QAFCO
TEXAS A&M *at* QATAR
CONFERENCE 2016

CO_2 MANAGEMENT AND RENEWABLE ENERGY

THURSDAY,
14 JANUARY 2016
HAMAD BIN KHALIFA UNIVERSITY
STUDENT CENTER
EDUCATION CITY, DOHA, QATAR

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QAFCO
شركة قطر للأسمدة الكيماوية
QATAR FERTILISER COMPANY

TEXAS A&M
UNIVERSITY *at* QATAR

WELCOME LETTER FROM INTERIM DEAN

On behalf of Texas A&M University at Qatar, it is my pleasure to welcome you to the Qatar Fertilizer Company – Texas A&M at Qatar Conference 2016.

This annual event is hosted by Texas A&M at Qatar and presented in collaboration with QAFCO. QAFCO has been a steadfast and dynamic partner to Texas A&M at Qatar through the years, and I thank QAFCO for its unwavering belief in the strength of our academic and research programs, our faculty, and our current and former students.

This important conference highlights the pressing need for industry and academia to work together to develop new knowledge and create scientific solutions that have direct impact on the world around us.

This year, we focus on managing CO_2 and renewable energies. Developing technology, industry and commercial applications have led to an increase in overall energy consumption, which has given rise to two important problems: energy resources and environmental pollution.

On one hand, fossil fuels such as oil, gas and carbon are diminishing, and research in renewable energy is more important than ever. Many solutions have been proposed and applied through the years, among which solar and wind power are the most promising and applicable. But such energy sources cannot continuously provide energy and instead are limited by daylight hours or windy conditions. At the same time, pollution caused by the use of fossil fuels — mainly due to the high emission of greenhouse gases, such as CO_2 — results in a series of problems such as global warming and poor air quality.

It is imperative to find new ways of managing CO_2 to make emissions friendlier to the environment and our health. The keynote lecture and all invited talks will provide different aspects of this theme, from fundamental, experimental and computational studies all the way to new process development with immediate industrial applications.

I thank our speakers for sharing their expertise with the professionals participating in this influential gathering of industry practitioners and scholars. Best wishes for a productive conference and thank you to QAFCO for their support and partnership in this meeting of international experts.

Best regards,
Dr. Ann Kenimer
Interim Dean and COO
Texas A&M University at Qatar

WELCOME FROM THE ORGANIZING COMMITTEE

On behalf of the Science Program and the Chemical Engineering Program at Texas A&M University at Qatar, we are pleased to welcome you to the annual QAFCO – Texas A&M at Qatar Conference 2016.

We are very proud of our partnership with QAFCO, which has generously supported us since 2007 in hosting the first conference series in Qatar. This series has attracted an impressive list of world-renowned scientists through the years, including 80 invited speakers from 18 countries. In addition, the list of speakers in previous years has included two Nobel laureates, Dr. Robert H. Grubbs and Dr. Ei-Chi Negishi.

The theme for this year's edition is CO_2 Management and Renewable Energy. We are glad to have Prof. Michael Graetzel, director of the Laboratory of Photonics and Interfaces in the Institute of Chemical Science and Engineering at the Ecole Polytechique Féderale de Lausanne (Switzerland), as keynote speaker of the 2016 edition of the conference. In addition, we have 14 distinguished invited speakers from the United States, Europe, Asia and Middle East.

We hope this conference will be an outlet for the exchange of scientific knowledge, sharing ideas, discussing future collaborations and building new projects. Your presence at this conference reaffirms our pursuits of cutting-edge chemistry and chemical engineering research in Qatar and the region. We wish you a very productive time at this event.

Best regards,
Hassan S. Bazzi
Co-chair, QAFCO – Texas A&M at Qatar Conference 2016
Assistant Dean for Research and Graduate Studies

Ioannis Economou
Co-chair, QAFCO – Texas A&M at Qatar Conference 2016
Professor, Chemical Engineering Program

Konstantinos E Kakosimos
Co-chair, QAFCO – Texas A&M at Qatar Conference 2016
Assistant Professor, Chemical Engineering Program

CO_2 MANAGEMENT AND RENEWABLE ENERGY

THURSDAY, 14 JANUARY 2016
HAMAD BIN KHALIFA UNIVERSITY STUDENT CENTER
EDUCATION CITY, DOHA, QATAR

8-8:45 a.m.	Registration and Light Breakfast
8:50-8:55 a.m.	**Dr. Hassan S. Bazzi,** **Assistant Dean for Research,** Texas A&M University at Qatar
8:55-9 a.m.	**Dr. Ann Kenimer,** **Interim Dean,** Texas A&M University at Qatar
9-9:05 a.m.	**Mr. Khalifa Al-Sowaidi,** **Vice Chairman and CEO,** Qatar Fertiliser Company (QAFCO)
9:05-10:10 a.m.	Keynote Lecture (Ballroom 1), Chair: Dr. Konstantinos E. Kakosimos) **Dr. Michael Graetzel,** Ecole Polytechique Féderale de Lausanne, Switzerland "Mesoscopic Photosystems for the Generation of Electricity and Fuels from Sunlight"

