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INTERNATIONAL ONLINE CONFERENCE ON FUNCTIONAL NANOMATERIALS

15—16 July 2020 | Online meeting

Abstract Book



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WELCOME MESSAGE

Dear colleagues and friends,

It is our pleasure to invite you to attend the International Online Conference on Functional Nanomaterials to be held on 15—16 July 2020. The conference brings together leading invited speakers and young researchers in solar cells and photo/catalysis. It aims to provide a high-profile and internationally renowned online conference for researchers to present the latest research results in solar cells and photo/catalysis science and technology. In addition, it offers an ideal and cordial setting for all participants worldwide to share experiences, to exchange views, to discuss the advancements and breakthroughs in relevant fields, and to promote friendships.

We'll be most pleased to welcome you in online and we hope you will enjoy a pleasant time along all the Conference, from both scientific and social points of view.

Sincerely Yours,



Dr. Saim Emin, Conference Chair University of Nova Gorica, Slovenia & European Nanoscience and Nanotechnology Association, Bulgaria



Dr. Alison B Walker Conference Co-Chair University of Bath, Bath, United Kingdom



Dr. M. V. Shankar Conference Co-Chair Yogi Vemana University, Kadapa, India

PROGRAM 15 July 2020

Session on Solar Cells

Session Chair: Saim Emin

- 12:00—12:10 Conference Opening / Session Introductory Remarks
- 12:10—12:40 Juan Bisquert Universitat Jaume I, Spain

"Impedance spectroscopy analysis of the physical response of perovskite solar cells"

- **12:40—13:10** Alison B Walker University of Bath, Bath, United Kingdom *"Working Principles of Perovskite and Organic cells"*
- **13:10—13:40** Ganesh Datt Sharma The LNM Institute of Information Technology, Jaipur, India *"Recent advances on organic solar cells based on non-fullerene acceptors: materials and device optimization"*
- **13:40—14:10 Stoichko Dimitrov** Queen Mary, University of London, United Kingdom "Applying time-resolved laser spectroscopy techniques for organic solar cell development"

PROGRAM 16 July 2020

Session on Photo/Catalysis			
Session Chair: Saim Emin			
12:00—12:10	Conference Opening / Session Introductory Remarks		
12:10—12:40	Richard E. Palmer — Swansea University, Swansea, United Kingdom		
	"Scaling-up Nanoparticle Beam Deposition for Green Synthesis of Advanced Materials"		
12:40—13:10	M. Mamatha Kumari — Yogi Vemana University, India		
	"Influence of different Nanostructured photocatalysts for solar H ₂ production"		
13:10—13:40	Sudhagar Pitchaimuthu — Swansea University, Wales, United Kingdom		
	"Sustainable Solar Hydrogen Fuel Generation: Recent progress in Materials Design and Solar Fuel Cell Architectures"		
13:40—14:10	M. V. Shankar - Yogi Vemana University, India		
14:10—14:30	"Hierarchical nanostructured photocatalysts for hydrogen production using industrial / domestic wastes" Break		

Session on Photo/Catalysis

Session Chair: Sudhagar Pitchaimuthu

- 14:30—15:00 Fernando Fresno IMDEA Energy Institute, Madrid, Spain
 "Selectivity modifications in CO₂ photoreduction over nanosized metal/semiconductor catalysts"
- **15:00—15:30** Artem Badasyan University of Nova Gorica, Nova Gorica, Slovenia *"Water reveals non-Arrhenius kinetics in protein folding experiments"*
- **15:30—16:00** Saim Emin University of Nova Gorica, Nova Gorica, Slovenia "Synthesis of iron phosphide nanoparticles and application in electrochemical hydrogen evolution"

16:00—16:10 Break

Presentation of Students

- **16:15—16:30** Waheed A. Adeosun King Abdulaziz University, Jeddah Kingdom of Saudi Arabia "Synthesis of polypyrrole doped polydopamine nanocomposite for non-enzymatic electrocatalytic oxidation of uric acid"
- **16:30– 16:45** *Hind Alshaikh -* King Abdulaziz University, Jeddah, Saudi Arabia "Novel Catalytic Transformations of Ionic polymer-supported Palladium Metal Nanoparticle Compounds"
- **16:45 17:00 Takwa Chouki -** University of Nova Gorica, Nova Gorica, Slovenia "Growth of MoSe₂ thin films and use in electrochemical hydrogen evolution"

INVITED SPEAKERS



Dr. Juan Bisquert

Jaume I University, Castelló, Spain

Title: "Impedance spectroscopy analysis of the physical response of perovskite solar cells"

Juan Bisquert is a professor of Applied Physics at Universitat Jaume I de Castelló. He is the director of the Institute of Advanced Materials, that develops research on materials, nanostructures and devices for production and efficient use of clean energies. He published 400 papers in research journals, and authored a series of books, including The Physics of Solar Energy Conversion (CRC Press, 2020). He has 30000 citations and h-index 97. He is a Senior Editor of the Journal of Physical Chemistry Letters. He has been distinguished in the list of Highly Cited Re-

searchers from 2014 to 2019.

