QAFCO
TEXAS A&M UNIVERSITY AT QATAR
CONFERENCE 2018

EMERGING FRONTIERS IN CHEMISTRY AND CHEMICAL ENGINEERING

قافكو
QAFCO
شركة قطر للأسمدة الكيماوية
QATAR FERTILISER COMPANY

TEXAS A&M
UNIVERSITY at QATAR

2018 PROGRAM

WELCOME FROM THE DEAN

DR, CÉSAR O. MALAVÉ

Dean, Texas A&M University Qatar

On behalf of Texas A&M University at Qatar, it is my pleasure to welcome you to the 10th Annual QAFCO–Texas A&M University at Qatar Conference. To celebrate this significant milestone, Texas A&M at Qatar and our longtime partners and supporters at the Qatar Fertiliser Company (QAFCO) present a slate of world-renowned speakers to address frontiers in chemistry and chemical engineering.

For 10 years, this important conference has highlighted the pressing need for policy makers, industry and academia to work together to develop new knowledge and create scientific solutions that have direct impact on the world around us. The 10th-anniversary conference features our highest-caliber speakers to date, including two Nobel Laureates: Robert H. Grubbs, 2005 Nobel Laureate in chemistry and the Victor and Elizabeth Atkins Professor of Chemistry at CalTech and Sir Fraser Stoddart, the 2016 Nobel Laureate in chemistry and the Board of Trustees Professor of Chemistry at Northwestern University.

We are glad that you have joined us in Doha for this important event, and we thank QAFCO for its support of our academic and research programs, our faculty, and our current and former students.

WELCOME FROM THE ORGANIZING COMMITEE

In February 2018, we celebrate the 10th edition of the longest conference series in Qatar, QAFCO-Texas A&M at Qatar Conference.

This annual event showcases cutting-edge research and hosts prominent speakers coming from all around the globe, including Nobel Laureates and National Academy members. The event is organized by faculty and staff at Texas A&M University at Qatar and it is fully supported with a generous sponsorship from Qatar Fertiliser Company (QAFCO). Our 10th edition features Prof. Robert H. Grubbs, Nobel Laureate in Chemistry in 2005 and the Victor and Elizabeth Atkins Professor of Chemistry, California Institute of Technology (USA), and Prof. Fraser Stoddart, Nobel Laureate in Chemistry in 2016 and Board of Trustees Professor of Chemistry, Northwestern University (USA).

Dr. Hassan S. Bazzi (Co-Chair)

Dr. Konstantinos Kakosimos (Co-Chair)

Dr. Ioannis Economou

Dr. Sherzod Madrahimov

Ms. Hala El-Dakak

Mr. Hamad Farooqi

ABOUT THIS CONFERENCE SERIES

UNDER THE PATRONAGE OF
H.E. DR. MOHAMMED BIN SALEH AL-SADA

Minister of Energy and Industry
State of Qatar

In partnership with the
American Chemical Society (ACS) Qatar Candidate Chapter

This conference series was initiated by Dr. Hassan S. Bazzi, then-chair of the Science Program at Texas A&M at Qatar, who chaired and organized the pilot edition in January 2007 (TAMUQ Chemistry Conference 2007) that showcased speakers from Qatar and the USA.

QAFCO, Qatar's first large-scale venture in the petrochemical sector, was the exclusive sponsor of the conference. Building on the success of the first edition and the large audience of chemists and engineers it attracted, QAFCO and Texas A&M at Qatar signed an agreement in February 2007 wherein QAFCO would become the exclusive sponsor of the conference series for 5 years and the event was renamed to "QAFCO-Texas A&M at Qatar Chemistry Conference." Between 2008 and 2013, the event grew to become a regional point of attraction for scientists and engineers and it covered different thematic areas, such as:

- **2008:** Polymers and Materials
- **keynote speaker:** Dr. Krzysztof Matyjaszewski, Carnegie Mellon University, USA
- **2009:** Organometallic Chemistry, Synthesis and Mechanisms
- **keynote speaker:** Dr. Robert G. Bergman, University of California, Berkeley, USA
- **2010:** Synthetic Methodologies in Organic Chemistry
- **keynote speaker:** Dr. Robert H. Grubbs, Nobel Laureate in Chemistry 2005, California Institute of Technology, USA
- **2011:** Computational Chemistry
- **keynote speaker:** Dr. Krishnan Raghavachari, Indiana University, USA
- **2013:** Green Chemistry and Green Engineering
- **keynote speaker:** Dr. Paul T. Anastas, Yale University, USA

Keynote speakers and invited speakers came from different countries all over the globe. The event kept collecting momentum in the local academic and industrial sectors, and the attendance increased over the years.

