPL-Caltech/Univ. Arizona, (Right) ESA/NASA/JPL/University of Arizona

Huygens showed us that Titan's surface has rivers, lakes, and even seas of liquid ethane and methane, as well as vast expanses of sand dunes. The climate of Titan is such that the methane can form clouds and even rain, as water does on Earth. Titan's atmosphere is composed primarily of nitrogen (about 95%), with some methane (about 5%) and small amounts of other carbon-rich compounds. Solar UV radiation induces a complex chemistry that forms organic compounds. The abundant complex organic material accessible on Titan's surface makes it an ideal destination to study the conditions necessary for the habitability of an extraterrestrial environment and the kinds of chemical interactions that occurred before life developed on Earth. As an analog to the very early Earth, Titan can provide clues to how life may have arisen on our planet.

DRAGONFLY

Dragonfly is a revolutionary mission concept capable of exploring diverse locations to characterize the habitability of Titan's environment, to investigate how far prebiotic chemistry has progressed, and even to search for chemical signatures that could indicate water-based and/or hydrocarbon-based life.

The dense, calm atmosphere and low gravity make flying an ideal way to travel to different areas of this moon. During its planned two-year mission, Dragonfly will fly to a variety of locations on Titan. In under an hour, Dragonfly will cover tens of miles or kilometers, farther than any planetary rover has traveled. With one hop per full Titan day (16 Earth days), the rotorcraft will travel from its initial landing site to cover areas several hundred kilometers away. Unable to use solar power under Titan's hazy atmosphere, Dragonfly will use a Multi-Mission Radioisotope Thermoelectric Generator (MMRTG), like the durable Curiosity rover on Mars. Flight, data transmission, and most science operations will be planned during Titan's daytime hours (eight Earth days), giving the rotorcraft plenty of time during the Titan night to recharge.

IMAGE CREDIT:Johns Hopkins APL

Despite its unique ability to fly, Dragonfly will spend most of its time on Titan's surface making science measurements. Dragonfly will explore diverse environments from organic dunes to the floor of an impact crater where liquid water and complex organic materials key to life once existed together for possibly tens of thousands of years. Its instruments will study how far prebiotic chemistry may have progressed. They also will investigate the moon's atmospheric and surface properties together with its subsurface ocean and liquid reservoirs. Additionally, instruments will search for chemical evidence of past or extant life.

Dragonfly's Instruments for Surface and Atmospheric Science measurements

Mass spectrometer: to analyze surface material as well as atmospheric samples (on the ground and in flight) and identify the chemical components and processes producing biologically relevant compounds
Neutron-activated gamma-ray spectrometer: to measure bulk elemental surface composition
Meteorology sensors: to monitor atmospheric and surface conditions, including diurnal and spatial variations
Cameras: to provide images of geologic features as well as aerial images of surface geology, and give context for surface measurements and scouting of sites of interest
Seismology instruments: to perform studies to detect subsurface activity and structure

THE DRAGONFLY TEAM

Led by the Johns Hopkins Applied Physics Laboratory, the Dragonfly team is comprised of leading Titan scientists and space system engineers as well as rotorcraft experts who have deep experience on missions to Saturn, Titan, the Sun, Pluto, and beyond.

Mission Leadership

Elizabeth "Zibi" Turtle [PI] (Johns Hopkins APL), Melissa Trainer [Deputy PI] (NASA GSFC), Jason Barnes [Deputy PI] (University of Idaho), Peter Bedini [Project Manager] (Johns Hopkins APL), Ralph Lorenz [Project Scientist] (Johns Hopkins APL), Scott Murchie [Deputy Project Scientist] (Johns Hopkins APL), Ken Hibbard [Mission Systems Engineer] (Johns Hopkins APL), Doug Adams [Spacecraft Systems Engineer] (Johns Hopkins APL).

