ASTROCHEMISTRY:

Discoveries to Inform the Chemical Sciences & Engineering Communities

The National Academies of Sciences, Engineering, and Medicine
500 Fifth Street NW, Washington, DC 20001
E Street Conference Room

November 8-9, 2018

Day 1: November 8, 2018

8:30 AM **Welcome and Opening Remarks**
Ellen Mantus, *Director, CSR*
Michael J. Fuller, *Chevron Energy Technology Company*

8:45 AM **Keynote Speaker**
Paola Caselli, *Max Planck Institute*; *University of Virginia*

Session I: The Chemistry of Space: Novel Chemicals and Reaction Mechanisms

9:30 AM **Introduction to Session I**
Eric Herbst, *University of Virginia*

9:45 AM **Detection of Exotic Species in Space and in the Laboratory**
Michael McCarthy, *Harvard-Smithsonian Center for Astrophysics*

10:15 AM **Observation of Organic Molecules in Disks around Young Stars**
Catherine Walsh, *University of Leeds*

10:45 AM **Break**

11:00 AM **PAHs and Fullerenes: Complex Carbon Species throughout the Universe**
Els Peeters, *University of Western Ontario*

11:30 AM **Production of Interstellar Molecules by Proton Bombardment of Ices**
Reggie Hudson, *NASA*

12:00 PM **Panel Discussion**
Panelists – Presenters 1-4

12:45 PM **Lunch**

Session II: Information from Remote Sensing through Spectroscopy

1:45 PM **Introduction to Session II**
Susanna Widicus Weaver, *Emory University*

2:00 PM **Where is the Carbon in the Solar System?**
Ted Bergin, *University of Michigan*

2:30 PM **Chemistry in Disks of Gas and Dust**
Ilse Cleeves, *University of Virginia*

3:00 PM **Break**

3:15 PM **Chemistry of Planetary Atmospheres**
Sarah Hörst, *Johns Hopkins University*

3:45 PM **Planetary Evolution**
Jonathan Fortney, *University of California Santa Cruz*

4:15 PM **Panel Discussion**
Panelists – Presenters 5-8

5:00 PM **Adjourn Day 1**

Day 2: November 9, 2018

Session III: Discoveries from Spacecraft Missions in the Solar System and from Laboratory Studies of Extraterrestrial Samples

8:30 AM **Introduction to Session III**
Stefanie Milam, *NASA*

8:45 AM **Origins of Complex Organics in Primitive Bodies**
Jamie Elsila, *NASA*

9:15 AM **Preservation of Organics on Mars**
Daniel Glavin, *NASA*

9:45 AM **Break**

10:00 AM **Searching for Habitability at the Extremes**
Amanda Stockton, Georgia Tech

10:30 AM **The Chemistry of Pluto as Revealed by New Horizons**
Mike Wong, *Caltech*

11:00 AM **Panel Discussion**
Panelists – Presenters 9-12

11:45 AM **Closing Remarks**
Michael J. Fuller, *Chevron Energy Technology Company*

12:00 PM **Workshop Concludes**

Speaker Biographies

Ted Bergin is a professor and chair of the Department of Astronomy at the University of Michigan. Dr. Bergin uses chemistry to probe the physics of star and planet formation and to trace the molecular origins of life. His current focus is the study of water and organics. He combines observation and theory to examine where and how molecules are formed and how they interact with radiation. His research aids in the understanding of chemistry but also increases the use of molecules as probes of the physics of star and planet formation. Dr. Bergin was a member of the team that showed that ice on the comet Hartley 2 has the same chemical composition as our oceans, supporting the theory that Kuiper-belt comets might have delivered a significant portion of Earth's water. He also helped detect vast quantities of cold water vapor in the outer reaches of the star TW Hydrae's planet-forming disk, which further supports that theory. Dr. Bergin received his PhD from University of Massachusetts.

