2024 WILLIAM H. NICHOLS DISTINGUISHED SYMPOSIUM & AWARD BANQUET

PHYSICAL CHEMISTRY AND SUSTAINABILITY

A distinguished symposium honoring

Professor Emily A. Carter
Princeton University

for groundbreaking quantum insights in sustainable catalysis

Date: Friday, April 12, 2024
Sonesta Hotel, White Plains, NY
Hotel website

Time: 1:30 PM – 9:00 PM
Download Brochure here
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Symposium Program

1:30 PM **Welcome**
Professor Ping Furlan, 2024 New York ACS Chair, US Merchant Marine Academy

1:35 PM **Opening of the Distinguished Symposium**
Professor Eric Chang, 2024 New York ACS Chair-Elect, Pace University

1:45 PM **Computational Discovery of Metal-Organic Frameworks for a Changing World**
Professor Laura Gagliardi, University of Chicago

Addressing the energy challenges that we face globally requires the coordinated efforts of scientists, engineers, and policy makers. Chemistry has the potential to drive quantum leaps in technology. With theory, computation, and machine intelligence we can accelerate the search for solutions to water scarcity, decarbonization, and clean energy. Metal-organic frameworks (MOFs) are versatile platforms for various applications including catalysis for complex reactions and water harvesting. I will first present our ongoing efforts to understand and design the water-filling mechanism for water-harvesting MOFs.[1]I will then describe our combined computational and data-driven study of MOF-supported catalysts. Utilization of machine learning algorithms in conjunction with experimental data can not only predict superior catalytic materials, but also under which experimental conditions they are most optimal.[2].

2:30 PM **Designing Metal-Oxide-Based thermochemical Redox Materials and Processes: Solar Fuels and Energy Storage**
Professor Ellen Stechel, Arizona State University

In this talk, we unveil cutting-edge developments in metal oxide-based thermochemical redox materials and processes[1], applicable to solar fuels and energy storage. We start by exploring how the high-temperature endothermic reduction of redox-active metal oxides, capable of releasing oxygen gas under achievable

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2:30 PM **Designing Metal-Oxide-Based thermochemical Redox Materials and Processes: Solar Fuels and Energy Storage (continued)**
Professor Ellen Stechel, Arizona State University

operating conditions, effectively converts thermal energy into stored chemical energy. A subsequent re-oxidation step then either recovers this energy as heat or drives further chemical reactions. The ability to indefinitely repeat these two steps opens the door to sustainable energy cycles. Here we will focus on two interrelated processes: reversible re-oxidation with oxygen and bond-breaking re-oxidation with CO2 and/or water. This presentation will also highlight the groundbreaking design of a novel perovskite metal oxide material, Ca2/3Ce1/3Ti1/3Mn2/3O3 (CCTM2112), specifically engineered for enhanced thermochemical hydrogen production. This material, predicted solely from theoretical considerations and validated experimentally, showcases a unique cation redox chemistry. Utilizing quantum-based modeling [2], we reveal how the deliberate manipulation of cation composition on both A and B sub-lattices leads to a material with optimal oxygen vacancy formation energies and superior redox dynamics to facilitate splitting of water and carbon dioxide. This presentation will delve into the intricacies of CCTM2112's thermodynamics, demonstrating its potential. Our findings not only introduce a high-performing material but also open new avenues in the design of redox-active materials through a deep understanding of their electronic characteristics.

3:15 PM *Coffee Break*

3:45 PM **Observing Molecular Transport through Living-Cell Membranes – Pushing the Boundary of Physical Chemistry toward Biology**
Professor Hai-Lung Dai, Temple University

Why should we store food in refrigerator to avoid bacteria contamination? But why refrigeration cannot keep the food fresh for a long period of time? How do bacteria develop antibiotic resistance? How are vesicles used for delivering mRNA vaccines into human body? All these questions can find answers from understanding molecular transport through cell membranes. Nonlinear light scattering in the form of Second Harmonic Generation, due to its symmetry properties, has been proven effective for observing molecular adsorption and transport at the surfaces of colloidal objects, including living biological cells. This method affords membrane specificity, real time resolution, and the ability to image single cells in examining molecule-membrane interactions. This talk will lay out the basic physical principles of the newly developed Second Harmonic Light Scattering (SHLS) method and illustrate how SHLS can be applied to examine molecular adsorption and transport at cell membranes. In addition to answering the questions above, this method has been used to determine the fundamental mechanism of the century-old Gram stain for classifying bacteria, understand effects of molecular structure and membrane structure in influencing molecular transport through cell membranes, and characterize membrane phase transition and membrane asymmetry.

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4:30 PM **A Physical Chemist's Journey to Combat Climate Change**
Professor Emily A. Carter, 2024 Nichols Medalist, Princeton University

When I first became fully cognizant of what fossil fuel burning was doing to our planet, I vowed to use my expertise full-time to transition the world to sustainable energy. But now it is terribly clear that to preserve the planet for future generations, this action – far from complete - is not nearly enough. We must stop emitting carbon into the atmosphere from all sectors, aiming not just for net-zero but net-negative emissions. More than 15 years ago, I pivoted my quantum simulation research to design materials for clean electricity (solar cells, fusion, fuel cells). More recently, we design catalysts for renewable fuels and chemicals production, via electro-/solar-thermo-chemical water splitting and photo/electro/solar-thermo-chemical carbon dioxide reduction. However, recycling CO2 is not enough; we must develop sustainable processes to convert and store CO2 in useful, durable products. I will describe our quantum embedding simulation methods that accurately simulate sustainable production of fuels and chemicals catalytically using electricity and/or light, and introduce its use for studying processes related to direct ocean capture of CO2 to form minerals, a strategy for getting to negative emissions.

5:45 PM *Social Hour*

6:45 PM **Medal Award Dinner**

Presiding;	**Dr. Ping Furlan** 2024 Chair, ACS New York Section
ACS Greetings:	**To be announced**
Introductory Address:	**Dr. Michael Berman** Air Force Office of Research
Medal Presentation:	**Dr. Ping Furlan**
Acceptance Address:	**Dr. Emily A. Carter** Nichols Medalist

THE WILLIAM H. NICHOLS MEDAL AWARD

Dr. William H. Nichols established this annual award, the first of its kind, in 1902 to honor a chemical scientist for original research. Since its inception, the New Yokr ACS has administered the award. It has been perpetuated through the generosity of Dr. Nichols, his family, and the Nichols Foundation, Inc. The award ceremony has evolved into a Distinguished Symposium and a Medal Award Banquet during which scientists can interact with their colleagues and with chemistry students. The Nichols Medal has been presented to 21 Nobel Laureates, and 23 National Medal of Science recipients.

Read more here

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