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INTERNATIONAL ONLINE CONFERENCE ON FUNCTIONAL NANOMATERIALS

19 May 2020 | Online meeting

Abstract Book



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Table of Contents

Welcome Message	4
Program	5
Invited Speakers	7
Abstracts Invited Speakers	9
Abstracts Regular Speakers	16
Posters	19
Authors Index	33
Upcoming event organized by ENNA	34
Organizing Company	35

WELCOME MESSAGE

Dear colleagues and friends,

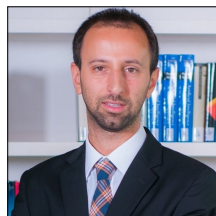
It is our pleasure to invite you to attend the International Online Conference on Functional Nanomaterials to be held on 19 May 2020. The conference brings together leading invited speakers and young researchers in photo/catalysis. It aims to provide a high-profile and internationally renowned online conference for researchers to present the latest research results in 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,



Prof. Dr. Saim Emin,
Conference Chair
University of Nova Gorica, Slovenia
&
European Nanoscience and Nano-
technology Association, Bulgaria



Prof. Dr. Giovanni Palmisano
Conference Co-Chair
Khalifa University of Science and
Technology, Abu Dhabi, United Arab
Emirates

PROGRAM 19 May 2020

Session on Photo/Catalysis

Session Chair: Saim Emin

- 12:00—12:10** Conference Opening / Session Introductory Remarks
- 12:10—12:35** **Maya Kiskinova** — Elettra Sincrotrone Trieste, Trieste, Italy
“Microscopic insights on properties of catalysts using synchrotronbased imaging and spectroscopy”
- 12:35—13:00** **Giovanni Palmisano** — Khalifa University of Science and Technology, Abu Dhabi, UAE
“Photocatalytic and energy-saving properties of stratified coatings for glass functionalization”
- 13:00—13:25** **Lourdes F. Vega** — Khalifa University, Abu Dhabi, UAE
“Understanding the performance of hierarchical carbon electrodes for lithium-air batteries by molecular dynamics simulations”
- 13:25—13:50** **Alexandre Loukanov** — Saitama University, Saitama, Japan
“Design of carbon nanodots as photo-catalytic nanozyme for oxygen reduction reaction”
- 13:50—14:10** **Break**

Session on Photo/Catalysis

Session Chair: Giovanni Palmisano

- 14:10—14:15** Session Introductory Remarks
- 14:15—14:40** **Carlos Jose Tavares**— University of Minho, Guimaraes, Portugal
“Photocatalytic Bi₂O₃/TiO₂:N Thin Films with Enhanced Surface Area and Visible Light Activity”
- 14:40—15:05** **Dr. Neus Domingo** — Catalan Institute of Nanoscience and Nanotechnology ICN2, Spain
“Ferrocatalysis: water splitting reactions on ferroelectric oxide surfaces”
- 15:05—15:20** **Habeebllah Oladipo**— Khalifa University of Science and Technology, Abu Dhabi, UAE
“Photocatalytic Hydrogen sulfide splitting over noble metal-free CdS/TiO₂ heterojunction”
- 15:20—15:35** **Saim Emin**— University of Nova Gorica, Nova Gorica, Slovenia
“Growth of transition-metal diselenides thin films and their application in electrocatalytic hydrogen evolution”

Poster Parade

- 15:35—15:38** **Corrado Garlisi** — Khalifa University of Science and Technology, Abu Dhabi, UAE
“Effect of Hafnium doping on photoelectrochemical properties of ZnO thin films”
- 15:38—15:41** **Ahmed Yusuf** — Khalifa University of Science and Technology, Abu Dhabi, UAE
“Photodegradation of Diclofenac Amide using N-TiO₂/Fe-TiO₂ in a recirculating Micro-slit photocatalytic reactor: Kinetic study and 3D simulation”
- 15:41—15:44** **Hind Alshaikh**— King Abdulaziz University, Jeddah, Saudi Arabia
“Ruthenium Nanoparticle Immobilized on Mesoporous Silica Functionalised Ionic Liquid Catalyst for Selective Hydrogenation”

- 15:41—15:44** **Samar Al Jitan**— Khalifa University of Science and Technology, Abu Dhabi, UAE
“rGO-(Pt/Cu-TiO₂) composite for the photocatalytic conversion of CO₂ into fuel: Activity in gas and liquid state”
- 15:44—15:47** **Pramod Vilas Shelar**— Haribhai Desai College, Maharashtra, India
*“Synthesis of Cu₂O nanoparticles using wheat-grass (*Triticum aestivum* L.) and investigation of its optical properties”*
- 15:47—15:50** **Sonia Siwatch**— Kurukshetra University, India
“Controllable synthesis of ZnO floweret by facile chemical bath deposition”
- 15:50—15:53** **Daniel Bahamon**— Khalifa University, Abu Dhabi, UAE
“Design of hybrid graphene oxide membranes via crown ether intercalation for water desalination”
- 15:53—15:56** **Amar Katkar**— Dr. B.N.Purandare Arts,Smt.S.G.Gupta Commerce and Smt.S. A. Mithaiwala Science College, Valvan, Maharashtra, India
“Growth of Longest Cr doped Core-Shell Ge/GeOX Nanowire”
- 15:56—15:59** **Artem Badasyan**— University of Nova Gorica, Nova Gorica, Slovenia
“Statistical mechanics of DNA adsorption on a carbon nanotube”
- 15:59—16:02** **Takwa Chouki**— University of Nova Gorica, Nova Gorica, Slovenia
“Iron phosphide thin films as an efficient electrocatalysts for hydrogen evolution reaction”
- 16:05—16:20** **Break**