10:10-10:30 a.m.	Coffee Break	
Session I	Chemistry	Chemical Engineering
	Chair: Dr. Ashfaq Bengali (Ballroom 1)	Chair: Dr. Patrick Linke (Ballroom 3)
10:30-11 a.m.	**Dr. Filippo De Angelis** Institute of Molecular Science and Technologies, Italy "Modeling Dye-sensitized and Perovskite Solar Cells from First Principles"	**Dr. Nazim Muradov** University of Central Florida, USA "Low-to-zero CO_2 Production of Hydrogen from Fossil Fuels: Status and Perspectives"
11-11:30 a.m.	**Dr. Nikos Hadjichristidis** King Abdullah University of Science and Technology, Saudi Arabia "Novel Strategies Toward Well-defined Polyethylenes"	**Dr. Perla B. Balbuena** Texas A&M University, USA "First-principles Analysis and Design of New Catalysts for CO_2-assisted Natural Gas Reforming"
11:30 a.m.-noon	**Dr. Stenbjörn Styring** Uppsala University, Sweden "Fuels from Solar Energy and Water: From Natural to Artificial Photosynthesis"	**Dr. Claire S. Adjiman** Imperial College London, UK "The Molecular Systems Engineering of Carbon Capture Processes"

Noon-1:30 p.m.	Lunch (Ballroom 2)	
Session II	Chair: Dr. Sherzod Madrahimov (Ballroom 1)	Chair: Dr. Ioannis Economou (Ballroom 3)
	Chemistry	Chemical Engineering
1:30-2 p.m.	**Dr. Suresh Valiyaveettil** National University of Singapore, Singapore "Synthesis and Characterization of Polyamines and Hybrid Materials"	**Dr. Berend Smit** Ecole Polytechnique Fédérale de Lausanne, Switzerland "The Materials Genome in Action"
2-2:30 p.m.	**Dr. Mahdi M. Abu-Omar** Purdue University, USA "New Mechanistic Paradigm and Cooperative Metal Catalysis for CO_2 Conversion to Fuels"	**Dr. Brian Norton** Dublin Institute of Technology, Ireland "Multifunctional Solar Energy Harnessing Systems for Building Facades"

2:30-3 p.m.	Coffee Break	
Session III	Chair: Dr. Ed. Brothers (Ballroom 1)	Chair: Dr. Marcelo Castier (Ballroom 3)
	Chemistry	Chemical Engineering
3-3:30 p.m.	**Dr. Anders Hagfeldt** Ecole Polytechnique Fédérale de Lausanne, Switzerland "The Versatility of Mesoscopic Solar Cells"	**Dr. Ioannis Kevrekidis** Princeton University, USA "No Equations, No Variables: Data and the Computational Modeling of Complex Systems"
3:30-4 p.m.	**Dr. Said Ahzi** Qatar Energy and Environment Institute, Qatar "Modeling of the Thermomechanical Behavior of PV Panels Under Service Conditions"	**Dr. Nimir O. Elbashir** Texas A&M University at Qatar, Qatar "Gas Processing Research at Texas A&M University at Qatar"

KEYNOTE LECTURE

Dr. Michael Graetzel

Ecole Polytechique Féderale de Lausanne, Switzerland

"Mesoscopic Photosystems for the Generation of Electricity and Fuels from Sunlight"

Abstract

Mesoscopic photovoltaics have emerged as credible contenders to conventional p-n junction photovoltaics. Separating light absorption from charge carrier transport, dye-sensitized solar cells (DSCs) were the first to use three-dimensional nanocrystalline junctions for solar electricity production, reaching currently a power conversion efficiency (PCE) of more than 14 percent in standard air mass 1.5 sunlight. Large-scale production and commercial sales have been launched on the multi-megawatt scale. DSCs have also engendered the meteoric rise of perovskite solar cells (PSCs) whose power conversion efficiency now attain 20.8 percent.

Methylammonium leadiodide ($CH_3NH_3PbI_3$) and related pigments have emerged as powerful light harvesters. Carrier diffusion lengths in the 100 nm to micron range have been measured for solution-processed perovskites. These photovoltaics show intense electroluminesence approaching the external quantum efficiency of silicon solar cells. As a consequence, very high Voc values close to 1.2 V for 1.55 eV band gap materials have been obtained under standard reporting conditions.

These high Voc values render perovskite-based mesoscopic photosystem very attractive for use in tandem cells and for generation of fuels from sunlight.

Biography

Dr. Michael Graetzel is a professor at the Ecole Polytechnique Féderale de Lausanne where he directs the Laboratory of Photonics and Interfaces. He pioneered the use of mesoscopic materials in energy conversion systems — in particular photovoltaic cells, lithium ion batteries and photo-electrochemical devices for the splitting of water into hydrogen and oxygen by sunlight.

He discovered a new type of solar cell based on dye-sensitized nanocrystalline oxide films. Mass production started in October 2009. He is author of more than 1,000 publications and two books, and inventor of more than 50 patents, and his work has been cited more than 148,000 times (h-index 176), making him one of the 10 most highly cited chemists in the world.

He has received prestigious awards, including the 2014 Samson Prime Minister Prize, the Balzan Prize, the Galvani Medal, the Faraday Medal, the Harvey Prize, the Gerischer Award, the Dutch Havinga Award and Medal, the International Prize of the Japanese Society of Coordination Chemistry, the ENI-Italgas Energy-Prize and the Year 2000 European Grand Prix of Innovation. His most recent awards include the 2012 Albert Einstein World Award of Science, 2011 Gutenberg Research Award, 2011 Paul Karrer Gold Medal and the 2010 Millennium Technology Grand Prize. He was selected by Scientific American as one of the 50 top researchers in the world. Graetzel received a doctor's degree in natural science from the Technical University Berlin and honorary doctoral degrees from 11 universities. He has been the Mary Upton Visiting Professor at Cornell University and a Distinguished Visiting Professor at the National University of Singapore. He was an invited professor at the University of California, Berkeley, the Ecole Nationale de Chachan (Paris) and Delft University of Technology.

In 2009 he was named Distinguished Honorary Professor by the Chinese Academy of Science (Changchun) and the Huazhong University of Science and Technology. He is a member of the Swiss Chemical Society and the European Academy of Science, a Fellow of the Royal Society of Chemistry, and an elected honorary member of the Société Vaudoise des Sciences Naturelles and the Bulgarian Academy of Science.