In order to closely align the event with the needs of Qatar and its industrial sector, the organizers decided to widen the scope and call the series "QAFCO-Texas A&M University at Qatar at Conference," QAFCO generously renewed its exclusive support with a $500,000 sponsorship agreement for another five years (2014-2018). Starting in 2014, the conference showcased parallel sessions in chemical engineering and chemistry. Topics ranged from:

- **2014:** Nanotechnology and Energy
- **keynote speaker:** Dr. Paul Alivisatos, Lawrence Berkeley National Laboratory, USA
- **2015:** Sustainable Chemical Processes
- **keynote speaker:** Dr. Peter Wasserscheid, University of Erlangen-Nuremberg, Germany
- **2016:** CO2 Management and Renewable Energy
- **keynote speaker:** Dr. Michael Graetzel, Ecole Polytechnique Federale de Lausanne, Switzerland
- **2017:** Water, Energy and Food Nexus
- **keynote speaker:** Dr. Michael Ladisch, Purdue University, USA
- **2018:** Emerging Frontiers in Chemistry and Chemical Engineering
- **keynote speakers:** Dr. Fraser Stoddart, Nobel Laureate in Chemistry 2016, Northwestern University, USA, and Dr. Robert H. Grubbs, Nobel Laureate in Chemistry 2005, California Institute of Technology, USA

PROGRAM SCHEDULE

QAFCO – Texas A&M University at Qatar Conference 2018
Emerging Frontiers in Chemistry and Chemical Engineering

Thursday, 15 February 2018
Texas A&M University at Qatar,
Education City, Doha Qatar, Lecture Hall 238

Time	Event
7:45–8:30 a.m.	Registration and Light Breakfast
8:30–8:35 a.m.	**Dr. Hassan S. Bazzi** Associate Dean for Research, Texas A&M University at Qatar
8:35–8:40 a.m.	**H.E. Dr. Mohammed Bin Saleh Al-Sada** Minister of Energy and Industry, State of Qatar
8:40-8:45 a.m.	**Dr. César O. Malavé** Dean, Texas A&M University at Qatar
8:45-8:50 a.m.	**Dr. Hamed A Al-Marwani** Chief Administration Officer, Qatar Fertiliser Company (QAFCO)

SESSION I

Chair: **Dr. Hassan S. Bazzi**

Time	Event
8:50-9:50 a.m.	**Sir Fraser Stoddart** 2016 Nobel Laureate in Chemistry Board of Trustees Professor Northwestern University, USA “My Journey to Stockholm”
9:50-10:50 a.m.	**Dr. Robert Howard Grubbs** 2005 Nobel Laureate In Chemistry Victor and Elizabeth Atkins Professor California Institute of Technology, USA “Synthesis of Polymers with Designed Structures”
10:50–11 a.m.	Coffee Break

SESSION II

Chair: **Dr. Konstantinos E Kakosimos**

Time	Event
11–11:30 a.m.	**Dr. John M. Vohs** University of Pennsylvania, USA “Advances in Ceramic Membrane Reactors: From Fuel Cells to Syngas Production”

11:30 a.m.–noon	**Dr. Maurice Brookhart** University of Houston, USA “Pd(II) and Ni(II) Catalysts for Copolymerization of Ethylene and Polar Vinyl Monomers”
Noon–12:30 p.m.	**Dr. Stratos Pistikopoulos** Texas A&M Energy Institute, USA “Multi-parametric Optimization and Control”
12:30–1:30 p.m.	Lunch

SESSION III

Chair: **Dr. Ioannis Economou**

Time	Event
1:30–2 p.m.	**Dr. Tobin Jay Marks** Northwestern University, USA “Surface Science Meets Homogeneous Catalysis”
2–2:30 p.m.	**Dr. Paul Anastas** Yale University, USA “Molecular and Synthetic Design for Us and Our Posterity“
2:30–2:50 p.m.	Coffee Break

SESSION IV

Chair: **Dr. Sherzod Madrahimov**

Time	Event
2:50–3:20 p.m.	**Dr. Peter Cummings** Vanderbilt University, USA “Molecular Studies of Ionic Liquids at Interfaces with Application to Supercapacitors”
3:20–3:50 p.m.	**Dr. David Bergbreiter** Texas A&M University, USA “Recyclable Polyolefins as Solvents and Tools in more Sustainable Homogeneous Catalysis”

NOBEL LAUREATE SPEAKER

SIR FRASER STODDART

2016 NOBEL LAUREATE IN CHEMISTRY

Board of Trustees Professor of Chemistry
Department of Chemistry
Northwestern University, USA

BIOGRAPHY

The academic career of Fraser Stoddart, who was born in the capital of Scotland on Victoria Day (May 24) in 1942, can be traced through thick and thin from the Athens of the North to the Windy City beside Lake Michigan with interludes on the edge of the Canadian Shield beside Lake Ontario, in the Socialist Republic of South Yorkshire, on the Plains of Cheshire beside the Wirral, in the Midlands in the Heartland of Albion, and in the City of Angels alongside the Peaceful Sea.