16:20—17:50 **Poster Session**

INVITED SPEAKERS



Prof. Dr. Maya Kiskinova

Elettra-Sincrotrone, Italy

Title: "**Microscopic insights on properties of catalysts using synchrotronbased imaging and spectroscopy**"

Maya Kiskinova was born in Sofia (Bulgaria). She graduated from Sofia State University "Kliment Ohridski" in 1972 with Master in Chemistry She received her Ph.D in 1977 and Sc. D. Habilitation in 1989 in Physical Chemistry. She had joint appointment in Bulgarian Academy of Science and Sofia State University before moving to Elettra Laboratory in 1990 to coordinate the microspectroscopy and imaging programs. Presently she is the Elettra Research Coordinator, teaches a PhD Course in the University of Trieste and lectures at international schools.

Maya Kiskinova is member of many scientific and review panels in Europe, USA and Asia, has chaired and co-chaired a number of international conferences, workshops and schools and is a member of numerous steering and program committees. Her research interests and achievements cover different aspects of nano-structured organic and inorganic materials, thin films, interfaces, surface reactions, mass transport, electronic and magnetic properties, chemical reactivity, fuel and solar cells, nano-toxicology and transient states of matter. Last two decades her research activities have been focused on exploring the properties and transient states of matter at sub-micrometer length scales and development of relevant synchrotron and FEL-based experimental set-ups.

She authored and co-authored over 300 articles in reviewed journals, 14 invited reviews, one book, three book chapters and 2 U.S. patents and has over 100 invited, keynote and plenary lectures at International Congresses, Conferences, Symposia and Workshops. H-index 50 (SCOPUS).



Prof. Dr. Carlos Jose Tavares

University of Minho, Braga, Portugal

Title: "**Photocatalytic Bi₂O₃/TiO₂:N Thin Films with Enhanced Surface Area and Visible Light Activity**"

Carlos Jose Tavares is a Professor of Physics at the Department of Physics, and researcher from the Center of Physics, at the University of Minho in Portugal. Has expertise in: Synthesis of nanostructured thin films by magnetron deposition (Physical vapor deposition – PVD) technologies; Production of transparent conductive oxide thin films for photovoltaic and thermoelectric applications; Study of photocatalytic thin films; Controlled release of insecticides/repellents from solar activated microcapsules; Deposition techniques for PdAg alloys for hydrogen-selective ceramic membranes; Design of wear resistant and very hard nano layered coatings for automobile motor parts. He is the author of 5 patents, and principal investigator of more than 20 funded research projects. Currently, is the Director of SEMAT/UM lab (www.semat.uminho.pt), President of the Portuguese Vacuum Society (www.soporvac.pt). He is also the representative of SOPORVAC in the Applied Surface Science division of the International Union for Vacuum Science, Technique and Applications (IUVSTA). Currently, supervises several PhD students (5), MSc students (1), Research Assistants (4).

Design of wear resistant and very hard nano layered coatings for automobile motor parts. He is the author of 5 patents, and principal investigator of more than 20 funded research projects. Currently, is the Director of SEMAT/UM lab (www.semat.uminho.pt), President of the Portuguese Vacuum Society (www.soporvac.pt). He is also the representative of SOPORVAC in the Applied Surface Science division of the International Union for Vacuum Science, Technique and Applications (IUVSTA). Currently, supervises several PhD students (5), MSc students (1), Research Assistants (4).

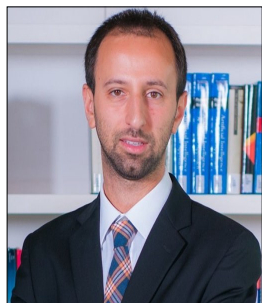


Prof. Dr. Alexandre Loukanov

Saitama University, Saitama, Japan

Title: "**Design of carbon nanodots as photo-catalytic nanozyme for oxygen reduction reaction**"

Alexandre Loukanov has completed his PhD from the Graduate University for Advanced Studies (SOKENDAI), Japan and DSc (Doctor of Sciences) from University for Mining and Geology, Sofia, Bulgaria. He is currently working as a Professor at Saitama University, Japan. He is also invited Professor at Arkansas University for Medical Sciences, USA and Vice President of the European Nanoscience and Nanotechnology Association.