Paola Caselli is the director of the Center for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics, a visiting professor in the Department of Astronomy at the University of Virginia, and Jubilee Professor at Chalmers University of Technology, Gothenburg, Sweden. At the Max Planck Institute, she has established a group working on observations, theory, and laboratory experiments of topics related to astrochemistry and star and planet formation. Her previous appointments are as a researcher at the Arcetri Astrophysical Observatory (Florence, Italy; 1996-2005), a visiting scholar and lecturer in the Department of Astronomy at Harvard University (2005-2007), and professor of astronomy at the School of Physics and Astronomy at University of Leeds (UK; 2007-2014). Dr. Caselli obtained her PhD in astrophysics from the University of Bologna, after spending a large portion of her time working with Dr. Eric Herbst on astrochemistry at the Ohio State University and working with Dr. Phil Myers on molecular cloud observations at the Harvard-Smithsonian Center for Astrophysics (CfA). She completed postdoctoral appointments at CfA and at the Max Planck Institute for Extraterrestrial Physics.

Ilse Cleeves is an assistant professor of astronomy and an assistant professor of chemistry at the University of Virginia. She studies the composition of molecule-rich disks around young stars that are potentially forming (or have recently formed) planetary systems. Using a combination of observations and simulations, she quantifies the chemical properties of these disks to shed light on the diversity of potential planetary compositions. Moreover, this same compositional information provides a powerful tool to constrain key disk physics—including temperature and radiation field—that might inform whether or not a disk can form planets efficiently. Dr. Cleeves received a PhD in astronomy from the University of Michigan.

Jamie Elsila is an astrochemist in the Astrobiology Analytical Laboratory at the Goddard Space Flight Center of the National Aeronautics and Space Administration (NASA). Her research focuses on stable isotopic signatures of extraterrestrial organic compounds, including amino acids in carbonaceous chondrites, lunar samples, and cometary material. She leads Goddard's Fundamental Laboratory Research (FLaRe) workgroup and is a scientific co-investigator for the NASA Astrobiology Institute at the Goddard Center for Astrobiology and a collaborator on the OSIRIS-REx asteroid sample return mission. Dr. Elsila received a PhD in chemistry from Stanford University.

Jonathan Fortney is a professor and the director of the Other Worlds Laboratory in the Department of Astronomy and Astrophysics at the University of California, Santa Cruz. Dr. Fortney is a planetary scientist that works to understand planets as classes of astrophysical objects. His current research is on modeling planetary atmospheres, interiors, and thermal evolution, from rocky terrestrial planets to gas giants. Exciting exoplanet observations are happening on two fronts: the close-in transiting planets that can be studied with

space-based and ground-based telescopes and the young warm Jupiter-class planets far from their parent stars that can be directly imaged. In his work on exoplanets, he makes connections between these distant planets and our solar system's planets. Dr. Fortney received his PhD in planetary sciences from the University of Arizona.

Daniel Glavin is the associate director for Strategic Science of the Solar System Exploration Division at the National Aeronautics and Space Administration (NASA). He co-founded the Astrobiology Analytical Laboratory at NASA Goddard, which specializes in the analysis of extraterrestrial amino acids and other organic compounds important to life in meteorites, lunar samples, and samples returned from asteroids and comets. Dr. Glavin is a co-investigator on the OSIRIS-REx asteroid sample return mission. He was selected to be a participating scientist on the Mars Science Laboratory mission in 2011 and was part of the team that discovered the first evidence of indigenous organic compounds on Mars using the Sample Analysis at Mars (SAM) instrument. In recognition of his meteorite research, the International Astronomical Union named an asteroid after him, asteroid (24480) Glavin. Dr. Glavin was awarded the Antarctica Service Medal of the United States, the Meteoritical Society's Nier Prize, and the NASA Goddard Internal Research and Development Innovator of the Year Award. He was also twice awarded the NASA Robert H. Goddard Exceptional Achievement Award for Science. He earned a PhD in earth sciences from the Scripps Institution of Oceanography.

Sarah M. Hörst is an assistant professor at Johns Hopkins University in the Department of Earth and Planetary Sciences. Her primary research interest is atmospheric chemistry, particularly the complex organic chemistry that occurs in the atmosphere or on the surface of bodies in the solar system. She is a recipient of the Gerard P. Kuiper Memorial Award from the Lunar and Planetary Laboratory at the University of Arizona. Dr. Hörst served as a member of the National Academies Standing Committee on Astrobiology and Planetary Science. She earned her PhD in planetary science from the University of Arizona and was a National Science Foundation astronomy and astrophysics postdoctoral fellow at the University of Colorado.

