



# The Astrochemistry Subdivision of the American Chemical Society

## Astrochemical Complexity in Planetary Systems

### 1. Chemical Complexity in Interstellar and Protostellar Environments (PHYS001A/ASTRO1)

Monday 5<sup>th</sup> April 2021. Morning, 9am-12pm PST (12pm - 3pm ET)

*Martin Cordiner and Christopher Bennett Presiding*

- 09:00 **Welcome and Introductory Remarks**  
*Martin Cordiner and Christopher Bennett (Organizers)*
- 09:05 **Complex Molecules in Space: The Interstellar Medium and Comets**  
*Steven Charnley (invited talk)*
- 09:30 **Alma and Rosina Detections of Phosphorus-Bearing Molecules: The Interstellar Thread Between Star-Forming Regions and Comets**  
*Victor M. Rivilla (contributed talk)*
- 9:45 **Nitrogen Isotopes in the Interstellar Medium: A Chemical Journey Across the Galaxy**  
*Laura Colzi (contributed talk)*
- 10:00 **Deuterated Methanol: From Theory to Observations in Low-Mass Star-Forming Regions**  
*Beatrice Marie Kulterer (contributed talk)*
- 10:15 *Intermission (15 minutes)*
- 10:30 **Untapped Reservoir of Complex Aromatic Carbon in Nascent Star and Planetary Systems**  
*Brett McGuire (invited talk)*
- 10:55 **Nuclear Spin Abundances of Water in the Orion Bar: A New Experimental Approach to Investigate the Role of Grains on the Nuclear Spin Populations of Water Molecules**  
*Thomas Putaud (contributed talk)*
- 11:10 **Carbon-Grain Sublimation: A New Top-Down Component of Protostellar Chemistry**  
*Merel van't Hoff (contributed talk)*
- 11:25 **Interstellar Prebiotic Soup: How Biomolecule Building Blocks Are Formed in Space**  
*Niels Ligterink (contributed talk)*
- 11:40 *End of Session (open to discussion until 12:00pm)*



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### 2. Experimental Techniques for Astrochemistry (PHYS001B/ASTRO2)

Monday 5<sup>th</sup> April 2021. Afternoon, 1pm-4pm PST (4pm - 7pm ET)

*Stefanie Milam and Christopher Bennett Presiding*

- 13:00 **Spectroscopy of and Radiation-Chemical Changes in Astronomical Ices**  
*Reggie Hudson (invited talk)*
- 13:25 **Building Biomaterials in Space: Organic Acids, Aminoalcohols, Amides, and Prebiotic Interstellar Chemistry**  
*Susanna Widicus Weaver (invited talk)*
- 13:50 **Experimental Determination of Reaction Product Branching Ratios at Low Temperatures for Astrochemistry**  
*Ian Sims (contributed talk)*
- 14:05 **Direct D Atom Incorporation in Radicals at Low Temperature: An Overlooked Pathway to Deuterium Fractionation?**  
*Nureshan Dias (contributed talk)*
- 14:20 *Intermission (15 minutes)*
- 14:35 **Investigating Potential Prebiotic Molecules Utilizing Ice Analogues in Space Simulation Experiments**  
*Andrew Turner (invited talk - ACS astrochemistry outstanding doctoral dissertation award winner)*
- 15:00 **Exploring the Chemistry Induced by Energetic Processing of the H<sub>2</sub> Bearing, CO-Rich Ice Layer**  
*Rafael Martin-Domenech (contributed talk)*
- 15:15 **Next-Generation Tools to Analyze Wideband Rotational Spectra of Complex Mixtures**  
*Michael McCarthy (invited talk)*
- 15:40 **Much Ado About Symmetry? - C<sub>60</sub> Ionization in Space**  
*Helgi Hrodmarsson (contributed talk)*
- 15:55 *End of Session (open to discussion until 4:00pm)*



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### 3. Chemistry of Protoplanetary Disks and Comets (PHYS001C/ASTRO3)

Tuesday 6<sup>th</sup> April 2021. Afternoon, 1pm-4pm PST (4pm - 7pm ET)

