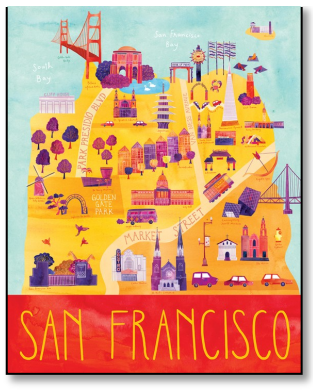
ACS DIVISION OF PHYSICAL CHEMISTRY
248th NATIONAL MEETING
San Francisco, California
10-14 August 2014



CALL FOR PAPERS

The Division of Physical Chemistry has organized the following topical oral symposia, consisting of both invited and contributed papers, as well as topical and general poster sessions. **The abstract deadline is 21 March 2014**. 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.

THE FUTURE OF COMPUTATIONAL CHEMISTRY

The future of computational chemistry hinges not only on the accuracy of its underlying models but also on the efficiency and efficacy of its algorithms and software. In all areas of molecular-level simulation, including not only traditional chemistry but materials and biomolecular science as well, recent theoretical advances have yielded unprecedented levels of accuracy and understanding for a broad array of fundamental chemical phenomena. However, the concomitant development of new, high-performance computing architectures—from now-common petascale computers to highly anticipated exascale systems—presents innumerable challenges for those implementing new methods in production-level software. This symposium will bring together experts in quantum chemistry, biomolecular simulation, and condensed-matter physics to highlight the current state of the art in both methodology and software design, and to explore paths forward toward sustainable and extensible codes that can take full advantage of the ever-changing landscape of cyberinfrastructure.
T. Daniel Crawford, *Virginia Tech, crawdad@vt.edu*
Theresa Windus, *Iowa State University, twindus@iastate.edu*

RENEWABLE ENERGY GENERATION AT THE INTERFACE BETWEEN THEORY AND EXPERIMENT

This symposium is designed to highlight the collaborative efforts of experimentalists and theoreticians in the area of renewable energy, spark cross-disciplinary discussions, and explore the relationship between computation and experiment more deeply. The topics for this symposium include the following: Artificial Photosynthesis, Proton-Coupled Electron Transport, Catalysis (water oxidation, carbon dioxide reduction, nitrogen reduction, and hydrogen generation), and Solar Cells (dye-sensitized solar cells, quantum dot solar cells, organic photovoltaics, and new cell architectures).
Amanda J. Morris, *Virginia Tech, ajmorris@vt.edu*
James T. Muckerman, *Brookhaven National Laboratory, muckerma@bnl.gov*

MOLECULAR AND NANOSCOPIC PROBES FOR BIOLOGICAL SYSTEMS

Biological systems are highly heterogeneous and dynamic, and the study of this topic has a cross-disciplinary impact on physical chemistry, biophysics, molecular and cell biology, materials science, translational medicine and multiple engineering fields. Recent developments show the critical importance of using molecular or nanoscopic probes to study the structure, diversity and function of various biological entities in cells or tissues. This symposium will present new advances in this vibrant research area. In particular, it will bring together experimentalists, theoreticians, and computational scientists to forge a scientific culture of fluid exchange of ideas and collaboration across disciplines and among laboratories.
Bozhi Tian, *University of Chicago btian@uchicago.edu*
Chen Yang, *Purdue University, yang@purdue.edu*

EXTREME BIOCHEMISTRY FROM SMALL MOLECULES TO LARGE PROTEINS: FORMATION, STABILITY, STRUCTURE AND FUNCTION

The origin and adaptability of life on Earth holds a fascination for most of us and is a central and compelling field of study for many scientists. Chemists have been involved in this field in many ways, including discovering how simple biomolecules, as building blocks for life, can be generated under prebiotic conditions, and how biomolecular processes can be adapted to extreme environmental conditions. More broadly, a study of extremophile biochemistry should, in principle, provide guidelines for the formation and evolution of life elsewhere, assuming that evolution is a general principle underlying the development of living systems on other planets besides Earth. In this symposium, we will combine members of the astrochemistry community with biochemists and chemists working on the properties of extremophiles to provide a broad picture of the latest results and insights into how, under extreme conditions, simple molecules become more complex, as well as how complex biomolecules (proteins, nucleic acids, etc.) adapt to inhospitable environments to enable and extend life in surprising habitats. Topics include interstellar chemistry, prebiotic terrestrial chemistry, and the properties and structures of extremophile proteins from extreme thermal, chemical and other challenging environments. The utilization of these studies to biotech applications will also be presented.
Yong Ba, *California State University at Los Angeles, yba@calstatela.edu*
Robert J. Stanley, *Temple University, rstanley@temple.edu*
Ralf Kaiser, *University of Hawaii, ralfk@hawaii.edu*

PHOTOINDUCED PROTON TRANSFER IN CHEMISTRY AND BIOLOGY

Proton transfer is one of the most fundamental chemical reactions in nature. However, understanding the ways in which the environment mediates proton dynamics remains a fundamental challenge. Excited-state proton transfer (ESPT), as well as more general photoinduced proton transfer (PPT), continues to provide a rich vein of new research activity. The range of systems that has pushed the limits of theory has greatly expanded in the past decade. The topics cover modern PPT theory, syntheses of novel photoacids and photobases, and studies of their PPT in a wide array of systems from gas phase to proteins and DNA. Numerous PPT applications will be discussed, including the utilization of reversible and irreversible pH-jumps using transient photoacids and PAGs, and recent advances in the development optically-active, intramolecular ESPT-based materials. A broad spectrum of PPT-related problems will bring together the leading specialists—not only from the world of physical chemistry, but theoreticians, biochemists, organic and material chemists from all over the world.
Pi-Tai Chou, *National Taiwan University, chop@ntu.edu.tw*
Kyril M. Solntsev, *Georgia Tech, solntsev@gatech.edu*