He was raised, an only child, on a mixed-arable farm a dozen miles south of Edinburgh. His formal education began with his attending the local village school in Carrington, Midlothian, when he was four. A rigorous introduction to the three Rs—namely, reading, writing and arithmetic—made it relatively easy for him to make the transition to Melville College, a high school in the middle of Edinburgh. He went to Edinburgh University in 1960 and graduated with a B.Sc. in 1964. During his time as a postgraduate student in the Department of Chemistry he cut his teeth in research investigating the nature of plant gums of the Acacia genus within the School of Carbohydrate Chemistry under Professor Sir Edmund Hirst.

In March 1967, Stoddart took his leave of the chemistry department at Edinburgh with a Ph.D. to spend the next three years as a National Research Council of Canada Postdoctoral Fellow at Queen's University with Professor J. N. Jones. No sooner had he arrived in Kingston, Ontario, than a communication appeared in the Journal of the American Chemical Society by Charles Pedersen (one of three Nobel Laureates in Chemistry in 1987) describing the synthesis of dibenzo[18]crown-6 in excellent yield as a consequence of the templating action of potassium ions. This seminal event marked the beginning of Fraser's fascination with chemistry beyond the molecule, which, combined with his interest in templation, has led to the template-directed synthesis, based on molecular recognition and self-assembly processes, of a wide range of mechanically interlocked molecules (e.g., catenanes and

rotaxanes), variants of which have found their way into molecular electronic devices, drug delivery systems, and molecular machines. Mechanically interlocked molecules – or MIMs for short – are discussed at length in "The Nature of the Mechanical Bond: From Molecules to Machines" written in conjuction with ex-graduate student, Carson Bruns, and published by Wiley in November 2016.

Fraser met Edinburgh graduate Norma Scholan (B.Sc. chemist/ Ph.D. biochemist) in 1966 while he was a postgraduate student in the Chemistry Department at Edinburgh and they started their married lives in Canada in 1968. In 1970, they returned to the United Kingdom so that Fraser could take up an Imperial Chemical Industries (ICI) Fellowship at Sheffield University where he worked briefly with Professor W. D. Ollis before being appointed as a Lecturer in Chemistry. After spending a three-year sabbatical (1978–1981) at the ICI Corporate Laboratory in Runcorn, he returned to Sheffield where he was promoted to a Readership in Chemistry. It was during his time at ICI that Stoddart developed his long-standing interest in bipyridinium units (constituents of the ICI herbicides Diquat and Paraquat) as redox-addressable building blocks for incorporation into bistable catenanes and rotaxanes. On 23 May 2013, Fraser published his 1,000th scientific paper; the total count has now reached 1,111. He has trained more than 400 graduate and postdoctoral students of which more than 90 have subsequently embarked on successful independent academic careers.

In 1990, he took up the chair of organic chemistry at Birmingham University where he was head of the School of Chemistry (1993–1997) before moving to the University of California, Los Angeles, as the Saul Winstein Professor of Chemistry in 1997. In 2002, Fraser became the Director of the California NanoSystems Institute and assumed the Fred Kavli Chair of NanoSystems Sciences. He joined the faculty at Northwestern University in 2008 as a Board of Trustees Professor of Chemistry and director of the Center for the Chemistry of Integrated Systems (CCIS).

Stoddart was appointed by Her Majesty Queen Elizabeth II as a Knight Bachelor in her 2007 New Year's Honours List for services to chemistry and molecular nanotechnology. In this same year, he won the King Faisal International Prize in Science. In 2010, he was the recipient of a Royal Medal, granted by Her Majesty Queen Elizabeth II and presented by Prince Philip, Duke of Edinburgh. He was awarded the Nobel Prize in Chemistry in 2016 for his design and synthesis of molecular machines.

NOBEL LAUREATE SPEAKER

ROBERT HOWARD GRUBBS

2005 NOBEL LAUREATE IN CHEMISTRY

Victor and Elizabeth Atkins Professor of Chemistry
Division of Chemistry and Chemical Engineering
California Institute of Technology, USA

BIOGRAPHY

Dr. Robert H. Grubbs is the Victor and Elizabeth Arkins Professor of Chemistry at the California Institute of Technology (Caltech) in Pasadena, Calif. (USA,) where he has been a faculty member since 1978. He earned a B.S. in chemistry in 1963 and an M.S. in chemistry in 1965 under Merle Battiste at the University of Florida. He earned a Ph.D. in chemistry under Ronald Breslow at Columbia University (USA) in 1968. He was an NIH Postdoctoral Fellow working with James P. Collman at Stanford University from 1968 to 1969.