Reggie Hudson is the lead scientist of the Cosmic Ice Laboratory at the Goddard Space Flight Center of the National Aeronautics and Space Administration. His research interests include the chemistry and physics of cosmic ices, especially those of Jupiter's and Saturn's satellites, trans-Neptunian objects, the Pluto-Charon system, Mars, comets, and the interstellar medium. His work also involves investigating the astrobiology of planetary systems, prebiotic chemistry, radiation chemistry, photochemistry, and thermal chemistry applied to astronomical problems, and molecular spectroscopy applied to molecular structure, bonding, and reactions of astronomical solids. Dr. Hudson was previously a professor of chemistry at Eckerd College. He received his PhD in physical chemistry from the University of Tennessee.

Michael McCarthy is the associate director of the Atomic and Molecular Physics Division of the Harvard-Smithsonian Center for Astrophysics. He was previously a member of the scientist staff and was appointed to a position as the Yoram Avni Distinguished Research Astronomer. His research interests include the spectroscopy of known and postulated astronomical carbon chains, carbon rings, and carbon clusters; the chemistry and physics of the interstellar medium; and molecular radio astronomy. He has co-authored over 200 scientific papers. Dr. McCarthy received his PhD in physical chemistry from the Massachusetts Institute of Technology.

Els Peeters is an associate professor in the Department of Physics and Astronomy at the University of Western Ontario and a research scientist at the SETI Institute in California. Her research focuses on the physics and chemistry of interstellar carbonaceous molecules and dust with an emphasis on polycyclic aromatic hydrocarbons (PAHs). She is an observational astronomer and has worked extensively with infrared observations from space-based telescopes, such as the Infrared Space Observatory (ISO), NASA's Spitzer Space Telescope and the Herschel Infrared Space Observatory, the Stratospheric Observatory for Infrared Astronomy (SOFIA), and ground-based telescopes, such as VLT and Gemini. Dr. Peeters obtained her PhD from the University of Groningen (The Netherlands) and completed postdoctoral appointments at the NASA Ames Research Center and the SETI Institute.

Amanda Stockton is an assistant professor in the School of Chemistry and Biochemistry in the Center for Space Technology and Research at Georgia Tech. Her research group focuses on analyzing extraterrestrial organic molecules in the search for life beyond Earth, fingerprinting life at Earth's extremes, and exploring the origins of biomolecules and the emergence of life. A primary thrust of the first theme is the development of in situ instrumentation to examine the organic chemical environment in the extraterrestrial environment through landed instruments, fly-by instruments, and impactor instruments. The group also examines organic molecules in extraterrestrial samples on Earth, including meteorites, interplanetary dust particles, and cometary grains returned by such missions as Stardust. The second theme involves field expeditions to volcanic and geothermal regions of Iceland and to the extremely acidic and saline Rio Tinto and analysis of samples from the Atacama Desert and Antarctic ice shelves. The third theme involves working with the Center for Chemical Evolution to explore the emergence of life in warm, wet pools on the surface of the early Earth. Her group also explores potential laboratory models of hydrothermal vent systems that mimic those now known to be present on the icy moons of the outer solar system, including Enceladus and Europa. Dr. Stockton obtained her PhD in chemistry from the University of California, Berkeley.

Catherine Walsh is a University Academic Fellow at the University of Leeds and based in the Astrophysics Group in the School of Physics and Astronomy. She studies molecules in space across the spectrum of molecular sources—from interstellar clouds (the birth places of stars) through protoplanetary disks and planetary atmospheres and even circumstellar envelopes around dying stars. She is interested in fundamental astrochemical processes, that is, how molecules are formed and destroyed in different environments and

how they can be used to probe the physical conditions in the diverse range of extreme environments in which they survive. She also makes use of high-spatial and high-spectral resolution observations with the Atacama Large Millimeter/Submillimeter Array (ALMA). Dr. Walsh is the co-principal investigator of a 100-hour ALMA Large Programme to investigate the chemistry of planet formation on spatial scales similar to the size of the solar system. She is also the principal investigator of four ALMA programs, two of which concern the investigation of the gas and dust structure of protoplanetary disks around intermediate-mass stars that also show signatures of embedded planets and ongoing planet formation. The second two programs are a deep search for the complex organic ice reservoir in disks around nearby sun-like stars to help answer questions regarding the origin of complex molecules in planetary systems. She received her PhD in astrophysics from Queen's University (Belfast, UK).

