Tuesday, March 19, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | R08
Making Stronger Connections to Students and Faculty | T. Holmes, *Presiding*

Change: Program will start at 8:30am.

8:30 AM. Necessity is the mother of invention. **M.D. Ellison**

8:55 AM. Allowing physical chemistry students to visualize spectroscopy and photochemistry using computational chemistry mini-projects. **A.S. Petit**

9:15 AM. Undergraduates using big data, machine learning and molecular docking tools to test and confirm protein function. **B. Hall**

9:40 AM. Studying kinetics through dissolving of spherical and non-spherical candies. **J.B. Dudek**

9:55 AM. Intermission.

10:10 AM. Math for PChem Foundation Module and its implemention in physical chemistry courses. **L. Jensen**, A. Driesbach, G. Camacho

10:30 AM. Kinetics experiments that are green and inexpensive. **R.C. Dudek**, M. Pawlak

10:55 AM. Universal Design for research training (UDRT): Adapting UDRL for diverse training in diverse communities in computational chemistry. **G. Lobodina**, S. Allen, J.R. Leszczynski, **G. Hill**

11:20 AM. Accelerating stem advancement among underprepared students at Jackson State University. **T. Sanders**, A. Williams, C. Smith, T. DeMeritte, N. Kirtman, A. Jennerjohn, M. Fadavi

11:40 AM. LABSIP: What we have learned so far from a growing community of physical chemistry instructors. **C.H. Londergan**, K. Takematsu, C. Baiz, R.F. Berger, J.C. De Paula, S.D. Fried, K. Donald, B. Rubenstein, G.Y. Stokes

Tuesday, March 19, 2024 | 2pm – 6pm session
Ernest N. Morial Convention Center | R08
Innovations in Lab| C. Jones, *Presiding*

2:00 PM. Introductory Remarks.

2:05 PM. Intermediate pK_a and spectrum of a polyprotic acid. **A. Mansell**

2:30 PM. Dimerization of propionic acid in gaseous phase (seemingly) contradicts what students learn about real gases' behavior: Activating previously learned knowledge to solve the dilemma. **B.H. Milosavljevic**

2:50 PM. Using eutectic mixtures and deep eutectic solvents as a framework for a physical chemistry laboratory. **T. Hopkins**

3:10 PM. A guided inquiry approach to measuring the equilibrium of methyl red in the physical chemistry laboratory. **R.R. Michelsen**

3:30 PM. Cureing Compchem: Facilitating meaningful research experiences and computational training via a project-based course in computational chemistry. **D. Sirianni**

3:55 PM. Intermission.
4:10 PM. Is it a stable molecule? A computational physical chemistry experiment. **A. Grushow**, S.S. Hunnicutt, R.M. Whitnell

4:30 PM. Marrying theory and experiment: Programming and computational chemistry in the year-long physical Chemistry Laboratory. **J.B. Schriber**

4:50 PM. Partnering a computational chemistry lab experiment with an organic chemistry cure. **P.M. Hare**, C. Rhodes, L. Ma

5:10 PM. Combining Raman spectroscopy, group theory and computational chemistry in the physical chemistry laboratory. **T.D. Varberg**

5:30 PM. Discussion.

5:55 PM. Closing Remarks.

PHYS Physical Chemistry
ACS Technical Division

Innovative Teaching in Physical and Computational Chemistry
Organizers: Ashley Ringer McDonald, Charlisa Daniels, Conrad Jones and Tiffani Holmes
Cosponsored by COMP
New Orleans, LA   **March 19-21, 2024**

Wednesday, March 20, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | R08
Innovations in Lab | A. Grushow, *Presiding*

8:00 AM. Introductory Remarks.