He was previously at Michigan Stare University from 1969 to 1978, achieving the rank of associate professor.

The Grubbs group discovers new catalysts and studies their fundamental chemistry and applications. Catalysts facilitate the transformation of organic molecules and are used widely in industry and academia for the preparation of important organic compounds and polymers. A family of catalysts for the interconversion of olefins, the olefin metathesis reaction has been discovered in the Grubbs laboratory. In addition to their broad usage in academic research, these catalysts are now used commercially to prepare new pharmaceuticals, composites for structural applications and for the conversion of biorenewable carbon sources into fuels and commodity chemicals. Catalysts for other useful transformations are also being developed and studied in detail.

His more recent awards have included the Nobel Prize in Chemistry (2005); Benjamin Franklin Medal in Chemistry (2000); Pauling Award Medal (2003); Havinga Medal (2006) from Leiden University; Golden Plate Award (2006) from the Academy of Achievement); eight ACS Awards, including Polymer Chemistry (1995), Arthur C. Cope Award

(2002), Award for Creative Invention (2009), ACS Roger Adams Award in Organic Chemistry (2011) and the Giulio Natta Award for Chemistry (2014). He was elected to the U.S. National Academy of Sciences (1989) and the U.S. National Academy of Engineering (2015); Fellow of the American Academy of Arts and Sciences (1994); Honorary Fellowship of the Royal Society of Chemistry (2006); and Fellow of the American Chemical Society (2009) and ACS Polymer Division Fellow (2010). He has received the Gold Medal of the American Institute of Chemists, Chemical Heritage Foundation (2010); National Academy of Inventors Fellows Medallion (2014); and the George A. Olah Award in Hydrocarbon or Petroleum Chemistry (2017). He has been awarded many honorary degrees, the most recent being an Honorary Degree of D.Sc. from University of Warwick, Coventry (2010); Honors Causa Doctrorate, Univerdidad de Huelva, Spain (2012); Commencement Speaker at KAUST, Jeddah, Saudi Arabia (2012); RWTH Aachen University Honorary Doctorate (Dr.rer.nat.h.c.) (2013); and Doctor of Science, honoris causa, from The Hong Kong Baptist University (2015). He has more than 620 publications and more than 150 patents based on his research.

INVITED SPEAKER

JOHN M. VOHS

CARL V. S. PATTERSON PROFESSOR
OF CHEMICAL ENGINEERING

Chair of the Department of Chemical and Biomolecular Engineering
University of Pennsylvania, USA

ABSTRACT

Advances in Ceramic Membrane Reactors: From Fuel Cells to Syngas Production

Reactors that use ceramic membranes that are either ionic or mixed ionic and electronic conductors are receiving increased attention due to the fact that such systems have the potential to have higher overall efficiencies and higher reaction selectivities than more conventional designs.

Solid oxide fuel cells (SOFC) which make use of a ceramic membrane that is an oxygen ion conductor are a good example of this technology. These systems exhibit high efficiency for electrical power generation and, at least in theory, are much more fuel flexible than other fuel cell designs. In this talk I will give an overview of our research program on the development of this type of reactor with an emphasis on the novel methods we have developed to control the structure and composition of the surfaces of the membranes. Much of the talk will focus on the use of infiltration techniques to synthesize high performance SOFC anodes that are fuel flexible allowing both hydrogen and hydrocarbons to be used to power the fuel cell. Our approach involves impregnating a porous matrix composed of the yttria-stabilized zirconia electrolyte with materials that have been optimized for both their catalytic and electronic properties. The influence of the microstructure of the electrode on catalytic performance and the development of thermally stable cathodes for SOFC and the use of mixed ionic and electronic conducting membranes for steam reforming of methane to produce hydrogen will also be discussed.

BIOGRAPHY

Professor John M. Vohs holds a Bachelor of Science from the University of Illinois and a Ph.D. from the University of Delaware, both in chemical engineering.

He joined the faculty at the University of Pennsylvania in 1989 where he is currently the Carl V.S. Patterson Professor of Chemical Engineering and chair of the Department of Chemical and Biomolecular Engineering. His research interests are in the areas of surface science, catalysis, membrane reactors, and solid-state electrochemistry, and his group specializes in elucidating structure-activity relationships for a variety of catalytic materials, including metals and metal oxides, and the development of anodes and cathodes for solid oxide fuel cells and electrolyzers. Current research projects in his group focus on supported metals catalysis, understanding the catalytic pathways for the reforming of bio-derived molecules, such as ethanol and glucose, to produce hydrogen and fuels, and using electrochemical techniques to characterize fuel cell and other catalysts. Professor Vohs has been author of 300 publications that have appeared in scientific journals and holds seven U.S. patents.