CHEMISTRY SESSION

Dr. Filippo De Angelis

Institute of Molecular Science and Technologies, Italy

"Modeling Dye-sensitized and Perovskite Solar Cells from First Principles"

Abstract

Organohalide lead-perovskites have revolutionized the hybrid/organic photovoltaics landscape.
Despite the fast efficiency increase, some of the materials properties related to their extraordinary photovoltaic performance remain largely not understood. Further advances in the perovskite solar cells (PSCs) field may be boosted by computational design and screening of new materials, with researchers examining material characteristics that can improve device performance and/or stability. Suitable modeling strategies may allow researchers to observe the otherwise inaccessible but crucial hetero-interfaces that control the operation of PSCs, allowing researchers the opportunity to develop new and more efficient materials and optimize processes. We illustrate here the performance of an integrated simulation toolbox, rooted into density functional theory and many body GW methods including spin-orbit coupling, that can provide atomistic electronic structure information on the materials properties and on the crucial perovskite absorbers/metal-oxide/hole transporter material heterointerfaces. We critically assess the accuracy of various computational approaches against the related experimental data and analyze the representative interfaces that control the device operational mechanism.
In particular, we describe the structural and electronic features of the methylammonium lead iodide perovskite with various metal oxide substrates (i.e., TiO_2, Al_2O_3 and ZnO) with emphasis on the influence of the substrate in determining the perovskite growth, the preference for specific surfaces and the underlying electronic interfacial properties.Defect migration and the influence of water in $MAPbI_3$ degradation mechanism are also discussed.

Biography

Dr. Filippo De Angelis is the founder and leader of the Computational Laboratory for Hybrid/Organic Photovoltaics, www.clhyo.org, and the deputy director of CNR Molecular Science and Technologies (CNR-ISTM) in Perugia, Italy. He is an expert in the development and application of first-principles computational methods to the simulation of inorganic and hybrid materials and related interfaces.

His main results are in the field of solar energy materials, with focus on dye-sensitized and perovskite solar cells. He holds four patents and has published more than 240 papers, with an h-index of 53, and five book chapters. He is member of the editorial advisory board of the Journal of Physical Chemistry and CNR delegate at CECAM. He is the 2007 recipient of the Nasini Gold Medal of the Italian Chemical Society.

Dr. Nikos Hadjichristidis

King Abdullah University of Science and Technology, Saudi Arabia

"Novel Strategies Toward Well-defined Polyethylenes"

Abstract

Access to well-defined (high degree of structural, molecular weight and compositional homogeneity) polyethylenes (PEs) and PE-based copolymers is necessary in order to elucidate the structure-properties relationships and evaluate potential applications. Polyhomologation, first discovered by Shea, is a borane-initiated living polymerization of ylides leading to well-defined polymethylenes (C1 polymerization). Our group is developing both novel borane initiators and ylide monomers and combines polyhomologation with other living polymerizations to synthesize model polymethylene (or PE)-based polymeric materials.

Biography

The research of Dr. Nikos Hadjichristidis focuses mainly on the synthesis of novel homopolymers, copolymers and hybrids (polymers/polypeptides, polymers/CNT) with well-defined complex macromolecular architectures (star, comb, cyclic, dendritic, etc.) by using anionic polymerization (AP) high-vacuum techniques, as well as combinations of AP with other polymerization methodologies (AP, ATRP, TEMPO, catalytic, etc). These polymers are ideal models for checking the theory, understanding and improving the performance of industrial polymers (e.g., polyethylene, polystyrene based thermoplastic elastomers) and are potential candidates for high-tech applications (e.g., nanolithography, drug delivery, high-temperature membranes). Hadjichristidis has published more than 450 scientific papers in referred scientific journals (citations until 30 Sept. 2015: 16994, h-index: 67, Web of Science; 20150, 68, Google Scholar), 19 patents, is the editor of three books and author of one book, Block Copolymers (Wiley 2003).

Dr. Mahdi M. Abu-Omar

Purdue University, USA

"New Mechanistic Paradigm and Cooperative Metal Catalysis for CO_2 Conversion to Fuels"

Abstract

Conversion of renewable feedstock to fuels and chemicals has received extensive attention as society shifts towards sustainable technologies. Carbon dioxide is an attractive synthon especially if it can be converted directly to methanol or dimethyl ether (DME). A new approach to upgrading CO_2 directly to DME via transition metal and ligand cooperation will be described through the use of metal oxo bifunctional organometallic catalysts. Simultaneous activation of dihydrogen on the metal and CO_2 by ligand allows for accelerated and selective addition. Through a combination of discovery research and mechanistic insights (spectroscopic characterization of intermediates, kinetics, and DFT computations), advances in catalyst design can be realized.

Biography

Dr. Abu-Omar earned his Ph.D. from Iowa State University and completed a postdoc at Caltech. He is the R. B. Wetherill Professor of Chemistry and Professor of Chemical Engineering at Purdue University, the associate director of the Center for Catalytic Conversion of Biomass to Biofuels (C3Bio), an Energy Frontiers Research Center, and the director of the Negishi-Brown Institute for Catalysis (NBIC). Mahdi is the founder and president of Spero Energy Inc., a green specialty chemicals company and a technology provider for the manufacture of high-value renewable chemicals from biomass. He is the author or co-author of more than 130 original research papers in peer-reviewed journals. Abu-Omar is a Fellow of the American Association for Advancement of Science (AAAS) .