The research activity of Juan Bisquert has been focused on materials and devices for production and storage of clean energies, in particular photovoltaic devices, based on nanostructured metal oxides, semiconductor quantum dots, organic and hybrid semiconductors, and related applications such as luminescence. The main contribution of Bisquert by which he established an international reputation is the application of measurement techniques and physical modeling in several areas of energy devices, relating the device operation with the elementary steps that take place at the nanoscale dimension: charge transfer, carrier transport, chemical reaction, etc., especially in the field of impedance spectroscopy, as well as device models, and the development of a general physical picture of solar energy devices. Since 2014, the research field has been largely influenced by the discovery of a new class of photovoltaic materials and devices, generally termed hybrid perovskites. These materials show excellent performance and radically new semiconductor properties. Unraveling the mechanisms of perovskite solar cells has established scientific work of high impact by Bisquert and coworkers in the last few years.



Dr. Alison B Walker

University of Bath, Bath, United Kingdom

Title: "Working Principles of Perovskite and Organic cells"

Alison Walker took her undergraduate and postgraduate degrees at the University of Oxford, followed by postdocs at Michigan State University in the US and at Daresbury Laboratory in the UK. Then she took up a lectureship at the University of East Anglia, Norwich, UK, moving to the University of Bath in 1998. A Royal Society Industry Fellowship was held with Cambridge Display Technology. Since then she coordinated four EU projects, including the currently running Horizon 2020 Innovative Training Network, Maestro,MAking pErovskiteS TRuly explOitable. She

is a partner in the Horizon2020 project EoCoE -II, Energy Oriented Centre of Excellence for Energy, towards exascale for energy and coleads the Centre for Doctoral Training in New and Sustainable Photovoltaics involving 7 UK universities. She is a member of the physics assessment sub panel for assessing UK research 2021. In 2019 she chaired the Solar Commission aimed at publicising the role of solar in the UK economy whose report can be found on her website https://people.bath.ac.uk/pysabw/.



Dr. Ganesh Datt Sharma

The LNM Institute of Information Technology, Jaipur, India

Title: "Recent advances on organic solar cells based on non-fullerene acceptors: materials and device optimization"

Prof. Ganesh Datt Sharma is working as Senior Professor of Physics and Dean (Research and Development) at The LNM Institute of Information Technology (Deemed University), Jaipur (Raj.), India since Nov 2015. Prof. Sharma obtained his Ph.D. degree from India Institute of Technology in 1985 and after then he had joined as Assistant Professor at JNV University, Jodhpur (Raj), India in Nov 1985. After then he had appointed as Professor of Physics and Electron-

ics in 2004, in the same university. In 1990 he was awarded a prestigious BOYCAST Fellowship by Department of Science and Technology, Government of India in 1990 to work as Visiting Scientist at the Department of Electrical and Computer Science, The State University of New Jersey for two years. His area of Research is Organic solar cells, nanocrystalline organic-inorganic hybrid solar cells and fuel cells, organic electronics, and nanomaterials for energy conversion and storage. He has delivered many invited/plenary lectures in many international conferences in India and abroad. Subject expert in project advisory committee, Department of Science and Technology, Govt of India, DRDO, Government of India. He is a Subject expert: European commission for project evaluation, Russian Science Foundation, Moscow. Prof. Sharma Published more than 300 research papers with citations of 6379, h-index:41 and ito:190.



Dr. Stoichko Dimitrov

Queen Mary, University of London, United Kingdom

Title: "Applying time-resolved laser spectroscopy techniques for organic solar cell development" Stoichko was appointed as Lecturer in Chemistry at Queen Mary in September 2019, where he leads a group in Photochemistry and Photophysics of functional nanomaterials and semiconductors. He has previously held positions as a research associate in the group of Prof James Durrant FRS at Imperial College London and Ser Cymru Fellow at the College of Engineering of Swansea University, investigating the nature of the excited state dynamics at organic donoracceptor interfaces. He has also worked at the Bulgarian Academy of Sciences and at a start-up

company developing photocatalytic water treatment reactors. Stoichko's PhD degree is in ultrafast laser spectroscopy of nanomaterials and DNA, completed at Boston College, USA in 2010. He has an integrated MSc degree from Sofia University, Bulgaria with a thesis focused on light induced complexation of photochromic dyes.



Dr. Richard E. Palmer

Swansea University, Swansea, United Kingdom

Title: "Scaling-up Nanoparticle Beam Deposition for Green Synthesis of Advanced Materials"

Richard is Head of the Nanomaterials Lab in the College of Engineering at Swansea, his hometown, and also Professor in the School of Physics of Nanjing University, China. His research on atomic clusters includes fundamental studies of atomic structure and dynamics as well as scale-up. Other well-established research topics include atomic manipulation in the STM and semiconductor nanofabrication. Richard was awarded an MA and PhD at Cambridge where he afterwards held 1851, Clare College and Royal Society Fellowships. At Birmingham (1994-

2017) he founded the UK's first centre for nanoscience. Honours include the IOP Boys Medal, an Honorary Doctorate from Hasselt University, the BVC Yarwood Medal, an EPSRC Senior Fellowship and Fellowships of the IOP, RSC and Learned Society of Wales. He has published >400 papers, h index 58; also 18 families of patent applications. Spin-out companies include Inanovate, Irresistible Materials and Grove Nanomaterials. He is Editor-in-Chief of the open-access journal Advances in Physics: X (2016-, Taylor and Francis) and Editor of the Elsevier Book Series 'Frontiers of Nanoscience'.