INVITED SPEAKER

MAURICE BROOKHART
PROFESSOR

University of Houston, USA
Adjunct Professor
University of North Carolina, Chapel Hill, USA

ABSTRACT

Pd(II) and Ni(II) Catalysts for Copolymerization of Ethylene and Polar Vinyl Monomers

Efficient transition metal-catalyzed copolymerization of ethylene with polar vinyl monomers represents a major challenge in the field of polymer chemistry. Numerous academic and industrial groups have sought solutions to this problem using late metal catalysts known to be more functional group tolerant than highly electrophilic early metal catalysts.

However, despite years of effort, little progress has been made in developing highly active, productive systems. This talk will focus on describing the barriers to such copolymerizations as well as reporting the successful development of Pd(II) and Ni(II) systems for copolymerization of ethylene with vinyltrialkoxysilanes. These copolymers(made by alternative routes) are crosslinkable and used to produce PEX-b, a material used for piping and wire coatings. Detailed mechanistic studies will be highlighted in this presentation.

BIOGRAPHY

Maurice Brookhart was born in 1942 and grew up in the Appalachian Mountains of Western Maryland.

He received his B.A. in 1964 from Johns Hopkins University and his Ph.D. in organic chemistry from the University of California, Los Angeles, in 1968. Following a NATO postdoctoral appointment at the University of Southampton, he joined the chemistry faculty of the University of North Carolina. After retiring from UNC in 2014 he joined the chemistry department at the University of Houston in 2015. Throughout his career, Brookhart's research efforts have focused primarily on fundamental investigations of the mechanisms of reactions of organometallic complexes. Recent work has involved invention of new late transition metal catalysts for polymerization of olefins to produce unique polymers and development of metal catalysts to activate carbon-hydrogen bonds as a means of modifying simple hydrocarbons derived from natural gas and petroleum to produce value-added materials.

INVITED SPEAKER

STRATOS PISTIKOPOULOS

TEES DISTINGUISHED RESEARCH PROFESSOR

Interim Co-director, Texas A&M Energy Institute
Editor-in-chief
Artie McFerrin Department of Chemical Engineering
Texas A&M University, USA

ABSTRACT

Multi-parametric Optimization and Control

Model based multi-parametric optimization provides a complete map of solutions of an optimization problem as a function of, unknown but bounded, parameters in the model, in a computationally efficient manner, without exhaustively enumerating the entire parameter space.

In a model-based predictive control (MPC) framework, multi-parametric optimization can be used to obtain the governing control laws – the optimal control variables as an explicit function of the state variables. The main advantage of this approach is that it reduces repetitive on-line control and optimization to simple function evaluations, which can be implemented on simple computational hardware, such as a microchip, thereby opening avenues for many applications in chemical, energy, automotive, and biomedical equipment, devices and systems. In this presentation, we will first provide a historical progress report of the key developments in multi-parametric optimization and control. We will then describe PAROC, a systematic framework and prototype software system which allows for the representation, modelling and solution of integrated design, operation and advanced control problems. Its main features include: 1) a high-fidelity dynamic model representation, also involving global sensitivity analysis, parameter estimation and mixed integer dynamic optimization capabilities; 2) a suite/toolbox of model approximation methods; 4) a host of multi-parametric programming solvers (POP –parametric Optimization] for mixed continuous/integer problems; 4) a state-space modelling representation capability for scheduling and control problems; and 5) an advanced control toolkit for multi-parametric/explicit MPC and moving horizon reactive scheduling problems. Algorithms that enable the integration capabilities of the systems for design, scheduling and control are presented along with applications in sustainable energy systems, process intensification, smart manufacturing and personalized healthcare engineering.

BIOGRAPHY

Professor Stratos Pistikopoulos is a TEES Distinguished Research Professor in the Artie McFerrin Department of Chemical Engineering at Texas A&M University.

He was a professor of chemical engineering at Imperial College London (1991-2015) and the director of its Centre for Process Systems Engineering (2002-2009). At Texas A&M, he is the interim co-director and deputy director of the Texas A&M Energy Institute, the course director of the Master of Science in Energy, the director of the Gulf Coast Regional Manufacturing Centre, and the Texas A&M principal investigator of the RAPID Manufacturing USA Institute on process intensification, co-leading the Modeling and Simulation Focus Area. He holds a Ph.D. from Carnegie Mellon University and worked with Shell Chemicals in Amsterdam before joining Imperial College London. He has been author or co-author of more than 400 major research publications in the areas of modeling, control and optimization of process, energy and systems engineering applications, as well as 10 books and twp patents. He is a co-founder of Process Systems Enterprise (PSE) Ltd, a Fellow of AIChE and IChemE, and the current editor-in-chief of Computers and Chemical Engineering. He is the current chair of the Computing and Systems Technology (CAST) Division of AIChE and he serves as a trustee of the Computer Aids for Chemical Engineering (CACHE) Organization. In 2007, Professor Pistikopoulos was a co-recipient of the prestigious MacRobert Award from the Royal Academy of Engineering. In 2012, he received the Computing in Chemical Engineering Award of CAST/AIChE. He received the title of Doctor Honoris Causa in 2014 from the University Politehnica of Bucharest and from the University of Pannonia in 2015. In 2013, he was elected Fellow of the Royal Academy of Engineering in the UK.