Dr. Stenbjörn Styring

Uppsala University, Sweden

"Fuels from Solar Energy and Water:
From Natural to Artificial Photosynthesis"

Abstract

The lecture will discuss the need for Solar Fuels and overview the different scientific paths to achieve this goal. Visions and strategies in research in the Swedish Consortium for Artificial Photosynthesis will be covered. Our research aims for the production of hydrogen from solar energy and water. Water shall be oxidized in a catalytic process using solar energy. The electrons from water shall be used in a second process to reduce protons to hydrogen. In our chemistry we use a photoactive Ru-center (instead of chlorophyll) that is coupled to synthetic water oxidation complexes. The lecture will describe a water oxidizing catalyst based on a cobalt nanoparticle. This nanoparticle has been linked to a photosensitizer to form a water-splitting photosensitizer-catalyst complex. Using MIMS we have recently managed to resolve the detailed catalytic mechanism in this nanoparticle. We also apply a biomimetic approach where we copy key principles from natural enzymes that accomplish partial reactions. To accomplish reduction of protons to hydrogen we mimic the di-iron center in hydrogenase enzymes. Some recent results on these biomimetic Fe-Fe complexes will be described.

Biography

Dr. Stenbjörn Styring works with natural and artificial photosynthesis and has about 250 publications. His research on photosynthesis has a strong biophysical profile dealing with mechanistic issues of the oxygen-evolving enzyme in Photosystem II. His main techniques are EPR and fluorescence spectroscopy. In artificial photosynthesis he focuses on synthesis and EPR spectroscopic studies of manganese, cobalt and ruthenium-manganese compounds intended for photo-catalytic oxidation of water.He has received the Svante Arrhenius medal from the Swedish Chemical Society and the Edlundska prize from the Royal Academy for Science. He was secretary (1988-1991) and president (1997-2000) of the Swedish Biochemical Society. Recently he evaluated strategic renewable energy research for the Helmholtz Association in Germany (2009; research for ca 200 MEuro) and the Irish Strategic Research Cluster for Solar Energy Conversion (SFI funded, ca 4 MEuro). He is a member of the scientific advisory board for Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg, Germany, and for the University Priority Program on Solar Light to Chemical Energy Conversion at University of Zurich. He is reviewer for numerous research councils and scientific journals.

Styring initiated the Swedish Consortium for Artificial Photosynthesis and has been its chairman since its start in 1994. The consortium is a major Swedish research initiative with approximately 50 researchers. He has since 1994 been PI for many large joint grants for the consortium, which has more than 300 joint publications, has supervised more than 40 Ph.D.s and has involved more than 120 researchers through the years.
are potential candidates for high-tech applications (e.g., nanolithography, drug delivery, high-temperature membranes). Hadjichristidis has published more than 450 scientific papers in referred scientific journals (citations until 30 Sept. 2015: 16994, h-index: 67, Web of Science; 20150, 68, Google Scholar), 19 patents, is the editor of three books and author of one book, Block Copolymers (Wiley 2003).

Dr. Suresh Valiyaveettil

National University of Singapore, Singapore

"Synthesis and Characterization of Polyamines and Hybrid Materials"

Abstract

Amine functionalized polymers are ubiquitous in nature, but not widely used in applications owing to increased reactivity, toxicity, sensitivity to air and moisture, low stability and processing difficulties. Recently, we reported a convergent strategy for the synthesis of polyamines and polyamine microparticles. Full structural characterization and properties of the materials are established using different spectroscopic and physicochemical methods. Polyamines gave porous films and spherical particles from chloroform and N,N-dimethylformamide on glass substrates, respectively. The synthesized polyamines and the microparticles were used for the liquid-liquid and solid-liquid extraction for removing dissolved pollutants such as metal nanoparticles, organic dyes and heavy metal ions from water. All materials showed good extraction efficiency towards both nanoparticles and organic dyes and they can be sued as potential adsorbents for water purification.

Recently, we have tried to extend biomimetic pathways for developing functional materials such as organo-inorganic hybrids from nanomaterials and soft polymers. We are also exploring liquid-liquid and solid-liquid interface chemistry to control the structure of polymers. In this approach, polymers are created at the interface of two immiscible liquids and variable such as concentration of monomers and nature of solvents are used to optimize the film properties. In addition, 3-D hybrid materials are synthesized through a selective polymerisation of both organic monomers and inorganic building blocks. Such materials are used for developing potential sensor for amines. Our approach tries to balance the structure-dimensionality-property triads of the materials towards the design of new functional materials. The talk will discuss synthesis, structural characterisation and potential application of the materials.

Biography

Dr. Suresh Valiyaveettil completed his undergraduate and postgraduate education in India and received his Ph.D. in supramolecular chemistry from the University of Victoria, Canada. After working at various universities around the world (including Cornell University, USA; University of Twente, The Netherlands; and the Max-Planck Institute for Polymer Research at Mainz, Germany), he joined the National University of Singapore (NUS) to set up a materials chemistry program. He has published more than 125 high-impact papers in peer-reviewed international journals in organic synthesis, polymer synthesis, nanomaterials, nanotoxicology and biomaterials, and has given more than 45 invited talks in international conferences. He has also organized a series of international symposia on various topics. He is a member of several national and international committees and editorial boards, and offers consulting in the above research areas. His group is exploring multidisciplinary projects in organic/polymer synthesis, biomaterials and nanomaterials/technologies at the Department of Chemistry at NUS.