Dr. M.V.Shankar YVU

Yogi Vemana University, Kadapa, India

Title: "Hierarchical nanostructured photocatalysts for hydrogen production using industrial / domestic wastes"

Prof. M. V. SHANKAR, is renowned for outstanding research contribution in the field of *Photocatalysis for Hydrogen fuel production*. He has developed several efficient photocatalysts by fine-tuning optical and surface-interface properties of semiconductors at nanoscale. He is successful in research projects sponsored by MNRE, New Delhi in collaboration with CSIR-IICT and CSIR-CECRI, India. The outcome of research work published in SCI journals (81), Pa-

tents (06) having h-index of 31. He is recipient of several awards, including Charted Chemist (CChem) and Fellow of Royal Society of Chemistry (FRSC), London.



Dr. Sudhagar Pitchaimuthu

Swansea University, Swansea, United Kingdom **Title:** "Sustainable Solar Hydrogen Fuel Generation: Recent progress in Materials Design and

Solar Fuel Cell Architectures"

Dr. Sudhagar graduated from Physics discipline, Bharathiar University, India in 2009. He was working as Research Assistant Professor during 2009-2013 under Prof. Yong Soo Kang at Center for Next Generation Dye-sensitized Solar Cells in Hanyang University, South Korea. Concurrently, he has been serving as visiting scientist to Department of Applied Physics, University of Jaume I, Spain from 2011. He was a recipient of JSPS award from Japan Society for the Promo-

tion of Science, Japan in 2013.

He is leading "Multifunctional Photocatalyst and Coating" research group at Swansea University. His research expertise is 'nanomaterial synthesis and coatings' towards constructing low-cost solar energy driven photoelectrochemical system/devices.



Dr. Fernando Fresno

IMDEA Energy Institute, Madrid, Spain

Title: "Selectivity modifications in CO₂ photoreduction over nanosized metal/semiconductor catalysts"

Fernando Fresno obtained his MSc in Chemistry at the *Autónoma* University of Madrid (UAM) in 2001 and his PhD from the same University in 2006, after carrying out a Doctoral Thesis in the Institute of Catalysis of CSIC, in collaboration with the Inorganic Chemistry department of UAM. He has worked as a postdoctoral researcher at CIEMAT and ICP-CSIC, and afterwards as Research Associate and Assistant Professor at the University of Nova Gorica, Slovenia. He has

spent visiting periods in IRCELYON and ICPEES (France) and in the Universities of Aberdeen (UK) and Niigata (Japan). His scientific activity focuses on the development of materials for an efficient use of solar energy in energy and environmental applications, mainly by photocatalytic and thermochemical processes. He has published more than 50 scientific papers (h=21) and contributed with more than 100 communications to scientific conferences. He is co-inventor in two patents in the field of photovoltaic and photocatalytic materials. He has co-edited the book "Design of Advanced Photocatalytic Materials for Energy and Environmental Applications" (Springer 2013, ISBN 978-1-4471-5060) and he is a member of the editorial board of Frontiers in Chemistry.



Dr. Artem Badasyan

University of Nova Gorica, Slovenia

Title:"Water reveals non-Arrhenius kinetics in protein folding experiments"

Artem Badasyan took his Bachelor (2000), Master(2002) and PhD (2005) degrees in Physics at Yerevan State University, Armenia, followed by postdocs at University of Toronto, Canada, University CaFoscari of Venice, Italy, Institute Jozef Stefan, Slovenia; in 2005-2006 he was adjunct scientist at National Institutes of Health, US. From 2013 to now, he is Assistant Professor at School of Science and Experienced Researcher at Materials Research Lab, University of Nova Gorica, Slovenia. His areas of expertise are Statistical Mechanics, Soft Condensed Matter Phys-

ics, Polymer Physics and Biophysics. Artem Badasyan is the author of more than 30 scientific publications in refereed journals and active University teacher.



Dr. Saim Emin

University of Nova Gorica, Slovenia

Title: "Synthesis of iron phosphide nanoparticles and application in electrochemical hydrogen evolution"

Saim Emin is a Professor at the University of Nova Gorica, Slovenia. Before joining the University of Nova Gorica in 2012 he obtained his PhD degree from Saitama University, Japan. His research focuses on the field of nanotechnology-related to renewable energy. Research on photo/ electrocatalytic hydrogen production and wastewater treatment. Supervision of PhD students Ms. Manel Machreki and Ms. Takwa Chouki. Participation in research projects related to photo-

catalysis, photovoltaics which cover quantum-dot-sensitized solar cells and organic-inorganic perovskite solar cells.