INVITED SPEAKER

TOBIN JAY MARKS

VLADIMIR N. IPATIEFF PROFESSOR
OF CATALYTIC CHEMISTRY

Professor of Materials Science and Engineering
Professor of Applied Physics
Professor of Chemical and Biological Engineering
Department of Chemistry
Northwestern University, USA

ABSTRACT

Surface Science Meets Homogeneous Catalysis

When chemisorbed upon certain surfaces, the reactivity of many types of organometallic molecules is dramatically enhanced in ways that historically have been poorly understood.

High activities for a variety of catalytic reactions are illustrative consequences of this altered reactivity. This lecture focuses on the intricate non-covalent and covalent multi-center interactions that modulate these catalytic processes, focusing primarily on polymerization and hydrogenation/dehydrogenation processes. Specific interrelated topics include:

- Catalytic chemistry of mononuclear and multinuclear d0 catalysts anchored on/activated by surfaces versus those in homogeneous solution
- Catalytic chemistry and cooperativity effects in multinuclear groups 4 and 6 catalysts in homogeneous solution
- Definitive structural characterization of these catalysts on “super-acidic” oxide surfaces and the broad scope of their catalytic properties
- Unusual catalytic chemistry of group 6 dioxo complexes adsorbed on activated carbon surfaces. It will be seen that the information obtained from these studies leads to design rules for next-generation homogeneous and supported catalysts, and for novel and useful polymerization and hydrogenation/dehydrogenation processes, such as the catalytic detoxification of gasoline, stereoselective aromatics hydrogenation, biofeedstock transesterification, and bio-alcohol dehydrogenation.

BIOGRAPHY

Professor Tobin Marks is the Vladimir Ipatieff Professor of Catalytic Chemistry, professor of materials science and engineering, professor of chemical and biological engineering, and professor of applied physics at Northwestern University.

His recognitions include the U.S. National Medal of Science, the Spanish Principe de Asturias Prize, the MRS Von Hippel Award, the Dreyfus Prize in the Chemical Sciences, the National Academy of Sciences Award in Chemical Sciences, and the American Chemical Society Priestley Medal. He is a member of the U.S., German and Indian National Academies of Sciences; the U.S. National Academy of Engineering; the American Academy of Arts and Sciences; and the U.S. National Academy of Inventors. He is a Fellow of the Royal Society of Chemistry. Marks has published 1,250 peer-reviewed articles and holds 265 U.S. patents. He received a B.S. from the University of Maryland and a Ph.D. from MIT.

INVITED SPEAKER

PAUL ANASTAS

DIRECTOR, CENTER FOR GREEN CHEMISTRY AND GREEN ENGINEERING

Teresa and H. John Heinz III
Professor in the Practice of Chemistry for the Environment
School of Forestry and Environmental Studies
Professor
Department of Chemistry
Yale University, USA

ABSTRACT

Molecular and Synthetic Design for Us and Our Posterity

The research at the Center for Green Chemistry and Green Engineering at Yale includes methods to design molecules that are inherently less hazardous and toxic through the use of computational models; the discovery of new molecules and methods that can use renewable biomass as a feedstock; and methods of enabling renewable energy with Earth-abundant catalysts.

While these technologies that will be reviewed are important steps toward making our chemistry more sustainable, this talk will focus on the types of transformations that need to take place on the civilization-wide level. There are trends emerging in the early 21st century that will inform and largely influence whether or not we as a society move closer to a sustainable world. These megatrends and the role that green chemistry and green engineering must play in forming this future will be presented.

BIOGRAPHY

Paul T. Anastas holds the Teresa and H. John Heinz III chair in Chemistry for the Environment at Yale University. He has appointments in the School of Forestry and Environmental Studies, Department of Chemistry, and Department of Chemical and Environmental Engineering. In addition, Professor Anastas serves as the director of the Center for Green Chemistry and Green Engineering at Yale, and director of the Sustainability Curriculum, MBA for Executives Program at Yale School of Management. He is widely known as the "Father of Green Chemistry" and is credited with establishing the field of green chemistry in 1991 during his time working for the U.S. Environmental Protection Agency where he served as chief of the Industrial Chemistry Branch.