Dr. Anders Hagfeldt

Ecole Polytechnique Fédérale de Lausanne, Switzerland

"The Versatility of Mesoscopic Solar Cells"

Abstract

In our work on solid-state, dye-sensitized solar cells (ssDSSC) we have recently shown that copper phenanthroline complexes can act as an efficient hole transporting material. We prepared ssDSCs with the organic dye LEG4 and copper(I/II)-phenantroline as redox system and achieved power conversion efficiencies of more than 8 percent, with open-circuit potentials of more than 1.0 V. The phenomenal breakthrough of the so called perovskite solar cells (PSC) originates from the ideas of replacing the dye layer adsorbed on the mesoporous oxide surface with an ultrathin inorganic perovskite layer and replacing the liquid electrolyte with a solid-state hole conductor. At present our best performance is achieved with a mixed composition of iodide/bromide and methyl ammonium/formamidinium. We will report on our work on optimizing the solar cell efficiency that at present shows a top result of 20.8 percent and certified at 19.9 percent. With the use of an ALD deposited SnO_2 compact underlayer we have constructed a planar perovskite solar cell with a hysteresis free efficiency of above 18 percent. Based on this configuration we have in collaboration with the group of Prof. Bernd Rech, Helmholtz Zentrum Berlin, prepared a monolithic Perovskite/Silicon-Heterojunction tandem solar cell with an efficiency above 18 percent, pointing out a promising direction for further improvement of tandem cells using PSCs as one of the constituents. Another possibility for a tandem system has been investigated in collaboration with Prof. Segawa and co-workers in which a spectral split-cell, using a combination of a DSSC cell (with a wideband dye DX3) and a perovskite cell, demonstrated an efficiency of 21.5 percent. We have also developed new hole conductor materials that reach efficiencies above 20 percent, similar to the conventional hole conductor spiro-OMeTAD but with the advantage of being more easily synthesized.

Biography

Anders Hagfeldt is professor at Ecole Polytechnique Fédérale de Lausanne (EPFL) in Switzerland, director of the laboratory of photomolecular science and co-founder of the company Dyenamo AB. He obtained his Ph.D. at Uppsala University in 1993 and was a postdoc with Dr. Michael Gratzel at EPFL (1993-1994). He has published more than 280 scientific papers that have received more than 22,000 citations (with an h-index of 72), and has eight patent applications.

He was ranked number 46 of the Top 100 material scientists of the past decade by Times Higher Education in 2011, and in 2012 he was awarded the Nature Award for Mentoring in Science. He is a member of the Royal Society of Sciences in Uppsala and the Royal Swedish Academy of Engineering Sciences in Stockholm. He is a visiting professor at Nanyang Technological University in Singapore and a Distinguished Adjunct Professor at King Abdulaziz University in Saudi Arabia.

Dr. Said Ahzi

Qatar Energy and Environment Institute, Qatar

"Modeling of the Thermomechanical Behavior of PV Panels Under Service Conditions"

Abstract

Solar energy is a very suitable alternate energy source owing to its natural existence and potential to replace the conventional sources. In the state of Qatar, photovoltaic (PV) devices are envisioned to be deployed within the next few years as a solar harvesting technology achieving the GW scale. Our objective is to develop a computational approach for the design and optimization of PV panels for climate conditions of Qatar and the golf region. For this, we propose first to address the thermal behavior and performance of photovoltaic panels under operation in harsh desert conditions using either a 1-D finite difference model or a 2-D finite element simulation. We apply such approaches to compute the through-thickness temperature distribution of a standard solar panel under different configurations of hot temperature service conditions such as in the Gulf region. Such conditions usually impact the electrical efficiency through the well-known thermal effect, among other particular degradation mechanisms. The three sub-models of the proposed multiphysics approach are the solar irradiance modeling which places the PV panel within an environment having direct sunlight, diffuse irradiance from the sky and ground-reflected irradiance (albedo); the thermal modeling, focusing mainly on the through-thickness temperature of the PV panel; and the electrical modeling, assuming a perfect yield of the I–V curves of the PV device. The thermal effects induce varying efficiency (h) during the simulation of relevant service periods. Note that this approach allows us to simulate the performance of PV panels assuming they are at their maximum electrical efficiency, and thus we can quantify the electrical power produced during the simulated service conditions. For these simulations, we use meteorological data from the Gulf region desert climate (Qatar and Saudi Arabia). The results will be presented in terms of temperature evolution of the panel as function of solar irradiance measured over a large period of time. The predicted efficiency results will also be presented as function of the atmospheric conditions. In addition, we will address the effects of degradation mechanisms such as dust-related effects, aging and thermal stresses.

Biography

Dr. Said Ahzi joined QEERI in August 2014. He came from the University of Strasbourg (France) where he held a position as distinguished professor (Exceptional Class 1). Ahzi received his Ph.D. (1987) and Habilitation (1995) degrees in physics and mechanics and of materials, both from the University of Metz, France. In January 2000, he joined the faculty of physics and engineering at the University of Strasbourg. He holds an adjunct professor position with the School of Materials Science and Engineering at the Georgia Institute of Technology in Atlanta (USA). He also was an associate research member with TEMA laboratory at the University of Aveiro, Portugal. From 1995 to 2000, he held the positions of assistant professor then associate professor in the Department of Mechanical Engineering at Clemson University (USA). He spent four years (1991-1995) as a research scientists/lecturer in the Department of Applied Mechanics and Engineering Sciences at the University of California, San Diego, USA. From 1987 to 1991, he was a postdoctoral research associate in the Department of Mechanical Engineering at the Massachusetts Institute of Technology (USA).

