



# ACS DIVISION OF PHYSICAL CHEMISTRY

## Fall 2022 National ACS Meeting

### Chicago, IL ☺ 21-25 August 2022

Meeting Theme: Sustainability in a Changing World



The Division of Physical Chemistry has organized the following oral symposia, consisting of both invited and contributed papers, as well as topical and general poster sessions.

**The abstract submission deadline is 14 March 2022.**

For those interested in an oral presentation, please submit abstracts to the appropriate symposium. For each symposium, the organizers (listed below) will select some contributed papers for oral presentations; contributions not selected for oral presentations will be assigned to the poster session.

#### Photochemistry Spotlight: Answering the Big Questions in Photochemistry

This symposium is designed to stimulate provocative discussions on big questions in photochemistry and spotlight the work of early career faculty. Photoexcitation is important for a range of applications and provides significant energy to drive chemical reactions. The sessions will highlight recent progress in the physical understanding, experimental tools, and application of photochemistry in molecules and molecular assemblies, at heterogeneous interfaces, and in nano and bulk materials.

**Jean-Luc Ayitou**, *Illinois Institute of Technology*, [ayitou@iit.edu](mailto:ayitou@iit.edu)

**Justin Caram**, *University of California, Los Angeles*, [icaram@chem.ucla.edu](mailto:icaram@chem.ucla.edu)

**Lisa Fredin**, *Lehigh University*, [laf218@lehigh.edu](mailto:laf218@lehigh.edu)

**John Swierk**, *Binghamton University*, [jswierk@binghamton.edu](mailto:jswierk@binghamton.edu)

#### Big Data & Computational Microscopy/Spectroscopy Applied to Chemical Characterization

Advancements in the hardware associated with physical chemistry have yielded more precise and larger datasets. At the same time, new analytical approaches from computer science and applied mathematics harness ideas from compressive sensing and neural networks. This symposium is aimed at sharing new hardware and software techniques from inside and outside the chemical field to boost further breakthroughs and nurture greater collaboration in the area of chemical microscopy and spectroscopy.

**Steve Baldelli**, *University of Houston*, [sbaldelli@uh.edu](mailto:sbaldelli@uh.edu)

**Elad Harel**, *Michigan State University*, [elharel@msu.edu](mailto:elharel@msu.edu)

**Kevin Kelly**, *Rice University*, [kkelly@rice.edu](mailto:kkelly@rice.edu)

#### Advances in Crystal Structure Prediction and Crystal Engineering

Crystal polymorphism is important for the pharmaceutical industry, and increasingly for organic electronics. Since changes in molecular packing between different polymorphs can result in large variations in targeted properties, one cannot optimize functionality of a material at the single-molecule level. While first-principles crystal structure prediction (CSP) is extremely challenging, it promises a means to identify stable polymorphs given only a molecular structure. The goal of this symposium is to bring together theorists advancing development of all aspects of crystal structure prediction with experimentalists engaged in research on molecular crystals.

**Gino Dilabio**, *University of British Columbia*, [gino.dilabio@ubc.ca](mailto:gino.dilabio@ubc.ca)

**Erin Johnson**, *Dalhousie University*, [erin.johnson@dal.ca](mailto:erin.johnson@dal.ca)

#### Quantum Chemistry: Current and Future Frontiers

Modern quantum chemistry plays a critical role in elucidating processes in diverse areas of research ranging from spectroscopy to materials science. New quantum chemical methods combined with state-of-the-art computer hardware now enable highly accurate simulations that seemed out of reach just two decades ago. This symposium will bring together a diverse community of quantum chemists to discuss recent advances in the field, current challenges, as well as prospects for future development.

**Francesco Evangelista**, *Emory University*, [francesco.evangelista@emory.edu](mailto:francesco.evangelista@emory.edu)

**Alexander Sokolov**, *The Ohio State University*, [sokolov.8@osu.edu](mailto:sokolov.8@osu.edu)

#### Open-source Software in Chemistry

Open-source software in physical chemistry underpins many aspects of theoretical method development and analysis, transcending production software and encompassing fundamental research codes that advance computational methods and provide new physical chemistry insight. This symposium will showcase new capabilities, algorithmic and theory development within existing open-source software packages, as well as up-and-coming software that seeks to find a broader audience. Additional topics include new analysis algorithms that help to interpret a variety of experimental characterization methods and the complex and multiscale information contained within simulation data.

**Aurora Clark**, *Washington State University*, [auclark@wsu.edu](mailto:auclark@wsu.edu)

#### Inorganic & Organometallic Astrochemistry

The inventory of metal-containing astrochemical molecules is growing, along with information about their spectroscopy, ionization rates, condensed phase behavior, and kinetics. This symposium will celebrate the interdisciplinary nature of astrochemistry. Topics will include terrestrial characterization and astronomical detection of novel astrochemicals; and improved mechanistic comprehension of how inorganic and organometallic molecules are produced or processed in interstellar environments.