8:05 AM. Introductory computational exercise for physical chemistry students. **M.D. Sonntag**

8:30 AM. Computational chemistry compliments kinetic experiments on cis-trans isomerization of 4-anilo-4'-nitrobenzene: A blended lab for use in undergraduate chemistry courses. **A.N. Migues**

8:50 AM. Development of a guided inquiry computational chemistry experiment: "Aromaticity! What is it good for?". **S.S. Hunnicutt**, A. Grushow, M.S. Reeves, R.M. Whitnell

9:10 AM. Motivating mastery of physical chemistry through problem solving and project work. **J.B. Foresman**

9:30 AM. Development and implementation of coal solar cell module for the two-level modular approach in physical chemistry laboratory course. **L. Wang**

9:55 AM. Intermission.

10:10 AM. Using quantum mechanics to understand the greenhouse effect. **P. Hall**, L. Gunning

10:35 AM. Computational chemistry assisting the identification of polymers. **C. Salter**, K. Range

10:55 AM. Characterizing fluorescence quenching in a model bio-sensing system: A novel pchem CURE. **J.J. Peterson**

11:15 AM. Generative AI in education and research: Opportunities, concerns, and solutions. **E. Alasadi**, C. Baiz

11:35 AM. Discussion.

11:55 AM. Closing Remarks.

Wednesday, March 20, 2024 | 2pm – 6pm session
Ernest N. Morial Convention Center | R08
Highlighting Innovations with Computational Tools | A. Ringer McDonald, *Presiding*

2:00 PM. Introductory Remarks.

2:05 PM. Assessing and improving computational thinking skills in physical chemistry at a women's HBCU. **M. Van Vleet**, T. Nelson, D. Hylton, S. Sung

2:25 PM. Using Python in quantum mechanics and nanoscience to explore concepts involving calculus. **T.R. Brewer**

2:45 PM. Reading scientific literature with large language models: a new approach for undergraduates in biophysical research. A.V. Vazquez, **F.X. Vazquez**

3:05 PM. Exploratory physical chemistry labs using Google Colaboratory: Random walkers and the Ising model. **J.H. Olshansky**

3:25 PM. Investigating the impact of student-generated Mathematica demonstrations developed using the compute-to-learn approach. **H.P. Hendrickson**, V. Venkatesh, T. Chua, T. Addy

3:45 PM. Intermission.

4:00 PM. Procedure for the *ab initio* computational study of amino acids. N. Tam, D. Abramov, **L. Tribe**

4:20 PM. Comparison of free and low-cost cloud gpu-based computing for exercises in introductory modecular dynamics simulations. **M.A. Kubasik**

4:40 PM. Project-based learning strategies with Python for developing code literacy and computational thinking in chemistry courses. **G. Grazioli**

5:00 PM. Teaching (experimental) chemists problem solving via programming. **C.J. Johnson**, **B.J. Lear**

5:20 PM. Introduction to computational chemistry using nanoHUB. **T. Simon**

5:40 PM. Discussion.

Thursday, March 21, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | R08
Innovations in Lecture | C. Daniels, *Presiding*

8:15 AM. Introductory Remarks.

8:20 AM. Pedagogical challenges and opportunities in a one semester physical chemistry class.
W.K. Gichuhi, G. Isham

8:45 AM. The flipped classroom as a tool to modernize the physical chemistry curriculum. **J. Duchimaza**

9:00 AM. Electrons on the move: An undergraduate introduction to time-dependent quantum mechanic.
T. Hua, R. Morehouse, K. Lopata

9:15 AM. Team-based learning in physical chemistry I lecture. **Y. Zhang**

9:40 AM. Achieving balance in physical chemistry laboratory through computational chemistry.
J.L. Sonnenberg

9:55 AM. Intermission.

10:10 AM. Exploring electron configurations of atoms and ions with WebMO and Gaussian. **K. Range**

10:25 AM. The importance of post-class homework in flipped classroom instruction for physical chemistry courses. T. Gomez, S. Villafane-Garcia, **M. Groves**

10:40 AM. Atmospheric reaction mechanisms as the focus of an intermediate-level computational chemistry course. **K.T. Kuwata**

10:55 AM. Implementing traditional and computational guided inquiry activities in the student-centered physical chemistry classroom. **A.L. Mifflin**

11:20 AM. Integrated physical chemistry. **C.M. Teague**

11:35 AM. Discussion.

11:55 AM. Concluding Remarks.