Physical Chemistry Research at Undergraduate Institutions

Organizers: Todd Hopkins and Carol Parish
March 23-26, 2026

Monday PM

Georgia World Congress Center | B310
C. A. Parish, *Organizer* | T. Hopkins, *Organizer, Presiding*

2:00 PM. Theoretical investigation of the radicaloid character of structurally diverse polycyclic aromatic hydrocarbons. **J.B. Schriber**

2:30 PM. Multi-configurational analysis of unusual features in x-ray absorption spectra of photoredox nickel complexes. **T. Scott**

3:00 PM. Formation of substituted benzenes in Titan's atmosphere and the spectroscopy of the reactive intermediates. **R.M. Huchmala**, V.J. Esposito

3:20 PM. Characterizing multiconfigurational polyradicals. **C.A. Parish**

3:40 PM. Computational astrochemistry at Chapman University: Anharmonic infrared spectra of polycyclic aromatic hydrocarbons. **V.J. Esposito**

4:10 PM. Intermission.

4:20 PM. Characterization of electron transport in molecular devices and wires using active space methods. **A. Sand**

4:50 PM. Spin-flip study of the diradical isomers of pyrrole, furan, & thiophene. **D. Sirianni**

5:20 PM. Symmetric or asymmetric structure, what happens to a triferrous extended metal atom chain upon reduction?. **J.E. Bates**, M.J. Lowe, H. Kristoffersen, J.N. McKeon, G. Guillet

5:40 PM. First-principles investigation of hole defects in B2C monolayers: A combined GA-NN-DFT approach. **M. Groves**, L. Zhang, D. Milla

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Tuesday PM

Georgia World Congress Center | B304
T. Hopkins, *Organizer* | C. A. Parish, *Organizer, Presiding*

2:00 PM. Exploring the molecular wonderland: How undergraduates drive computational research in the Baker lab at The College of New jersey. **J.L. Baker**

2:30 PM. Development of a coarse-grained model of nucleic acids for studying folding in the presence of polycationic peptides. **K.M. Lebold**

2:50 PM. Current research topics in the shields lab at Furman university: Atmospheric aerosols and opioid conformations. **C.S. Glick**, G.C. Shields

3:10 PM. Illuminating interfaces: Experimental and theoretical insights into atmospheric chemistry on aerosol surfaces. **J.G. Navea**

3:40 PM. Engaging the next-generation of computational chemists: Vignettes from an undergraduate research group at a liberal arts college. **H.P. Hendrickson**

4:10 PM. Intermission.

4:20 PM. Competing ions regulate sulfate affinity at model marine aerosol interfaces. **J. Patterson**

4:50 PM. Assessing amyloid polymorphism for disease-related and functional amyloids using the phasor approach to FLIM. **S. Sohail**, J. Chen, A. Buendia

5:10 PM. Approaches to structure-activity relationships for 1,3-dipolar cycloaddition reactions of criegee intermediates with carbonyls. **A.W. Harrison**

5:30 PM. Exploring reactive oxygen species for ethylene epoxidation. **A. Baber**

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Wednesday AM

Georgia World Congress Center | A310
T. Hopkins, C. A. Parish, *Organizers* | L. Jarocha, *Presiding*

8:00 AM. Designing enantioselectivity with ternary chiral deep eutectic solvents. **T. Hopkins**, H.J. Teague, A.T. Lake

8:20 AM. Reactivity and phase behavior of atmospherically-relevant organic acids at the air-water interface. **R. Rapf**, K. Holt, B. Rugeley, E. Peterson

8:50 AM. Undergraduate research into predicting pK_a Using machine learning and quantum mechanical workflows. M. Meduna, M.J. Petroff, **P. Patel**

9:10 AM. Solvent control of proton transfer in photoacids. **K. Takematsu**

9:40 AM. Undergraduate research in computational reaction path dynamics. **L. Bladow**

10:00 AM. Intermission.

10:10 AM. Harnessing lewis photoacidity for CO_2 capture and release. H. Harkins, B. Delibas, S. Sahu, J. Dawlaty, **A.S. Petit**

10:30 AM. Intermission.

10:50 AM. Carbones as potential players in organocatalysis: Mechanistic insights from computations and data science. **M. Ogba**

11:20 AM. Quantifying atmospheric ozonolysis reaction mechanisms with quantum chemistry and statistical rate theory. **K.T. Kuwata**, L. Valin, A. Converse, C. Martin, K. Zhang

Physical Chemistry Research at Undergraduate Institutions

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Wednesday PM

Georgia World Congress Center | B5 - EXHIBIT HALL ChemPod 8
T. Hopkins, C. A. Parish, *Organizers* | R. Rapf, *Presiding*

2:00 PM. Driving Student engagement through a tailored approach to MOF synthesis and characterization. **M.R. Hudson**

2:30 PM. Characterization of wave patterns as a function of the BZ chemical environment. **D. Yengi**, S.L. Small, A. Hoch, N. Divins, S. Nkomo

2:50 PM. Photocatalysis mechanisms of bi and Bi-Sn alloy nanoparticles. **P. Lyu**, E. Stephens, L. Hoffman

3:10 PM. Characterizing the interactions between brooker's merocyanine and mordenite using experimental and computational methods. **J.S. Holt**, D. Virgo

3:40 PM. Structures and properties of doped silicon and magnesium hydride clusters. **J.T. Lyon**

4:00 PM. Intermission.

4:10 PM. Investigating intermolecular interactions and structural effects in thin films of functional materials. **C. Mauck**

4:40 PM. Exploration of MOF surface chemistry in research and teaching labs at the University of San Diego. **L.B. Benz**, A. Dela Merced, J. Meyer, H. Pham, A. Loney, M. Beam

5:10 PM. Shining light on perovskites (and other compounds). **R. Berger**

5:40 PM. Thermodynamics of the (Fe^{3+}/Fe^{2+}) oxidation-reduction of heme-fluoride complexes in hemoglobin and myoglobin: Oxygen binding implications and redox pathways. **J. Cerda**, K.G. Flanders, S. Sheppard, D. Lukoss

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Thursday AM

Georgia World Congress Center | A316
T. Hopkins, C. A. Parish, *Organizers* | J. B. Schriber, *Presiding*

8:00 AM. Probing vibrational fingerprints of strong hydrogen bonds: The case of Bihalide ions. **J. Tan**, D. Rienzo

8:30 AM. Investigation of diatom light-harvesting using fluorescence spectroscopy. **S.C. Massey**

8:50 AM. Researching ultrafast dynamics with undergraduate Students. **C.J. Stromberg**, E.J. Heilweil

9:10 AM. Toward accessible ultrafast spectroscopy: A blueprint for phase-resolved second harmonic generation to track interfacial chemistry. **N.M. Gonzalez**, F. Geiger

9:30 AM. Diabatic valence-hole state: A unifying concept in the global electronic structure of the second and third row diatomic molecules. **J. Jiang**

10:00 AM. Intermission.

10:10 AM. First electronic spectra of vanadium hydride (VH): Experimental analysis and astronomical implications. **T.D. Varberg**

10:40 AM. Rotational spectroscopy of methoxy-substituted heterocycles reveals conformational dynamics. **T. Barnum**, L. Baker, N. Gestring, N. Riordon

11:00 AM. Broadband microwave spectroscopy of highly functionalized 5-membered ring organic molecules. **A.O. Hernandez-Castillo**

11:30 AM. Fluorescence-based methods to detect and optimize the performance of radical pair-based magnetosensors. **L. Jarocha**

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