Dr. M. Mamatha Kumari

Yogi Vemana University, Kadapa, India

Title: "Influence of different Nanostructured photocatalysts for solar H₂ production"

Dr. M.Mamatha Kumari, is working as Assistant Professor at Department of Materials Science and Nanotechnology, Yogi Vemana University, Kadapa, Andhra Pradesh. She holds Ph.D. in Photocatalysis from Indian Institute of Technology, (IITM) Madras, Chennai Tamil Nadu. She has significantly contributed in the area of design and development of various functional nanomaterials and nanostructures for energy, and environmental applications. She has to her credit over 30 research publications in reputed international peer reviewed journals of high impact, three book

chapters and has 2 international Patents. She is Associate Fellow of Andhra Pradesh Academy of Sciences, also fellow of several prestigious academic and research bodies in India.

She has expertise in areas such as novel process development for synthesizing nano-materials (nanostructures, nanocomposites), for solar hydrogen production, photocatalytic decomposition of organic pollutants. She has research collaboration in leading research groups in India and Abroad.

Invited Talks

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Impedance spectroscopy analysis of the physical response of perovskite solar cells

Juan Bisquert

Institute of Advanced Materials, Universitat Jaume I, Castelló, Spain. E-mail: bisquert@uji.es

The dynamic response of metal halide perovskite devices shows a variety of physical responses that need to be understood and classified for enhancing the performance and stability and for identifying new physical behaviours that may lead to developing new applications. These responses are the outcome of complex interactions of electronic and ionic carriers in the bulk and at interfaces. Based on a systematic application of frequency modulated techniques and time transient techniques to the analysis of kinetic phenomena, we present a picture of the dominant effects governing the kinetic behaviour of halide perovskite devices. First with impedance spectroscopy we provide an interpretation of capacitances as a function of frequency both in dark and under light, and we discuss the meaning of resistances and how they are primarily related to the operation of contacts in many cases. Working in samples with lateral contacts, we can identify the effect of ionic drift on changes of photoluminescence, by the creation of recombination centers in defects of the structure.¹ We also address new methods of characterization of the optical response by means of light modulated spectroscopy. The IMPS is able to provide important influence on the measured photocurrent.² We apply the dynamic picture to the characterization of perovskite memristors.³ A memristor is a device that has different metastable states at a voltage V. It has a resistance that depends on the history of the system, and the states can be switched by applied voltage. It is simpler than a transistor in that the control occurs by 2 contacts. As a summary we suggest an interpretation of the effects of charge accumulation, transport, and recombination, how these effects influence the currentvoltage characteristics and time transient properties, and we suggest a classification of the time scales for ionic/electronic phenomena in the perovskite solar cells.

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Working Principles of Perovskite and Organic cells

Alison B Walker^a

^a Department of Physics, Department of Physics, University of Bath, Bath BA2 7AY, UK E-mail: pysabw@bath.ac.uk

The physics of perovskite and organic cells is dominated by light harvesting, charge and energy transport and extraction, all process that take place at the nanoscale. I will describe the operation of these cells, how these technologies can compete with crystalline silicon and other thin film solar technologies, and discuss the barriers that need to be overcome for their exploitation.

Recent advances on organic solar cells based on non-fullerene acceptors: materials and device optimization

Ganesh Datt Sharma

Department of Physics, The LNM Institute of Information Technology (Deemed University) Jamdoli, Jaipur 302031, India E-mail address: gdsharma273@gmai.com and gdsharma@Inmiit.ac.in

Organic solar cells (OSCs) consist of a bulk heterojunction (BHJ) active layer of carbon-based donor (D) and acceptor (A) materials, have many environmental advantages compared to other inorganic counterparts' technologies. In active layer employed in OSCs, charge generation is accomplished using BHJ of electron donors and acceptors, where the charge transfer occurs at the donor/acceptor interfaces [1]. Fullerene and its derivatives have been widely used as electron acceptors for many years, while the electron transfer from polymer/small molecule donors is considered as the major channel for photocurrent generation and the power conversion efficiency (PCE) of these OSCs is limited only upto 11 % [2] due to several drawbacks, such as weak absorption in visible region of the solar spectrum, high synthesis costs, limited tailoring of energy levels and high voltage loss. In an effort to overcome these obstacles, in the past three years a great deal of attention has been paid to the development of non-fullerene acceptors (NFAs), especially small molecule acceptors (SMA) [3, 4, 5]. After the limited time of research work on the designing of new SMA, the overall PCE of more than 18% [6, 7] achieved for single junction and are on the road to the commercial reality.

This talk deals with the recent advance in the binary and ternary active layer OSCs based on non-fullerene acceptor along with the conjugated polymers and small molecules donors, in terms of designing and optimization of molecular structures, active layer morphology optimization and interface engineering.