*Merel van't Hoff and Amanda Hendrix Presiding*

- 13:00 **Organic Chemistry in Protostellar Disk Systems**  
*Jennifer Bergner (invited talk)*
- 13:25 **From Disk Midplane to Planet Atmosphere: The Chemical Link**  
*Christian Eistrup (invited talk)*
- 13:50 **Deciphering the Origin and Evolution of Our Solar System From the Chemical Composition of 67P**  
*Kathrin Altwegg (invited talk)*
- 14:15 **Heavy Nitrogen Isotopic Composition of Comet 67p/Churyumov–Gerasimenko**  
*Susanne Wampfler (contributed talk)*
- 14:30 *Intermission (15 minutes)*
- 14:45 **Organic Matter in Comet 67P: Low and High Molecular Weight Molecules**  
*Hervé Cottin (invited talk)*
- 15:10 **Remote Studies of Organics in Cometary Comae**  
*Stefanie Milam (contributed talk)*
- 15:25 **Building a Taxonomy of Comets Based on Native Ice Compositions**  
*Michael DiSanti (contributed talk)*
- 15:25 **Pre- and Post-Perihelion Observations of the Co-Dominated Comet C/2016 R2 (PanSTARRS)**  
*Adam McKay (contributed talk)*
- 15:40 *End of Session (open to discussion until 4:00pm)*



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### 4. Advances in Computational Approaches for Astrochemistry (PHYS001D/ASTRO4)

Wednesday 7<sup>th</sup> April 2021. Afternoon, 1pm-4pm PST (4pm - 7pm ET)

*Reggie Hudson and Jamie Elsila Presiding*

- 13:00 **Advances in Modeling Interstellar Grain-Surface Chemistry**  
*Robin Garrod (invited talk)*
- 13:25 **Hypervelocity Sampling of Ice-Borne Biosignatures in Space Missions: First-Principles Based in Silico Study**  
*Andres Jaramillo-Botero (contributed talk)*
- 13:40 **Recent Progress in the Mixed Quantum/Classical Calculations of Collisional Energy Transfer Between the Molecules of Astrochemical Relevance**  
*Dmitri Babikov (contributed talk)*
- 13:55 **Expanding the Astrochemical Catalog: Novel Gas Phase N-Heterocycle Formation Pathways Identified with an *Ab Initio* Nanoreactor**  
*Sommer Johansen (contributed talk - withdrawn)*
- 14:10 *Intermission (15 minutes)*
- 14:25 **Infrared Signatures for the Molecular Building Blocks of Planets**  
*Ryan Fortenberry (invited talk)*
- 14:50 **Molecular Polarizability in Astrochemistry of Complex Organic Compounds: Isomeric Species, PAHs, Polyynes, and Fullerenes**  
*Denis Sabirov (contributed talk)*
- 15:05 **Investigating the Relative Importance of Low-Energy (< 20 eV) Electrons in Astrochemistry**  
*Hannah Anderson (contributed talk)*
- 15:20 **Monte Carlo Simulations of Low-Energy (< 20 eV) Electrons in Astrochemistry**  
*Olivia Adamczyk (contributed talk)*
- 15:55 *End of Session (open to discussion until 4:00pm)*



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### 5. Complex Chemistry in Planetary and Satellite Systems (PHYS001E/ASTRO5)

Thursday 8<sup>th</sup> April 2021. Afternoon, 1pm-4pm PST (4pm - 7pm ET)

*Jennifer Bergner and Ryan Fortenberry Presiding*

13:00 **Carbon Complexity at Saturn: What the Rings Tell Us About Carbon in the Saturn System?**  
*Jack Waite (invited talk)*

13:25 **Multi-Spectral Observations of Saturn's Icy Moons to Probe Exogenic Effects**  
*Amanda Hendrix (invited talk)*

13:50 **Measuring Effects of Hypervelocity Impact on Spectral Signatures of Enceladus Ice Grain Analogues**  
*Morgan Miller (contributed talk)*

14:05 **Molecular Solids on Titan: New Insights into Hydrogen Cyanide and Butadiene**  
*Robert Hodyss (contributed talk)*

14:20 *Intermission (15 minutes)*

14:35 **Recent Molecular Detections in the Atmosphere of Titan**  
*Alexander Thelen (contributed talk)*

14:50 **Mass Spectrometry as a Tool for Detecting Organics on Mars (and Beyond)**  
*Jennifer Stern (invited talk)*