He has experience in business (co-founded three companies), the not-for-profit sector (co-founded the Green Chemistry Institute) and government, having served in the administrations of the past four U.S. presidents, including serving in the White House Office of Science and Technology Policy in the Clinton and Bush Administrations, and as assistant administrator of the Office of Research and Development and chief scientist at the U.S. Environmental Protection Agency in the Obama Administration.

Professor Anastas has published 13 books on sustainable technology. He has received numerous awards including the Heinz Award, the Rachel Carson Prize, the E.O. Wilson Prize and the Emanuel Merck Medal.

INVITED SPEAKER

PETER CUMMINGS

JOHN R. HALL PROFESSOR
OF CHEMICAL ENGINEERING

Vanderbilt University in Nashville, USA

ABSTRACT

Molecular Studies of Ionic Liquids at Interfaces with Application to Supercapacitors

In order to be self-sufficient with relatively constant energy output, renewable energy sources, such as solar and wind, require that energy be stored during periods of high energy production so that it can be available during periods of low or zero energy production. Among the many choices for energy storage devices, electrical double layer capacitors (EDLCs), also called supercapacitors, are attracting considerable attention.

Supercapacitors store electrical energy via ion electrosorption directly in the EDLs at the electrolyte-electrode interface, suggesting that such liquid-solid interfaces play a dominant role in the underlying energy storage mechanism and the resulting device performance. Because electrical energy in supercapacitors is stored based on physical phenomena rather than chemical reaction (as in batteries), supercapacitors have fast rates of charge/discharge and a virtually limitless number of charge cycles (unlike batteries, which are often limited to 104 or less cycles). Much of the goal of supercapacitor research is aimed at increasing the amount of energy stored (energy density is the strong point in favor of batteries), which in turn focuses attention on the electrolyte, the nature of the electrode, and the electrode-electrolyte interactions.

To date, ionic liquids (ILs) have become emerging candidates for electrolytes used in supercapacitors, due to their exceptionally wide electrochemical window, excellent thermal stability, nonvolatility, and relatively inert nature; meanwhile carbons are the most widely used electrode materials in supercapacitors, due to their high specific surface area, good electrical conductivity, chemical

stability in a variety of electrolytes, and relatively low cost. To improve the energy density and the transport properties of the charge carriers in supercapacitors, carbons have been developed in diverse forms such as activated carbons, carbon nanotubes (CNTs), onion-like carbons (OLCs), carbode-derived carbons and graphene. Using molecular modeling combined with molecular experimental probes, such as SAXS, SANS, NMR, and AFM, we report on our investigations into the interfacial phenomena occurring between the IL electrolytes and electrodes of varying geometries to understand the energy storage mechanism of supercapacitors that rely on EDLs established at IL-electrode interfaces.

BIOGRAPHY

Peter T. Cummings is the John R. Hall Professor of Chemical Engineering at Vanderbilt University. He also holds the position of associate dean for research in the Vanderbilt University School of Engineering.

For 20 years (1994-2013), he was associated with Oak Ridge National Laboratory (ORNL) at levels of effort ranging from 40 to 50 percent. Most recently (2007-2013), he served as the chief scientist (with title principal scientist) of the ORNL Center for Nanophase Materials Sciences (CNMS). He was previously the founding director of the Nanomaterials Theory Institute, the theory program within the CNMS, and one of the four principal investigators who wrote the proposal to establish the CNMS. His research interests include statistical mechanics, molecular simulation, computational materials science, computational and theoretical nanoscience, and computational biology. He is the author of more than 400 refereed journal publications and the recipient of many awards, including the 1998 Alpha Chi Sigma award given annually to the member of the American Institute of Chemical Engineers (AIChE) with the most outstanding research contributions over the previous decade; the 2007 AIChE Nanoscale Science and Engineering Forum Award; the 2010 AIChE Founders Award for Outstanding Contributions to the Field of Chemical Engineering in recognition of his “outstanding contributions through research, service to the Institute, and national leadership on behalf of the profession”; the 2012 Yeram S. Touloukian Award from the American Society of Mechanical Engineers; and the 2013 John Prausnitz award, the most prestigious research award in chemical engineering thermodynamics presented every three years. He has been elected fellow of the American Physical Society, the American Association for the Advancement of Science and the American Institute of Chemical Engineers.

INVITED SPEAKER

DAVID BERGBREITER

Professor
Texas A&M University, USA

ABSTRACT

Recyclable Polyolefins as Solvents and Tools in More Sustainable Homogeneous Catalysis

Recycling ligands, catalysts, and solvents remains a challenge for homogeneous catalysis. This talk will describe how polyolefins can be used to molecularly engineer more sustainable homogeneous catalysis systems. The studies we will discuss show that terminally functionalized polyisobutylene (PIB) oligomer ligands and catalysts can be readily prepared and that such species have chemistry that is identical to that of conventional ligands and catalysts.