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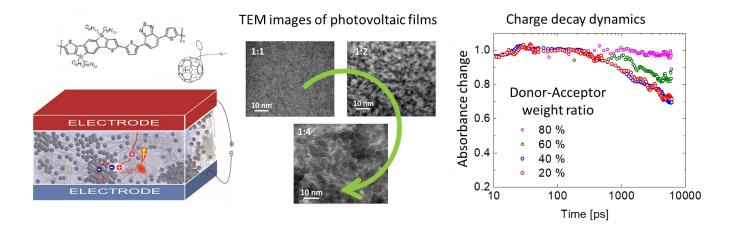
Excited state dynamics at donor-acceptor interfaces for performance and stability enhancement of organic solar cells

Stoichko Dimitrov

School of Biological and Chemical Sciences, Queen Mary University of London, E1 4NS, London, United Kingdom

E-mail: s.dimitrov@qmul.ac.uk

The performance of organic solar cells has rapidly increased for the past five years demonstrating the potential of this technology to compete with inorganic and perovskite solar cells. There are however challenges with respect to operation and stability which continue to be unresolved and require further analysis. The most debated question has been the mechanism of charge photogeneration in bulk-heterojunction devices and this is because of inconclusive experimental and theoretical results producing two main contradictory models for electron-hole separation. This presentation will discuss our recent findings in the understanding of exciton and charge transfer dynamics in polymer:fullerene solar cell blends. Using a combination of transient absorption and electroluminescence and photoluminescence spectroscopy experiments, we identify how interfacial enthalpy and morphology on the nanometre length scale control the electron-hole separation dynamics on the pico- and nanosecond time scales, allowing us to conclude that the apparently contradictory studies on electron-hole separation can be explained by the presence of both bound and unbound charge transfer states in the same blend. Furthermore, our analysis of the electron-hole dynamics identify two oxygen-induced degradation pathways in polymer:non-fullerene solar cell devices, thereby, developing design guidelines for more stable materials.



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Scaling-up Nanoparticle Beam Deposition for Green Synthesis of Advanced Materials

Richard E. Palmer

Nanomaterials Lab, College of Engineering, Swansea University, UK E-mail: r.e.palmer@swansea.ac.uk

The deposition of size-controlled nanoparticles (atomic clusters) onto supports from the beam is a solventfree, green route to small-scale manufacturing of functional nanomaterials. To translate the beautiful physics and chemistry of clusters into practical applications, e.g., coatings, catalysts, biochips, biomaterials and photonic materials, **significant scale-up** of the rate of deposition is needed [1,2], while reducing the loss of material in the process (to say 1-10%). For example, the deposition rate needed for industrial catalyst R&D is 10mg/hour of clusters, while for bespoke pharmaceutical manufacturing 1-10g/hour is required. In this talk I will discuss both the fundamental aspects of deposited clusters at the atomic-scale – as revealed by aberration-corrected scanning transmission electron microscopy [3,4] – and the status of efforts to meet the scale-up challenge, with emphasis on our "Matrix Assembly Cluster Source" (MACS) [5]. Some first practical demonstrations [6-10] of deposited clusters in heterogeneous and electrocatalysis will be presented, showing attractive activities and selectivities [1, 6-10], as an illustration of what might be done in fields as diverse as surface engineering, theranostics, photonics and neuromorphics.

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Influence of different Nanostructured photocatalysts for solar H₂ production

M Mamatha Kumari

Nanocatalysis and Solar Fuels Research Laboratory, Department of Materials Science & Nanotechnology, Yogi Vemana University, Kadapa – 516 005, Andhra Pradesh, INDIA. E-mail: mamatha@yogivemanauniversity.ac.in

Photocatalysts generate hydrogen through water splitting by utilizing solar energy, contribute to environmentally friendly programs due to their properties such as zero emissions. Among the photocatalysts, TiO_2 is a promising candidate because of its relatively low cost, non-toxicity, stability and suitable band edge positions for redox reactions. However, TiO_2 can absorb only UV light (nearly 5% of solar light). Further, the photoinduced electrons and holes in TiO_2 may experience rapid recombination, which causes significant decrease in the efficiency of the photocatalytic reaction.

Additions of different nanostructures such as functionalized carbon nanotubes, Carbon nanohorns to TiO_2 extend the absorption into the visible region (nearly 50% of solar light). Also, the present talk briefs about morphology of TiO_2 such as nanoparticles, Nanotubes, Nanowires, Nanobelts and core-shell structures influence the photovatalytic activity by minimizing the electron-hole recombination.

References:

[1] Mamatha Kumari. et al, Int. J. Hydrog. Energy, 40(2015)1665-1674

Sustainable Solar Hydrogen Fuel Generation: Recent progress in Materials Design and Solar Fuel Cell Architectures

Sudhagar Pitchaimuthu,

Multi-functional Nanocatalyst & Coatings Group, SPECIFIC, College of Engineering, Swansea University (Bay Campus) Swansea SA1 8EN Wales, United Kingdom E-mail: S.Pitchaimuthu@swansea.ac.uk