**Nathan DeYonker**, *University of Memphis*, [ndyonker@memphis.edu](mailto:ndyonker@memphis.edu)

**Leah Dodson**, *University of Maryland*, [ldodson@umd.edu](mailto:ldodson@umd.edu)

#### Standing Out in the Crowd: Dynamics of Biomolecules in Complex Environments

Recent technological advancements have enabled experimental and computational investigations of the composition, physical, and electronic structures of biomolecules at atomic, molecular, and macro scales in relevant environments. This session will highlight new methods, sample preparation approaches, theories, and analyses that are being developed to study biomolecules under more complex conditions related to both biology and biomaterials. Of particular interest are emerging areas including, but not limited to, quantum biology, phase separation, viruses, and drug delivery.

**Julie Biteen**, *University of Michigan*, [jsbiteen@umich.edu](mailto:jsbiteen@umich.edu)

**Caitlin Davis**, *Yale University*, [c.davis@yale.edu](mailto:c.davis@yale.edu)

**Lydia Kisley**, *Case Western Reserve University*, [lydia.kisley@case.edu](mailto:lydia.kisley@case.edu)

#### Structure and Dynamics in the Carbon-based Nanostructure Superfamily

From carbon dots to melanin, lab-made and naturally occurring carbon-based nanostructures are of great interest for energy conversion and storage, catalysis, and bioelectronics but are challenging to study due to their structural complexity and multiscale dynamics. This symposium welcomes researchers seeking unifying concepts and first-principles understanding of hallmark properties in the broad family of carbon-based nanostructures of natural and synthetic origin. Topics include chromophore generation, light-to-charge conversion, radical chemistry, redox-gated functions, charge transport and storage, photochemistry, and excited-state dynamics.

**Dirk M. Guldi**, *Friedrich-Alexander University*, [dirk.guldi@fau.de](mailto:dirk.guldi@fau.de)

**Bern Kohler**, *The Ohio State University*, [kohler.40@osu.edu](mailto:kohler.40@osu.edu)

**Clara Santato**, *Polytechnique Montreal*, [clara.santato@polymtl.ca](mailto:clara.santato@polymtl.ca)

#### Spectroscopy, Imaging, & Dynamics of Energy Related Materials

The frontier in energy related materials research lies in designing new functionalities from nanostructured and molecular components. A major challenge is how to integrate functional entities to achieve optimal energy flow over multiple time (fs-ms) and length (nm-mm) scales. This symposium will feature advances in experimental techniques that probe structure and dynamics with energy, structural, temporal, and spatial resolutions and new theoretical approaches to address the complex and multiscale interactions in these materials.

**Libai Huang**, *Purdue University*, [libai-huang@purdue.edu](mailto:libai-huang@purdue.edu)

**Jenny Lockard**, *Rutgers University - Newark*, [jlockard@newark.rutgers.edu](mailto:jlockard@newark.rutgers.edu)

#### Advances in Single-Particle Imaging: From Single Molecules to Nanomaterials

The past decade has witnessed tremendous advances in super-resolution, photothermal, electron beam, and scanning probe characterization tools that span across a wide domain of energies, spatial resolutions, and time scales. It is the purpose of this symposium to bring together both junior and senior experimentalists and theoreticians leading this effort to overview the latest advances in the field and to foster new ideas to probe electronic, vibrational, magnetic, optical, and thermal phenomena below the diffraction limit of light.

**Stephan Link**, *Rice University*, [slink@rice.edu](mailto:slink@rice.edu)

**David Masiello**, *University of Washington*, [masiello@u.washington.edu](mailto:masiello@u.washington.edu)

**Katherine A. Willets**, *Temple University*, [kwillets@temple.edu](mailto:kwillets@temple.edu)

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#### PHYS Division Research Awards and PHYS/JPC Lectureship Awards

The four winners of the PHYS Division Research Awards and the three winners of the PHYS/Journal of Physical Chemistry Lectureship Awards will present talks at this half-day symposium on Tuesday, August 23rd.

#### Division of Physical Chemistry Poster Session

Contributions from all areas of physical chemistry are highly encouraged for the poster session (*likely* to be held Wednesday, 24 August), from 6:00 to 8:00 PM. Up to six awards with monetary prizes will be given for exemplary work. To be eligible for the awards, the presenting author must be a graduate or undergraduate student at the time of the poster presentation and must be present during judging.

On-Line Abstract Submission Deadline: 14 March 2022

<https://callforabstracts.acs.org/acsfall2022/PHYS>

#### DIVISION OF PHYSICAL CHEMISTRY YOUNG INVESTIGATOR RESEARCH AWARDS

Four PHYS Division Young Investigator Research Award talks will be presented during the relevant PHYS technical symposia. See <http://phys-acs.org/all-awards/>

**Prof. Christy Landes, Program Chair**

**Rice University, Department of Chemistry (713) 348-4232 [cflandes@rice.edu](mailto:cflandes@rice.edu)**

FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEBSITE: <http://phys-acs.org/>