Science and Engineering Team

Will Brinckerhoff (GSFC), Morgan Cable (JPL), Carolyn Ernst (Johns Hopkins APL), Caroline Freissinet (LATMOS), Kevin Hand (JPL), Alex Hayes (Cornell), Sarah Horst (JHU), Jeff Johnson (Johns Hopkins APL), Erich Karkoschka (University Arizona), Jack Langelaan (PSU), David Lawrence (Johns Hopkins APL), Alice LeGall (LATMOS), Juan Lora (Yale University), Shannon MacKenzie (Johns Hopkins APL), Chris McKay (NASA Ames), Catherine Neish (PSI/University West Ontario), Claire Newman (Aeolis Research), Marty Ozimek (Johns Hopkins APL), Jose Palacios (PSU), Mark Panning (JPL), Ann Parsons (GSFC), Patrick Peplowski (Johns Hopkins APL), Jani Radebaugh (BYU), Scot Rafkin (SwRI), Mike Ravine (MSSS), Lev Rodovskiy (Johns Hopkins APL), Duane Roth (JPL), Sven Schmitz (PSU), Chris Scott (Johns Hopkins APL), Jason Soderblom (MIT), Angela Stickle (Johns Hopkins APL), Ellen Stofan (Smithsonian), Cyril Szopa (LATMOS), Tetsuya Tokano (University of Koln), Benjamin Villac (Johns Hopkins APL), Colin Wilson (Oxford), Aileen Yingst (PSI), Kris Zacny (Honeybee Robotics).

Hydrogenated Polycyclic Aromatic Hydrocarbons (H_nPAHs) as Catalysts for Hydrogenation Reactions in the Interstellar Medium: a Quantum Chemical Model

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The sticking of H atoms onto dust grains and large hydrocarbon molecules has received considerable attention because it is thought to govern the formation of H_2 and other H-containing molecules in the interstellar medium. Using the density functional theory (DFT) approximation, we have investigated the capacity of neutral hydrogenated polycyclic aromatic hydrocarbons (HnPAH) to catalyze simple hydrogenation reactions by acting as a source of atomic hydrogen. In particular, the interaction of OH and CO with H_1-anthracene (singly hydrogenated) and H_{14}-anthracene (fully hydrogenated) to form H_2O and HCO was modeled following the Eley-Rideal mechanism. In this process, a hydrogen atom is abstracted from the HnPAH molecule forming the corresponding hydrogenated compound. The results were compared to the most known case of the HnPAH-catalyzed formation of H_2. It was observed that whereas H_2 is formed by overcoming activation barriers of approximately 0.02 and 0.10 eV with H_1-anthracene and H_{14}-anthracene, respectively, H_2O is produced in a barrierless fashion with both hydrocarbon molecules. The production of HCO was found to be a highly unfavorable process (with activation barriers of 0.73 eV and 3.13 eV for H_1- and H_{14}-anthracene, respectively). Complementary calculations performed using the rest of the H_n-anthracene molecules (from 2 to 13 extra H atoms) showed that in all the cases the reaction with OH is barrierless as well. This efficient mechanism could therefore be a possible route for water formation in the cold interstellar medium.

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Phys. Chem. Chem. Phys. 2019, 21, 12012-12020

https://pubs.rsc.org/en/content/articlelanding/2019/cp/c9cp02329a#!divAbstract

On the Structure, Magnetic Properties, and Infrared Spectra of Iron Pseudocarbynes in the Interstellar Medium

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Carbon chains, especially polyynes, are the building blocks of complex molecules such as polycyclic aromatic hydrocarbons and fullerenes, and polyynes are observed in circumstellar and interstellar (CIS) environments. Yet these same CIS environments show only low levels of gaseous iron despite it being the fourth most abundant element in the solar abundance pattern. In this study we explore the structure, magnetic properties, and synthetic infrared (IR) spectra of iron bound to polyynes, yielding what we call iron pseudocarbynes. We find that polyynes of all lengths are characterized by an IR-active C-H stretching feature at $\lambda \sim 3$ µm, and an IR-active CCH/CCC bending feature at $\lambda \sim 16$ µm. The CCH bending feature exhibits a redshift in iron pseudocarbynes such as Fe_{12}-C_2H_2, appearing at $\lambda \sim 15.8$ µm with an IR intensity that is reduced by a factor of $\sim$5. Similarly, iron pseudocarbynes with different carbon-chain lengths such as Fe_{13}-C_2H_2 and Fe_{13}-$(C_2H_2)_6$ also show IR features at nearly the same wavelengths with reduced IR intensities. Iron pseudocarbynes may have been overlooked because, based on calculations, their IR spectra are, within experimental uncertainties, identical to astronomically observed, iron-free species. The occurrence of iron pseudocarbynes in CIS environments would enhance Fe depletion, facilitate production of thermodynamically stable long-chain polyynes, provide a catalytic bridge over the composition gap between molecules containing nine or fewer carbon atoms and complex molecules, and supply a potential mechanism for the modulation and polarization of magnetic fields in CIS environments.