Michael Wong is a PhD candidate at the California Institute of Technology who studies astrobiology, habitability, and planetary atmospheres with Professor Yuk L. Yung and researchers at Caltech and the Jet Propulsion Laboratory. Mr. Wong hosts a podcast called Strange New Worlds, which examines science, technology, and culture through the lens of Star Trek.

Planning Committee Biographies

Michael J. Fuller is a Completions Fluids and Stimulation Advisor at Chevron. His current role in Chevron's Energy Technology Company includes applications, development, and troubleshooting of fluids and materials for productivity enhancement, acid stimulation, hydraulic fracturing, and drilling and completions, including sand control. His contributions span deepwater projects, unconventionals (including shale and tight-rock), and other challenging reservoir conditions. In his former roles at Schlumberger, his accomplishments comprised development, engineering, and troubleshooting of chemical products, fluids, and materials in upstream oil and gas disciplines. Dr. Fuller has multiple publications and patents in the areas of hydraulic fracturing of shale and conventional reservoirs; sand control applications and fluids; formation damage and response to upstream fluids; productivity enhancement; and general drilling and completions applications and fluids. Dr. Fuller received his PhD in chemistry from Northwestern University.

Franz M. Geiger is a professor of chemistry at Northwestern University where he leads major collaborative research projects that involve experimental and computational methods to study the special role that surfaces and interfaces play in the world. He is a Fellow of the Alfred P. Sloan Foundation, the American Association for the Advancement of Science, and the Royal Society of Chemistry. Most recently, he is the recipient of the 2017 Friedrich Wilhelm Bessel Prize of the Alexander von Humboldt Foundation and the 2016 Faculty Diversity Award from Northwestern University's Graduate School. He serves as senior editor of the Journal of Physical Chemistry, as Chair-Elect of the newly established Experimental Physical Chemistry subdivision of the American Chemical Society Physical Chemistry Division, as a member of the Science Board of the Telluride Science Research Center, and as a member of the International Advisory Board of the Pacific Conference on Spectroscopy and Dynamics. Dr. Geiger received his PhD in chemistry from Georgetown University.

Eric Herbst is Commonwealth Professor of Chemistry at the University of Virginia, with courtesy appointments in astronomy and physics. He has held faculty positions at The College of William and Mary in chemistry, at Duke University in physics, and at The Ohio State University in physics and astronomy. His current major interest is in the chemistry that occurs as stars and planets form. Dr. Herbst is a Fellow of the American Physical Society and the Royal Society of Chemistry (RSC) and received the Centenary Prize in 2004 from the RSC. He has also received the Max Planck Research Prize and prizes from the French, Norwegian, and Czech physical chemical societies. He served as a scientific editor of *The Astrophysical Journal* from 1998-2007 and has recently become an associate editor of the new American Chemical Society journal *Earth and Space Chemistry*. Dr. Herbst received his PhD in physical chemistry from Harvard University.

Stefanie Milam works in the Astrochemistry Laboratory at the NASA Goddard Space Flight Center. She conducts high-resolution spectroscopic studies of evolved stars, star-forming regions, and the Galactic interstellar medium with an emphasis on isotopic fractionation and astrobiology of primitive materials. Specifically, her key research objective is to study the isotope composition of evolved stars to determine the nucleosynthetic processes that have taken place, chemical enrichments that might occur in the mass-loss process, and how the enrichment is distributed to the interstellar medium, star-forming regions, and planetary systems. She also has a laboratory dedicated to simulate interstellar/cometary/planetary ices and detect trace species by using the same techniques used for remote observations to help constrain the chemical complexity of the ices, the amount of processing that occurs, and interpret past and present data from missions that observe ice features. Dr. Milam maintains a renowned observational program with radio telescopes located around the world and with space-based observatories to observe comets. She was selected as the James Webb Space Telescope (JWST) Planetary Science Liaison for solar system observations. Dr. Milam received her PhD in chemistry from the University of Arizona.

Susanna Widicus Weaver is an associate professor and director of graduate studies in the chemistry department at Emory College of Arts and Sciences. Her research focuses on astrochemistry and molecular spectroscopy. She was the vice-chair of the American Chemical Society Astrochemistry subdivision in 2016 and has served on the editorial board for the *Journal of Molecuar Spectroscopy*. A few of her several awards include the Flygare Award in Molecular Spectroscopy, the National Science Foundation Career Award, and the Eugene M. Shoemaker Impact Cratering Award. Dr. Weaver received her PhD in chemistry from the California Institute of Technology.