Our studies have also shown that these PIB oligomers are readily recycled and separated as oligomers. However, we also show that if necessary we can some functionalized PIB oligomers to substituted arenes under very mild conditions (i.e., in minutes at 25°C). In a typical of PIB-bound catalysts, these catalysts are dissolved and used in miscible alkane/cosolvent mixtures. After a reaction, a physical or chemical perturbation forms biphasic mixtures where the catalyst and product phases are separated by density. This chemistry typically uses heptane as an alkane solvent. However, we have also shown that heptane can be replaced by more sustainable poly([]-olefin) (PAO)g solvents. Those studies show that nonvolatile and nontoxic PAOs are more recyclable and sustainable than heptane and that PAOs are more efficient in recovering PIB-bound catalysts or catalyst surrogates. Ongoing studies also suggest that alkane-solubilized polymers can even serve as alternative recyclable cosolvents, partly or fully replacing conventional solvents used in these solvent mixtures leading to even more sustainable solvent systems for catalysis chemistry.

BIOGRAPHY

Professor David Bergbreiter has published more than 260 papers and made more than 640 presentations in his independent career. These research accomplishments are the product of his collaborations with more than 150 undergraduate, graduate and postdoctoral students.

The results he has reported have included seminal contributions to understanding regio- and stereoselectivity in azaallyl anion formation, the invention of new synthetic methodology, the development of new methods and strategies for syntheses of functional surfaces, and work that elucidated the basis of and that later used the Hofmeister effect in studies of polymeric materials that exhibit stimuli-responsive solubility. His group has been especially successful and are leaders in studies of phase separable catalysts that control reaction rates (e.g., "smart" catalysts) or that facilitate the reuse and/or separation of homogeneous catalysts from products. This work has emphasized pioneering studies that have explored new ways to use soluble polymers to recover and reuse homogeneous catalysts. This included the first description of thermomorphic liquid/liquid solvent systems for catalyst systems and ongoing work that is elucidating the principles that make such systems efficient and workable. His varied contributions in research have been recognized with a local university-level research award in 2008, receipt of the 2008 ACS Southwest Regional award, recognition as a fellow of the AAAS in 2006, and recognition as an ACS Fellow in 2011.

He has taught more than 30 different courses in his career at Texas A&M University, including freshman, sophomore, senior and graduate lecture classes, laboratory courses at all levels, as well as seminar-style classes for entering undergraduates, freshmen students, honors students, chemistry majors and graduate students. He also has extensively mentored undergraduates in research, with 25 of these 60 students being coauthors on peer-reviewed publications or patents. He has also been recognized with every award for teaching at Texas A&M given by faculty/student committees.

His involvement in research and education has been matched by service to both ACS and to the profession of chemistry more broadly. Within ACS, he has served locally as chair of the local section and he has been the local section councilor for nearly 20 years. He has served on several ACS committees, including the Minority Affairs Committee. He is currently a member of the Joint Board Council Committee on Publications. He served as secretary general of the Catalysis and Surface and Science Secretariat in 2000. He has organized or participated in symposia in more than 100 ACS national, regional or divisional meetings.

ABOUT QAFCO

QAFCO was founded in 1969 as a joint venture between the government of Qatar and a number of foreign shareholders. The country's first large-scale venture in the petrochemical sector, QAFCO was established with a view to diversify the economy and utilize the nation's enormous gas reserve. After successfully implementing several expansion projects over the past three decades, the Company has evolved into a world-class fertiliser producer. QAFCO is now owned 75 percent by Industries Qatar (IQ) and 25 percent by Yara Nederland. QAFCO has two subsidiaries, Gulf Formaldehyde Company (70 percent) and Qatar Melamine Company (60 percent).

With a sizable annual production capacity of 3.8 million MT of ammonia and 5.6 million MT of urea from, QAFCO is now the world's largest single-site producer of ammonia and urea. This enabled Qatar to be a key player in the global fertilizer market and the largest exporter of urea in the world with about 15 percent share of the world urea supply.

OUR DOWNSTREAM OPERATIONS

Gulf Formaldehyde Company

The Gulf Formaldehyde Company (GFC) was created in 2003 and began operations in 2004. The GFC plants A&B are designed to produce 82 tons per day of Urea Formaldehyde (UFC-85), a viscous liquid with 60 percent formaldehyde, 25 percent urea and 15 percent of water. Eighty percent of the UFC-85 produced is consumed by QAFCO and is used as an anti-caking agent in the production of urea.

Qatar Melamine Company

QAFCO has utilized its expertise in fertilizer plant operations to operate and manage a production plant of premium grade Melamine. The plant has design capacity to produce 60,000MT of Melamine annually. This is one of the largest plants in the region.