Light driven catalysis using semiconductors to produce clean fuels such as hydrogen is recognized as emerging route to mitigate environmental issues caused by the depletion of fossil fuels to meet increasing worldwide demands for energy.¹ In this context semiconductor nanomaterials shows promising performance as photoabsorbers and catalysts in photoelectrochemical (PEC) hydrogen generation. The merits of nanostructured semiconductor interfaces in producing large fraction of solar light photon harvesting to the PEC reaction as well as rapid charge separation are anticipated to contribute high quantum yield of hydrogen generation in PEC cells. However, intricacy of how the semiconductor interface /water interface control both the energetics and kinetics of a photoelectrode needs to be understood. Exploration of nanostructured semiconductor interfaces might lead future trends in the application of autonomous water splitting in tandem solar fuel cells as well as simultaneous pollutant removal and fuel generation. This talk will focus on fundamental and advanced development of nanoscale photoelectrocatalysts in fuel generation. Particularly discussing about how the material design (interfacial layer, passivation layer, co-catalyst decoration and Pt-free cathode) influence the solar to fuel conversion efficiency.²

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Hierarchical nanostructured photocatalysts for hydrogen production using industrial / domestic wastes

Muthukonda Venkatakrishnan Shankar^a*, Vempuluru Navakoteswara Rao^a, Murikinati Mamatha Kumari^a, Parnapalle Ravi^b, Marappan Sathish^b

 ^aNanocatalysis and Solar Fuels Research Laboratory, Department of Materials Science & Nanotechnology, Yogi Vemana University, Kadapa-516005, Andhra Pradesh, India.
 ^bFunctional Materials Division, Central Electrochemical Research Institute (CSIR-CECRI), Karaikudi-630003, Tamil Nadu, India.
 E-mail: shankar@vogivemanauniversity.ac.in

Hydrogen can be a reliable alternative renewable energy source that has a potential to replace the fossil fuels to mitigate the present energy crisis, thanks to its high energy content and zero emission. Hydrogen (H_2) production from photocatalytic water splitting under solar irradiation represents a promising process for the direct conversion of light-energy into clean fuels, but the key issue is to develop quantum efficient and stable materials. This process often works well under ambient conditions and produces H_2 via detoxifying industrial wastewater, which ensures the environmental cleaning and energy production is a novel approach to reform industrial waste. In our research group more than 20 efficient and stable photocatalysts for H_2 production utilizing organic and inorganic sacrificial agents under visible/solar light irradiation. Hierarchical structures (core-shell with nanosize shell thickness) used in the present work have demonstrated enhanced H_2 production efficiencies and catalytic stability. Although handful of literature reports are available on these type of materials, choice of synthesis method, experimental skills and processing conditions have significant impact on material properties.

My talk highlight the utilization of industrial by-product crude glycerol generated as a part of vegetable oil production. Hydrogen (H_2) generation from biomass derived by-products (crude glycerol) is a clean and green approach to full-fill the global energy demand. Alternatively, my talk will focus on utilization of wastewater containing sulphide ion from sewage treatment plant.

This talk also highlights the challenges, recent developments and opportunities ahead for development of efficient photocatalytic systems. Finally, major achievements on photocatalytic H₂ production in our research group and cost benefit analysis on utilization of crude glycerol form biomass industry will be elaborated.

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Selectivity modifications in CO₂ photoreduction over nanosized metal/semiconductor catalysts

Fernando Fresno,^a Patricia Reñones,^a Laura Collado,^{a,b} Mariam Barawi,^a Ana Iglesias-Juez,^c Minoo Tas-bihi,^d Ulla Simon,^d Freddy E. Oropeza,^a Elena Alfonso-González,^a Cristián Huck-Iriart,^e Ignacio J. Villar-García,[†] Víctor A. de la Peña O'Shea.^a

^a Photoactivated Processes Unit, IMDEA Energy, Móstoles, Madrid, Spain.

^b Department of Chemical and Environmental Technology, Universidad Rey Juan Carlos, Móstoles, Madrid, Spain. [°] Instituto de Catálisis y Petroleoquímica (CSIC), Madrid, Spain.

^d Technical University Berlin, Berlin, Germany.

^e Universidad Nacional de San Martín, San Martín, provincia de Buenos Aires, Argentina.

^f ALBA Synchrotron, Cerdanyola del Vallès, Barcelona, Spain.

E-mail: fernando.fresno@imdea.org

One of the keys to carrying out a successful energy transition lies in the development of robust technologies to achieve the efficient conversion of small, low-energy molecules like H₂O, N₂ and CO₂ into fuels and chemicals using only renewable energy sources, solar par excellence [1]. A promising pathway to convert CO₂ into renewable fuels is artificial photosynthesis using semiconductor photocatalysts, based on the red-ox reactivity of electron-hole pairs created upon irradiation with light of photon energy equal to or greater than the semiconductor band gap. One of the cornerstones in photocatalytic CO_2 reduction is to control the selectivity, not only towards the different possible products of CO_2 conversion, but also towards CO_2 reduction against the water splitting reaction that competes for conduction band electrons [2]. Metals nanoparticles, e.g. Pt, Pd, Au, Ag, and Rh, can act as electron sinks that promote multi-electron transfer reactions that are crucial for photocatalytic efficient reduction of CO₂ and, at the same time, can modify the surface chemistry of the photocatalyst, both factors leading to modifications in the selectivity of the reaction with respect to the use of bare semiconductors [3].