CHEMICAL ENGINEERING SESSION

Dr. Nazim Muradov

University of Central Florida, USA

"Low-to-zero CO_2 Production of Hydrogen from Fossil Fuels: Status and Perspectives"

Abstract

Currently, more than 95 percent of all industrial manufacturing of hydrogen is based on fossil fuels, primarily, natural gas and coal. As a consequence, hydrogen production plants are and, most likely, will remain for the foreseeable future among major CO_2 emitters. Even the "cleanest" of H2 production processes, steam methane reforming (SMR), produces in excess of 10 kg of CO_2 per kg of H2 product. This fact greatly diminishes the environmental appeal of hydrogen as environmentally clean fuel. Thus, there is an urgent need to drastically reduce or, preferably, eliminate CO_2 emissions from fossil fuel-based hydrogen production processes. The main technological approaches to the low-to-zero CO_2 production of hydrogen from fossil fuels are:

1. The integration of fossil fuel-based hydrogen production plants (e.g., SMR, plants) with CO_2 capture and storage (CCS),
1. Production of CO_2-free hydrogen via dissociation of methane, and
2. The combination of fossil fuel-based hydrogen production processes with non-carbon energy sources such as nuclear and solar.

In a typical modern SMR plant, CO_2 could be captured from three streams: shifted gas, PSA tail gas and flue gas. Challenges facing the SMR-CCS approach include the high cost of CCS, weak incentives for implementation (uncertain climate regulations, carbon tax), and long-term ecological uncertainties of CO_2 geological or ocean storage. The methane dissociation approach eliminates CO_2 production and produces a value-added marketable byproduct — clean carbon. Among major challenges to this approach are catalyst deactivation problem and need for sufficiently large markets for carbon byproduct. According to several technical evaluations, the SMR process has a great potential for the integration with both solar and nuclear high temperature heat sources. Future developments in this area will focus on efficient solar-receiver reactors with improved solar radiation absorption characteristics, integrated thermal energy storage systems, the use of advanced materials, etc. Current status, existing and emerging technological trends in drastically reducing CO_2 emissions from fossil fuel-based manufacturing of hydrogen and outlook for the near- to mid-term future are analyzed in this presentation.

Biography

Dr. Nazim Muradov is a research professor at the Florida Solar Energy Center at the University of Central Florida. He holds an M.S. in petrochemical engineering, a Ph.D. in catalysis and a Doctor of Science in physical chemistry. He has been author of two books, six book chapters, close to 100 research articles and 49 patents in the area of hydrogen energy and technology.

Muradov is a member of the Board of Directors of the International Association for Hydrogen Energy (IAHE) and an associate of the International Journal of Hydrogen Energy. He has received several Excellence in Research awards. In 2010, he was granted the honorary title of the IAHE Fellow and in 2014 received the international R&D 100 Award.

Dr. Perla B. Balbuena

Texas A&M University, USA

"First-principles Analysis and Design of New Catalysts for CO_2-assisted Natural Gas Reforming"

Abstract

Converting CO_2 into useful products is one of the important themes that are expected to significantly contribute to controlling CO_2-derived environmental pollution. Among the various proposed technologies, the reaction of CO_2 with natural gas to produce syngas ($CO + H_2$) is especially attractive in regions where there is abundance of natural gas and at the same time a large production of CO_2 from industrial processes. However, this so-called "dry reforming" reaction consumes significant energy and the usual catalysts suffer from rapid deactivation due to the formation of coke that covers the active surface. Recently a new series of alumina-coated catalysts have been developed using atomic layer deposition techniques. The porous thin coating allows reactants to reach the catalytic surface and efficiently combine CO_2 and methane while suppressing coke formation. But the reasons for the success of these catalysts are not yet totally clear. In this talk I will discuss a first-principles based analysis of the full process: deposition of the alumina film on metal or metal-oxide catalysts, growth of an alumina layer and reactivity of the coated catalyst. Our analysis allows us to determine alternative catalytic materials and/or synthesis methods that would further improve the efficiency of the process.

Biography

Dr. Perla Beatriz Balbuena is the GPSA Professor in the Artie McFerrin Department of Chemical Engineering at Texas A&M University with a joint appointment in the Department of Materials Science and Engineering. Her research focuses on understanding and predicting thermodynamic, transport and kinetic properties of materials using state-of-the-art first principles computational chemistry and physics methods. Her work centers on design of nanomaterials used as catalysts and electrolytes in power sources devices, such as lithium-ion and lithium-sulfur batteries and fuel cells. She has contributed to an improved design of power sources and to the development of new materials for catalytic processes. Balbuena's work with lithium-ion batteries — used in laptop computers, cell phones and electric vehicles — involves elucidating fundamental mechanisms related to interfacial reactions, and designing chemistries that are less toxic and work more efficiently than those currently used. Her work with fuel cells, called the power source of the future, involves studying how reactions take place on the surface of the nanocatalytic particles to improve the cells' efficiency and cost. Other current projects include the design of new nanomaterials for catalysis and gas separation processes and evaluation of the phase behavior of shale gas mixtures.

Balbuena joined the Texas A&M chemical engineering department as a professor in 2004. She earned her bachelor's degree from the Universidad Tecnologica Nacional in Rosario (Argentina), a master's degree from the University of Pennsylvania, and a Ph.D. from the University of Texas at Austin, all in chemical engineering. She has published 210 peer-reviewed articles and has co-edited five books in her areas of specialization. In 2013 she was elected AAAS Fellow for "distinguished contributions to the theory of interfacial processes, through molecular simulation of electrochemical reactions and materials properties at the nanoscale." Her work is supported by the U.S. Department of Energy, the U.S. National Science Foundation and Qatar National Research Foundation.

