Arousal of reversible and irreversible pH syntheses of novel photoacids and photobases, 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. 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 extreme environmental 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 new ways. Topics include interstellar chemistry, photosynthetic habits, and structures of extremophiles from extreme thermal, chemical and other challenging environments. The utilization of these studies to biotech applications will also be presented.

Yong Ba, University of Chicago btyou@uchicago.edu

EXEMPLARY PROBES FOR BIOLOGICAL SYSTEMS

Biological systems are highly heterogeneous and dynamic, and the study of this topic has a complex impact on physical chemistry. Biopolymers, molecular and cell biology, materials science, medicinal chemistry, and many other engineered fields. Recent developments show the importance of understanding the role of molecules, 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 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 extreme environmental 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 new ways. Topics include interstellar chemistry, photosynthetic habits, and structures of extremophiles 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, btyou@uchicago.edu

Robert J. Stanley, Temple University, rstanley@temple.edu

Rafi Kaisar, University of Hawaii, rafi@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 topic of PPT theory, syntheses of novel photocatalysts and photoswitching, and studies of their PPT in a wide array of systems from gas-phase to protic solvents is rapidly growing. The focus will be on understanding the utilization of reversible and irreversible pH jumps using transient photocatalysts and PAGs, and recent advances in the development optically-active, intramolecular ESPT-based materials. A broad spectrum of applications in materials and fundamental problems will be addressed.

Pi-Tai Chou. National Taiwan University, choupntu@ntu.edu.tw

Kyril M. Sokolov, Georgia Tech, sokolov@chemistry.gatech.edu

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 materials and biomolecular simulations but also chemistry, the underlying advances in the development of the algorithms for energy, stability, and structure, are critical to the overall progress of the field. 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; selections not selected for oral presentations will be assigned to the poster session.

Daniel Crawford, Virginia Tech, dcrawford@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 generation. The goal is to discuss the challenges and opportunities involved in the design, synthesis, and evaluation of materials for clean-energy technologies. The focus will be on the development of novel concepts and strategies for the efficient generation and conversion of solar energy, with an emphasis on the fundamental principles governing the synthesis, structure, and properties of materials.

Zahid Qureshi, University of Chicago, qureshi@uchicago.edu

Ulrike Scherwiede, Lawrence Berkeley National Laboratory, ulrike.scherwiede@lbl.gov

Molecular and Nanoscopic Probes for Biological Systems

Biological systems are highly heterogeneous and dynamic, and the study of this topic has a complex impact on physical chemistry. Biopolymers, molecular and cell biology, materials science, medicinal chemistry, and many other engineered fields. Recent developments show the importance of understanding the role of molecules, 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 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 extreme environmental 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 new ways. Topics include interstellar chemistry, photosynthetic habits, and structures of extremophiles from extreme thermal, chemical and other challenging environments. The utilization of these studies to biotech applications will also be presented.

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Kyril M. Sokolov, Georgia Tech, sokolov@chemistry.gatech.edu

PHYSICAL CHEMISTRY OF IONIC LIQUIDS

From fundamental studies to applications in energy, materials, 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 aims to bring together the leading experts 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, photolyis and radiolysis, ultratop to ultra-slow spectroscopy, separations and solubility, interfaces with bulk and nanomaterials, and catalysis.

Edward W. Caser, Jr., Rutgers University, ed.caser@ruters.edu

Edward J. Maginn, University of Notre Dame, edj@nd.edu

Claudio J. Margulis, University of Texas at Austin, margulis@琊 תמיד nhé uma vida.

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 origin of the majority of the Earth’s atmosphere due to its early stages of formation, the mechanism by which the atmosphere and its composition are influenced by solar radiation, 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 techniques 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 PHYSICISTS?

The 20th century was a great age of physical chemistry, with those prominent figures like Linus Pauling, who were honored with the first Nobel Prize in Chemistry in 1901 to Harald Hahn and the continued evolution to 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 truly advanced, it needs to be both internal and external. Fortunately, there are many living physical chemists who are bringing the excitement of these foundational achievements to the current membership of PHYS. This symposium will feature many leaders of physical chemistry who are truly excited about revitalizing the field in dynamic ways.

Gary D. Patterson, Carnegie Mellon University, gdp@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, catalysis, 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, ultraviolet, and magnetic resonance spectroscopies of both gas- and condensed phase systems.

Caroline Chick Jarrold, Indiana University, cjarrold@indiana.edu

John F. Stanton, University of Texas, f Stanton@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, PhysAcowskoph@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

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