PHYSICAL CHEMISTRY OF IONIC LIQUIDS

From fundamental studies to applications in energy, catalysis and separations, ionic liquids are permeating all aspects of modern chemistry. Physical chemistry plays a leading role in understanding chemical reactivity, relaxation phenomena, structure and interfacial behavior in these diverse materials. This symposium will present the latest advances in the physical chemistry of ionic liquids on a range of topics that include the relationships between ionic liquid structure and physical and transport properties, volatility and thermal stability, electron transfer, photolysis and radiolysis, ultrafast to ultra-slow spectroscopy, separations and solubility, interfaces with bulk and nanomaterials, and catalysis.
Edward W. Castner, Jr., *Rutgers University, ed.castner@rutgers.edu*
Edward J. Maginn, *University of Notre Dame,* ed@nd.edu
Claudio J. Margulis, *University of Iowa, claudio-margulis@uiowa.edu*
James F. Wishart, *Brookhaven National Laboratory, wishart@bnl.gov*

FUNDAMENTAL PROCESSES OF ATMOSPHERIC CHEMISTRY

Although several decades of research have greatly advanced our understanding of the physical chemistry of the atmosphere, there remain many outstanding research areas that are poorly understood. These questions include the potential for organic oxidation to recycling radical species, the chemical mechanisms and kinetics behind the oxidation of organic and inorganic compounds, gas-particle partitioning of multi-generational oxidation products, and the potential for compounds in the atmosphere to affect the radiative balance of the planet through the formation of cloud and ice condensation nuclei, light scattering of aerosol particles, and absorption by brown and black carbon. Research approaches into these problems include ambient observations, laboratory experiments and theoretical studies. The development of new chemical detectors and *in situ* perturbation studies are leading to new measurements and new insights that are driving the development of models. Recent advances have led to better predictions of atmospheric chemistry and its effects on the atmosphere's radiative properties.
Delphine Farmer, *Colorado State University, Delphine.Farmer@colostate.edu*
Frank Keutsch*, University of Wisconsin, keutsch@chem.wisc.edu*

WHAT DOES 20TH CENTURY PHYSICAL CHEMISTRY HAVE TO SAY TO 21ST CENTURY PHYSICAL CHEMISTS?

The 20th century was the great age of physical chemistry. It started with the first Nobel Prize in Chemistry in 1901 to van't Hoff and continued right up to the close of the century with Zewail in 1999. Many paradigms were established for all time—not just for the 20th century. Indeed, for any field to be dynamic, it needs to both move forward and to remember its roots. Fortunately, there are many living physical chemists who are bringing the excitement of these foundational achievements to the current membership of PHYS. Thus, this symposium will feature many leaders of physical chemistry who are truly excited about revisiting the history of physical chemistry in dynamic ways.
Gary D. Patterson, *Carnegie Mellon University, gp9a@andrew.cmu.edu*

COMPUTATIONAL SPECTROSCOPY

Experiments in spectroscopy have laid the foundation for current understanding of, for example, the electronic and magnetic properties of molecules, reactive intermediates, combustion chemistry, materials, and surface and interfacial chemistry. This Computational Spectroscopy Symposium will highlight the significant impact that computational chemistry has made on the interpretation and prediction of spectroscopic measurements. Since many of the more recent important advances have been achieved through close collaborations between theorists and experimentalists, prominent and emerging scientists representing both theory and experiment will be invited to give talks in areas of electronic, vibrational, ultrafast, and magnetic resonance spectroscopies of both gas- and condensed phases.
Caroline Chick Jarrold, *Indiana University, cjarrold@indiana.edu*
John F. Stanton, *University of Texas, jfstanton@mail.utexas.edu*

PHYS DIVISION RESEARCH AWARDS AND JPC LECTURESHIP AWARDS

The four winners of the PHYS Division Research Awards and the three winners of the Journal of Physical Chemistry Lectureship Awards will present talks at this one-day symposium.

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP FOR UNDERGRADUATE CHEMISTRY MAJORS

The Workshop for Undergraduate Chemistry Majors is targeted for current junior chemistry majors, who will be seniors at the time of the San Francisco meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the San Francisco meeting. In addition, they will be expected to present posters on their research as part of the PHYS poster session. More information and application materials can be found at http://phys-acs.org/ugrad_workshop/2014.html. The application deadline is 10 February 2014.
Carol Parish, *University of Richmond, PHYSworkshop@richmond.edu*

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, 13 August 2014. See the announcement below for information about the Physical Chemistry Student Poster Awards.
Nancy Levinger, *Colorado State University, Levinger@lamar.colostate.edu*

On-Line Abstract Submission Deadline: 21 March 2014
http://abstracts.acs.org

POSTDOCTORAL RESEARCH AWARDS

PHYS Division Postdoctoral Research Awards and invited talks will be presented at the relevant PHYS Symposia**.**

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

Six awards with monetary prizes will be awarded for posters presented by students at the Physical Chemistry Poster Session on Wednesday evening of the meeting.
To be eligible for the awards, the **presenting author** must be a graduate or undergraduate student at the time of the poster presentation.
Poster presenters will be contacted by e-mail and invited to declare their eligibility (student status) and desire to participate in the student poster award competition.

NANCY LEVINGER, PROGRAM CHAIR

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