Dr. Claire S. Adjiman

Imperial College London, UK

"The Molecular Systems Engineering of Carbon Capture Processes"

Abstract

The performance of a carbon capture processes depends on the flowsheet structure, the design of the equipment and the operating conditions, and on the choice of processing materials such as catalysts and solvents. By using a different solvent, for instance, one can change the rate of a given reaction by several orders of magnitude. In practice, processing materials are often selected in the early stages of process development, and considered as fixed for the purpose of process/equipment design. This can lead to sub-optimal designs: for example, a solvent which leads to the best absorption capacity may incur significant recovery costs and therefore not be cost-effective from a process-wide perspective. It is thus desirable to extend the boundary of process design to include processing materials in the set of design variables. Given the number of potential solutions to this extended design problem and the complexity of the task, computer-aided design can play an important role in identifying promising areas of the solution space. A key objective is thus to identify candidate molecules and/or mixtures that should be investigated experimentally, thereby providing focus for experimental studies and reducing their cost. In this talk, a methodology for computer-aided integrated molecular and process design is discussed, with applications to high-pressure separation and reaction systems. The methodology presented here follows the general blueprint of computer-aided molecular design with two important features. First, we seek to develop or use advanced property prediction techniques, such as quantum mechanics or molecular equations of state, in order to address problems that had previously been out of reach. Second, we treat the design problem as a single optimization problem, in which all decision variables are considered simultaneously. Applications are presented to the design of carbon dioxide capture processes and reaction systems. A difficulty in addressing these problems is to capture the impact of the solvent on the phase equilibrium, chemical equilibrium or reaction kinetics in a way that is both computationally tractable and transferable from solvent to solvent. Through the applications discussed, integrated molecular and process design is shown to be effective in guiding experimental work towards promising molecules.

Biography

Dr. Claire Adjiman, FREng, is professor of chemical engineering at Imperial College London and founding co-director of the Institute for Molecular Science and Engineering. She holds an M.Eng. from Imperial College and a Ph.D. from Princeton University, both in chemical engineering. Her research interests lie in the area of integrated process and molecular/materials design, including the development of design methods, property prediction techniques and optimization algorithms. She is the recipient of several prizes, including a RAEng-ICI Fellowship (1998-2003), the Philip Leverhulme Prize for Engineering (2009) and the SCI Armstrong Lecture (2011). She holds an EPSRC Leadership Fellowship (2012-2017) and was elected Fellow of the IChemE in 2013 and Fellow of the Royal Academy of Engineering in 2015. She has been author of more than 150 refereed publications. In 2011, she co-edited a book, Molecular Systems Engineering, published by Wiley-VCH.

Dr. Berend Smit

Ecole Polytechnique Fédérale de Lausanne, Switzerland

"The Materials Genome in Action"

Abstract

In the past few years there has been a surge in the number of published nanoporous materials. For a long time zeolites were the preferred crystalline nanoporous materials, but recently novel classes of nanoporous materials — such as metal-organic frameworks (MOFs) or porous polymer networks (PPNs) — have been discovered. These materials are very interesting as millions of different materials can, in principle, be synthesized by combining different molecular building blocks in varying topologies. In analogy with the human genome in which a small number of building blocks (e.g., amino acids) can be combined to yield the nearly infinite variety of biology, one can envision a nanoporous materials genome. In practice, however, due to limits on time and resources, only a small set of the possible materials will ever be synthesized and tested. Computational method can help screening all possible materials to find the most optimal material for a given application. In this presentation we show how these computational methodologies can be used to find the best material for some energy related applications.

Biography

Dr. Berend Smit received an M.Sc. in chemical engineering in 1987 and an M.Sc. in physics, both from the Technical University in Delft (The Netherlands). He received his Ph.D. in chemistry cum laude in 1990 from Utrecht University (Tthe Netherlands). He was a (senior) research physicist at Shell Research from 1988 to 1997 and professor of computational chemistry at the University of Amsterdam (The Netherlands) from 1997 to 2007. In 2004 Smit was elected director of the European Center of Atomic and Molecular Computations (CECAM) in Lyon, France. Since 2007 he has been professor of chemical engineering and chemistry at the University of California, Berkeley, and faculty chemist in the Materials Sciences Division of the Lawrence Berkeley National Laboratory. Since 2014 he has been director of the Energy Center at Ecole Polytechnique Fédérale de Lausanne. Berend Smit's research focuses on the application and development of novel molecular simulation techniques, with emphasis on energy related applications. He wrote the textbook Understanding Molecular Simulations with Daan Frenkel and the textbook Introduction to Carbon Capture and Sequestration with Jeff Reimer, Curt Oldenburg and Ian Bourg.

Dr. Ioannis Kevrekidis

Princeton University, USA

"No Equations, No Variables: Data and the Computational Modeling of Complex Systems"

Abstract

I will first briefly review how a computational framework involving matrix-free algorithms, and in particular, timestepper-based matrix-free methods can functionally link fine-scale simulators with coarse-grained, systems-level numerical tasks (such as coarse stability and bifurcation computations) for complex dynamical models.

I will then discuss what we are currently concerned about/working on in my group: the use of data mining (the "variable-free" component) in the overall computational process. Processing the results of brief bursts of multiscale simulations with manifold learning tools such as diffusion maps can suggest good macroscale observables (variables) in terms of which macroscopic equations can in principle be written/solved. Performing scientific computation in terms of these "data-mining–based" variables poses a number of interesting questions/challenges that I will outline and discuss.

Biography

Dr. Ioannis Kevrekidis has been the Pomeroy and Betty Perry Smith Professor of Engineering at Princeton University since 1994. His research interests have centered on the dynamics of physical and chemical processes, types of instabilities, pattern formation, and their computational study. More recently he has developed an interest in multiscale computations and the modeling of complex systems. He has been co-author of more than 350 journal publications and cited more than 14,000 times. He has been a Packard Fellow, an NSF PYI and the Ulam Scholar at Los Alamos National Laboratory. He holds the Colburn and Wilhelm Awards of the AIChE, the Crawford prize of SIAM/DS and a Humboldt prize. He has been the Gutzwiller Fellow at the Max Planck Institute for the Physics of Complex Systems in Dresden, a senior Hans Fischer Fellow at IAS-TUM in Munich and an Einstein Visiting Fellow at FU/Zuse Institut Berlin.