In this work, we report on the performance of different metal/semconductor systems for photocatalytic CO₂ reduction, with particular attention on the selectivity modifications caused by the charge transfer and surface chemistry properties induced by the presence of metal nanoparticles (Aq, Au, Pt) on the surface of the semiconductors (TiO₂, Nb-Ta perovskites). Ex-situ and in-situ spectroscopic analyses with different techniques like NAP-XPS, FTIR, static and time-resolved fluorescence or electrochemical impedance spectroscopy have been carried out to shed light on the mechanistic pathways leading to the observed selectivity changes.

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Water reveals non-Arrhenius kinetics in protein folding experiments

Artem Badasyan^a

^a Materials Research Laboratory, University of Nova Gorica, Slovenia. E-mail:abadasyan@gmail.com

Statistical theories describe systems in equilibrium, and cannot be used to study kinetics. However, the theories are based on coarse-grained parameters, that include assumptions regarding the underlying kinetics. If such assumptions are incorrect, the theoretical expressions, used to process the experimental data, will not fit. I report on one such case we have met within the application of Zimm-Bragg [1] theory to process folding experiments, and discuss the reasons and consequences.

Studies of relaxation phenomena in glass-forming liquids by default account for the shift in temperature by some value, corresponding to the glass formation temperature, t_g . In particular, temperature $t - t_g$ shift appears in hydrated proteins because of the presence of partially glassy states giving rise to non-Arrhenius relaxation times $\log \tau \sim [2]$. $t_g/(t - t_g)$

A phenomenological approach was suggested by Adam and Gibbs as early as in 1965 to describe the sudden increase of viscosity and the slowing down of the collective modes in super-cooled liquids as the temperature is approaching[3]. The t_g key idea of Adam-Gibbs theory was to consider the supercooled liquid as a set of clusters (cooperatively rearranging regions) of different sizes that change with temperature, giving rise to the shift in re- $t - t_g$ laxation time. The temperature shift factor is present in many theories describing properties of water. Thus, Truskett and Dill had to include the Adamm-Gibbs temperature shift into their simple analytical model of water to achieve the agreement with experimental data on the temperature dependence of self-diffusion coefficient [4]. Later, Schiro and Weik have summarised recent in vitro and in silico experimental results regarding the role of hydration water in the onset of protein structural dynamics, and have reported the presence of super-Arrhenius relaxation region above the "protein dynamic transition" temperature [4]. Recently, Mallamace et al have used the Adam-Gibbs theory in their NMR measurements of protein folding-unfolding in water [4] and to rationalise the complicated pressure-temperature diagrams in these glass-forming systems.

Motivated by the considerations above, and taking into account the $s(t) \sim 1/\tau$ relationship between the unimolecular rate of folding in water and the relaxation time 45, we introduce the $t - t_g$ temperature shift into the formulas used to fit experimental data on hydrated polypeptides.

By doing so we resolve the paradox and complete the new method of processing the Circular Dichroism experimental data on protein folding.

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Synthesis of iron phosphide nanoparticles and application in electrochemical hydrogen evolution

T. Chouki, M. Machreki, **S. Emin**,*

Materials Research Laboratory, University of Nova Gorica, Nova Gorica 5000, Slovenia *E-mail: saim.emin@ung.si

We report the solvothermal synthesis of iron phosphide electrocatalysts using a low-cost phosphorus precursor. The synthetic protocol allows for the preparation of a Fe₂P phase at 300°C and FeP phase at 350°C. To enhance the catalytic activities of obtained iron phosphide particles, heat-treatments were carried out at elevated temperatures. Annealing at 500°C induced structural changes in the samples: (i) Fe₂P provided a pure Fe₃P phase (Fe₃P-500°C) and (ii) FeP transformed into a mixture of iron phosphide phases (Fe₂P/FeP-500°C). The electrocatalytic activities of heat-treated Fe₂P-450°C, Fe₃P-500°C, and Fe₂P/FeP-500°C catalysts were studied for hydrogen evolution reaction (HER) in 0.5 M sulfuric acid (H₂SO₄). The lowest recorded overpotential of 110 mV at 10 mA cm⁻² vs. a reversible hydrogen electrode was achieved with Fe₂P/FeP-500°C catalyst. The present approach allows preparation of immobilized iron phosphide catalyst onto carbon support which is essential for application purpose. The procedure developed by us is an elegant approach to tune the composition of iron phosphide catalyst and control the morphology of particles.

Posters

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Synthesis of polypyrrole doped polydopamine nanocomposite for non-enzymatic electrocatalytic oxidation of uric acid

Waheed A. Adeosun*^{a,b}, Abdullah M. Asiria^{a,b}, Mohammed M. Rahman^{a,b} and Hadi M. Marwani^{a,b}

^a Department of Chemistry, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia ^bCentre of Excellence for Advanced Materials Reserach, King Abdulaziz University, Jeddah, Saudi Arabia. *E-mail: <u>dsnwaheed1@gmail.com</u>*

Uric acid is mainly produced from metabolism of purine nucleotide in human body and have several medical importance in human system. It is therefore very imperative to develop a sensitive and accurate method of its detection. This study aimed to develop uric acid biosensor based on polydopamine-co-polypyrole (PDA-co-PPY) nanocomposite decorated on glassy carbon electrode.