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ApJ, 2019, 879, 2

https://iopscience.iop.org/article/10.3847/1538-4357/ab22b7

You can also find the press release on this work here

Interactions of Atomic and Molecular Hydrogen with a Diamond-like Carbon Surface: H_2 Formation and Desorption

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Institute of Low Temperature Science, Hokkaido University

The interactions of atomic and molecular hydrogen with bare interstellar dust grain surfaces are important for understanding H_2 formation at relatively high temperatures (>20 K). We investigate the diffusion of physisorbed H atoms and the desorption energetics of H_2 molecules on an amorphous diamond-like carbon (DLC) surface. From temperature-programmed desorption experiments with a resonance-enhanced multiphoton ionization (REMPI) method for H_2 detection, the H_2 coverage-dependent activation energies for H_2 desorption are determined. The activation energies decrease with increasing H_2 coverage and are centered at 30 meV with a narrow distribution. Using a combination of photostimulated desorption and REMPI methods, the time variations of the surface number density of H_2 following atomic and molecular hydrogen depositions are studied. From these measurements, we show that H_2 formation on a DLC surface is quite efficient, even at 20 K. A significant kinetic isotope effect for H_2 and D_2 recombination reactions suggests that H-atom diffusion on a DLC surface is mediated by quantum mechanical tunneling. In astrophysically relevant conditions, H_2 recombination due to physisorbed H-atoms is unlikely to occur at 20 K, suggesting that chemisorbed H atoms might play a role in H_2 formation at relatively high temperatures.

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ApJ, 2019, 878, 1

https://iopscience.iop.org/article/10.3847/1538-4357/ab1e4e

CALL FOR ABSTRACTS

Atmospheric Processes, Particles, and Chemistry (P003)

AGU 2019 FALL MEETING
December 9-13, 2019 – San Francisco, CA

Abstract submission deadline: 31 July 2019, 11:59 pm EDT

We are excited to invite you to submit an abstract to a **cross-disciplinary session on** **Atmospheric Processes, Particles, and Chemistry (P003)** at the AGU 2019 Fall Meeting in San Francisco, CA (December 9-13, 2019).

The goal of this session is to stimulate communication across disciplines and spark new scientific collaborations between the **Earth** and **Planetary** communities (lab, theory, model, observations). With this in mind, we invite presenters who have already made these types of connections, as well as others who have a technique to offer or a problem in search of a new perspective to submit their abstracts. **We intend to use the short talk format to allow maximum visibility.**

P003 - Atmospheric Processes, Particles, and Chemistry
Many of the chemical and microphysical processes occurring in planetary atmospheres have direct similarities to those studied in the Earth's atmosphere. The aim of this session is to bring together atmospheric expertise from the Earth and planetary communities to share knowledge and techniques across traditional boundaries. We encourage submissions from all areas of atmospheric studies, including but not limited to experimental and/or theoretical studies of gas phase composition, chemistry, dynamics, and particle (aerosols and clouds) formation and evolution. We encourage reports of existing cross-disciplinary efforts as well as abstracts describing techniques that could be applied to other bodies, and submissions describing a gap in knowledge that could be addressed collaboratively. We intend to use the "short talk" format to maximize information exchange and encourage participants to initiate conversations that could lead to future collaborations and new research investigations.

Conveners: Laura Iraci (NASA Ames), Ella Sciamma-O'Brien (NASA Ames), Alexandria Johnson (Brown University), and Erika Barth (Southwest Research Institute).

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