Dr. Brian Norton

Dublin Institute of Technology, Ireland

"Multifunctional Solar Energy Harnessing Systems for Building Facades"

Abstract

By changing innovative thermophysical characteristics of an adaptive façade a building it is possible without additional heating or cooling to satisfy the thermal and lighting comfort conditions required by occupants throughout the significant different weather conditions encountered over a year in many climates. The changing characteristics are embodied in building facade elements that, in different ways, can collect and store solar energy as heat and/or electricity, provide daylight and induce ventilation air flows. Associated with such adaptive facades are systems and mechanisms by which heat, daylight and ventilation are conveyed from the facade to deeper into a building. This presentation discusses innovations in switchable opacity glazings, highly insulating high-transmittance vacuum glazing, luminescent concentration of diffuse solar energy and high-energy density energy storage using phase change materials. For differing conditions depending on weather, climate, building type and occupancy adaptive facades systems combining these features have the potential to achieve near zero energy buildings by inclusion in coherent functional architectural designs. Incorporating other enabling technologies such as photovoltaics with battery storage and integrated wireless antenna enables autonomous modular operation whilst providing environmental control via interactions between modules and the building energy management system. Possible future directions are discussed for research that combine these technologies in multifunctional facades (as shown in the diagram) with controlled complex time-varying characteristics that produce environmentally sustainable building performance responsive to occupant's requirements and the prevailing weather conditions.

Biography

Dr. Brian Norton is president of the Dublin Institute of Technology. He is the author or co-author of six books (including two sole-authored major advanced texts) and more than 400 papers, including more than 170 in learned journals. He has supervised more than 40 doctorates and serves on several international journal editorial boards. He is editor-in-chief of Foundations and Trends in Renewable Energy. He has been an invited plenary speaker to major international conferences and to ministerial meetings. Norton has chaired and served on the board of many bodies, and is currently chair of the board of Action Renewables, which is responsible for developing renewable energies in Northern Ireland.

He has a B.Sc. (Hons) in physics from the University of Nottingham; an M.Sc. in engineering experimentation and a Ph.D. in applied energy, both from Cranfield University; and a D.Sc. from the University of Nottingham. He is a Fellow of the Irish Academy of Engineering, the Energy Institute and Engineers Ireland, as well as the Higher Education Academy. He is a Chartered Engineer both in the UK and Ireland. Among his awards are the Napier Shaw Medal of the Chartered Institute of Building Services Engineers (CIBSE) and the Roscoe Award of the Energy Institute and the Honorary Fellowship of the CIBSE, the highest honor for his professional discipline. Previously he was professor of built environmental engineering and dean of engineering and built environment at the University of Ulster. He is an honorary professor at Harbin Institute of Technology, University of Ulster, University of Houston and Bejing Wuzi University.

Dr. Nimir O. Elbashir

Texas A&M University at Qatar, Qatar

"Gas Processing Research at Texas A&M University at Qatar"

Abstract

Qatar made major investments in the gas processing technologies to build one of the world's most advanced existing plants in the field of liquefied natural gas (LNG) and gas-to-liquid (GTL) technology. Texas A&M at Qatar built world-class research facilities in the GTL field to support research activities aimed at improving the design of reactors and reformers for the GTL process, conversion of CO_2 generated from Qatar's gas processing plants to chemical precursors for production of ultra-clean fuels and value-added chemicals, and the formulation of new generations of synthetic fuels and chemicals obtained from natural gas via the GTL technology. All of the aforementioned projects are aimed at supporting Qatar's research and development activities and building the skilled scientists, engineers and technical staff required to sustain and further improve Qatar's gas processing plants. Many of these projects have been conducted in collaboration with Qatari national companies and world-leading energy corporations by building unique industry-academia research collaboration models that involve several esteemed universities from the States, Europe, and the region. This presentation will highlight a few examples of these collaboration projects with a brief description of their outcome as led by Dr. Elbashir's research team. The topics covered will be on the advancement of reactor design for Fischer Tropsch (FT) synthesis, and the development of correlations between the synthetic fuels composition and their critical physical and chemical properties as well as the design of new generation of synthetic fuels and surrogates.

Biography

Dr. Nimir Elbashir is an associate professor of chemical engineering and petroleum engineering at Texas A&M University at Qatar and the director of the TEES Gas and Fuels Research Center, a major research center that involves 19 faculty members from both the Qatar and College Station campuses of Texas A&M University. His research activities is focused on design of reactors and catalysts for gas-to-liquid (GTL) technology, petrochemical conversions and CO_2 utilization. He has more than 16 years of research and teaching experience. Before joining his current position he was part of BASF Catalysts R&D team in Iselin, N.J. He is leading multimillion dollar research projects in collaboration with academia and industry with a focus on the design of advanced reactors, processes, and products in XTL technology (gas-to-liquid, coal-to-liquid, and biomass-to liquid). He holds several U.S. and European patents and numerous publications. The scholarship of his research activities has been recognized by awards from the Gordon Research Conferences, BASF Corp., the American Institute of Chemical Engineers, Texas A&M University and the 2012 Qatar Foundation's Best Energy and Environment Program of the Year. In addition, Elbashir is the director of Texas A&M at Qatar's Fuel Characterization Lab, a research lab that is supporting major research activities in the advancements of synthetic fuels and chemicals obtained from natural gas in collaboration with GE (Oil& Gas), OryxGTL and Shell, and world-leading academic institutions.

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