The conductive polymer PDA/PPY was electrochemically synthesized and casted on glassy carbon electrode (GCE). The synthesized PDA-co-PPY was characterized by Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), electrochemical impedance spectroscopy (EIS), energy dispersive x-ray spectroscopy (XEDS) and x-ray photoelectron spectroscopy (XPS).

After the electrochemical synthesis and deposition on glassy carbon electrode, the mass of copolymeric film (PDA-co-PPY) deposited was 0.3 μ g. As synthesized PDA-co-PPY modified GCE showed good response towards electrocatalytic oxidation of uric acid with low limit of detection (0.1 μ M, S/N =3), good linearity (0.5-40 μ M) and high sensitivity (2.1 μ A μ Mcm⁻²). It was also found that PDA-co-PPY modified GCE displayed stable current response for uric acid unaffected by common interferents (electroactive substances). Also, when used for uric acid detection in human serum and urine, it showed a good recovery of 90-110%. The developed PDA-co-PPY nanocomposite is proposed as a promising biosensor for uric acid for human health protection.

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Novel Catalytic Transformations of Ionic polymer-supported Palladium Metal Nanoparticle Compounds

Hind Alshaikh^{ab}, Julian Knight^b, Simon Doherty^b

^a Department of Chemistry, King Abdulaziz University, Jeddah, Saudi Arabia ^bDepartment of Chemistry, Newcastle University, Newcastle upon Tyne, The United Kingdom *E-mail: hfalshakh@kau.edu.sa*

Metal nanoparticles are increasingly used in catalysis due to their high surface area and increased density of surface active sites compared to bulk metal.¹ Ionic liquids have been shown to stabilized nanoparticles towards aggregation and also, in some cases, to enhance the catalytic activity or selectivity.² In this project cross-linked ionic copolymers were prepared by radical polymerisation of imidazolium-functionalised styrene monomers together with styrene carrying a neutral pyrrolidinone derivative designed to interact with metal nanoparticles.

The ionic polymer was loaded with $PdCl_4^{2^-}$ by anion exchange and then hydrogenation produced a Pd (0) loaded polymer which was characterized by TEM, microanalysis, ICP-OES, XPS, XRD, and SEM. These palladium-immobilised ionic polymer-supported nanoparticles were demonstrated to be active catalysts for Suzuki cross coupling reactions, and we will explore the efficiency of palladium nanoparticles in a broader range of reactions including the selective hydrogenation of α , β -unsaturated aldehydes and ketones as well as the decompositions of formic acid to CO₂ and H₂.

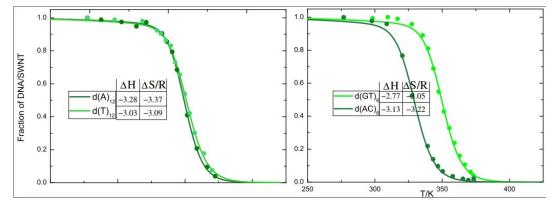
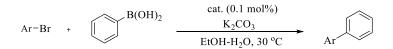
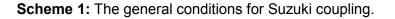


Figure 1. Fit results. Points are experimental points, lines are fitted theory. Parameters of fit shown in tables; enthalpy in kcal/(mol base) units. Errors of fit (not shown) in the range of several percents

Figure1: The structure and SEM image of the palladium loaded ionic polymer.





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Growth of MoSe₂ thin films and use in electrochemical hydrogen evolution

T. Chouki^a, B. Donkova^b, S. Emin^{a,*}

^a Materials Research Laboratory, University of Nova Gorica, Nova Gorica 5000, Slovenia ^b Faculty of Chemistry and Pharmacy, University of Sofia, 1 James Bourchier Blvd., Sofia 1164, Bulgaria. *E-mail:* saim.emin@ung.si

We present the chemical vapor deposition (CVD) approach to grow $MoSe_2$ thin films using colloidal molybdenum nanoparticles (Mo NPs). The synthetic protocol of Mo NPs was achieved using a wet-chemical method. The obtained Mo NPs were spin-coated on graphite substrates and heat-treated in the presence of selenium vapors at several temperatures (\geq 750 °C). The electrocatalytic activities of heat-treated MoSe₂ thin films were studied for hydrogen evolution reaction (HER) in 0.5 M sulfuric acid (H₂SO₄). The lowest recorded overpotential of 218 mV at 10 mA cm⁻² vs. a reversible hydrogen electrode was achieved with MoSe₂–800°C catalyst. In addition, electrochemical impedance spectroscopy (EIS) was performed to access the chargetransfer resistance of the MoSe₂ films. The colloidal approach combined with CVD is a promising route to produce carbon supported MoSe₂ electrocatalyst for HER.

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