15:15 **Formation of Complex Organic Molecules (COMs) From Polycyclic Aromatic Hydrocarbons (PAHs): Top-Down Synthesis of Organics in Planetary Systems**  
*Andrew Mattioda (contributed talk)*

15:30 **Automated Spectroscopic Detection of Molecular Species in Planetary Atmospheres Using Machine Learning**  
*David Josephs (contributed talk)*

15:45 *End of Session (open to discussion until 4:00pm)*



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### 6. Organics in the Inner Solar System, Asteroids and Meteorites (PHYS001F/ASTRO6)

Friday 9<sup>th</sup> April 2021. Morning, 9am-12pm PST (12pm - 3pm ET)

*Martin Cordiner and Jennifer Stern Presiding*

- 09:00 **Analysis of Organics in Solar System Samples**  
*Jamie Elsila (invited talk)*
- 09:25 **OSIRIS-REx Sample Return Mission - Looking for Signs of Primitive Astrochemical Complexity in Asteroid (101955) Bennu**  
*Scott Sandford (invited talk)*
- 09:50 **An Experimental and Theoretical Investigation into the Reactivity of Fluoranthene Under Asteroidal Conditions**  
*Claudia-Corina Giese (contributed talk - withdrawn)*
- 10:05 **Synthetic pathways to interstellar C<sub>60</sub>: A link to presolar grains**  
*Jacob Bernal (contributed talk)*
- 10:20 *Intermission (10 minutes)*
- 10:30 **Coordinated Analysis Using AFM-IR, STXM/XANES and NanoSIMS for Organic Petrology in Complex Planetary Materials**  
*Yoko Kebulkawa (invited talk)*
- 10:55 **Novel Infrared and Raman Spectroscopic Methods for Studying Organic Matter Within Meteorites**  
*Mehmet Yesiltas (invited talk)*
- 11:20 **Revealing Origin of Chemical Complexity in Extraterrestrial Matter by Combining Multiple Characterization Techniques: HR-L<sup>2</sup>MS, ToF-SIMS, and MicroRaman Spectroscopy**  
*Claire Pirim (invited talk)*
- 11:45 **Characterization of Sedimentary Organic Matter Using Laser Desorption-Ionization Mass Spectrometry**  
*Siveen Thlajeh (contributed talk)*
- 12:00 *End of Session (open to discussion until 12:00pm)*



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### 7. The Primordial Earth, Exoplanet Atmospheres, and Novel Instrumentation for Planetary Science (PHYS001G/ASTRO7)

Monday 12<sup>th</sup> April 2021. Afternoon, 1pm-4pm PST (4pm - 7pm ET)

*Robin Garrod and Christopher Bennett Presiding*

- 13:00 **Exploring the Complexity of Prebiotic Organic Chemistry using Combined Computational and Experimental Approaches**  
*Henderson Cleaves (invited talk)*
- 13:25 **Model Primordial Peptides with Diverse Monomer Compositions, Sequences, and Structures**  
*Jay Forsythe (invited talk)*
- 13:50 **Fate of Glycine Traced by Quantum Chemical Simulations: From Its Interstellar Formation to Its Polymerization in Planetary Environments**  
*Albert Rimola (contributed talk)*
- 14:05 **Glycine Condensation Chemistry Under Extreme Conditions**  
*Nir Goldman (contributed talk)*
- 14:20 *Intermission (15 minutes)*
- 14:35 **Integrated Stellar, Atmospheric, Planetary, and Surface Chemistry to Identify Habitable Worlds**  
*Steven Benner (invited talk)*
- 15:00 **Photochemical Haze Formation in Exoplanetary Atmospheres: Insight From Laboratory Simulations**  
*Chao He (invited talk)*
- 15:25 **H<sub>2</sub>SO<sub>4</sub> And Organosulfur Compounds Revealed in Laboratory Analog Aerosols by Orbitrap Mass Spectrometry**  
*Veronique Vuitton (contributed talk - withdrawn)*
- 15:40 **ORIGIN: A Novel Laser Desorption Mass Spectrometry Concept for the *in Situ* Detection of Biomolecules on Planets and Moons**  
*Niels Ligterink (contributed talk)*
- 15:55 **Concluding Remarks**  
*Martin Cordiner and Christopher Bennett (Organizers)*