Prof. Dr. Giovanni Palmisano

Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates

Title: "**Photocatalytic and energy-saving properties of stratified coatings for glass functionalization**"

Dr. Giovanni Palmisano earned his MSc in Chemical Engineering and his PhD in Chemical and Materials Engineering from the University of Palermo, Italy. Before joining Khalifa University (Masdar Campus), Dr. Palmisano's research activities were mainly developed in Italy and Spain and concern photo-catalytic processes for organic chemistry, hydrogen production, water and air remediation, and self-cleaning coatings, with a special attention to materials characterization, kinetics, modelling of photo-reactors and radiant fluxes. From 2009 to 2012, he was administrator, chief engineer and safety manager at Hedera Engineering Srl – an Italian company operating in design and construction of photovoltaic plants in Italy. From 2008 to 2013 he has held free-lance consulting activity for private companies and Italian municipalities. Dr. Palmisano has co-authored ca. 95 highly cited papers in peer-reviewed international journals, and he has to his record seven patents, six books and six invited book chapters.



Dr. Neus Domingo

Catalan Institute of Nanoscience and Nanotechnology ICN2, Spain

Title: "**Ferrocatalysis: water splitting reactions on ferroelectric oxide surfaces**"

Neus Domingo is born in Igualada (Catalonia), 1977. Graduated in Physics at Universitat de Barcelona (UB) in 1997, where she also obtained PhD in 2005 in the field of molecular magnetism and Single Molecular Magnets with a FPU fellowship from the MECED (Spain).

Interested on the study of phenomena of nanoscale objects at the nanoscale, she joined the CIN2 in 2008 under a Juan de la Cierva Fellowship where Neus Domingo focused her research on surface nanostructuring. In 2011 she integrated into ICN2 as a Ramon y Cajal Researcher

to provide the Oxide Nanophysics Group with her complementary skills on magnetism and force microscopy, and leading the research lines devoted to nanoscale studies. From 2016, Neus Domingo lead her own research group "Advanced AFM Lab", a Research Platform of the Institut Català de Nanociència i Nanotecnologia (ICN2), CSIC and the Barcelona Institute of Science and Technology (BIST).



Prof. Dr. Lourdes F. Vega

Khalifa University, Abu Dhabi, UAE

Title: "**Understanding the performance of hierarchical carbon electrodes for lithium-air batteries by molecular dynamics simulations**"

Dr. Lourdes F. Vega is a Professor in Chemical Engineering and Director of the Research and Innovation Center on CO₂ and H₂ (RICH Center) at Khalifa University in Abu Dhabi, UAE, as well as an Independent Member of the Board of Directors of the company ERCROS, SA, in Spain. Prof. Vega obtained her Ph.D. in Physics from the University of Seville, Spain, in collaboration with the Chemical Engineering Department, University of Southern California, USA. She has developed her career between academia and industry, with academic positions in the USA, Spain and the UAE. She was the General Director of MATGAS, R&D Director of Carburros Metálicos, Technology Manager of Air Products and Chemicals and Founder and CEO of AlyaTech. She is the Editor in Chief of the Journal of Molecular Liquids. With more than 200 publications and 5 patents under exploitation, she is internationally recognized for her contributions in molecular thermodynamics by applying fundamental knowledge to industrial problems. She has received several prestigious awards, including the Mohammed Bin Rashid (MBR) Medal for Scientific Distinguishment in 2020 for her contributions in clean energy and sustainable products, and the Physics, Innovation and Technology Prize awarded by the BBVA Foundation and the Royal Spanish Society of Physics in 2013, among others. She is Academician of the Academy of Mathematics, Physical Chemistry and Natural Sciences of Granada and an a member of the Mohammed Bin Rashid Academy of Sciences in the UAE.

Invited Talks

Contents

Microscopic insights on properties of catalysts using synchrotronbased imaging and spectroscopy	10
<i>Maya Kiskinova</i>	
Photocatalytic and energy-saving properties of stratified coatings for glass functionalization	11
<i>Giovanni Palmisano</i>	
Understanding the performance of hierarchical carbon electrodes for lithium-air batteries by molecular dynamics simulations	12
<i>Lourdes F. Vega</i>	
Design of carbon nanodots as photo-catalytic nanozyme for oxygen reduction Reaction	13
<i>Alexandre Loukanov</i>	
Photocatalytic Bi₂O₃/TiO₂:N Thin Films with Enhanced Surface Area and Visible Light Activity	14
<i>Carlos Jose Tavares</i>	
Ferrocatalysis: water splitting reactions on ferroelectric oxide surfaces	15
<i>Neus Domingo</i>	

Microscopic insights on properties of catalysts using synchrotronbased imaging and spectroscopy

Maya Kiskinova*,

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Heterogeneous catalysis, one of the crucial technologies employed in the chemical and energy industries, is exclusively controlled by processes occurring at the interface between the catalyst and gas or liquid phase that require issues of complexity at various microscopic length scales to be faced and understood. In this respect the complementary capabilities of synchrotron-based methods in terms of imaging, spectroscopy, spatial and time resolution and variable probing depths have opened unique opportunities to explore the catalysts' structure and chemical composition at relevant length and time scales and correlate them to the actual fabrication or operating conditions. The topics that will be addressed in the talk are the events occurring with metal, alloy and composite catalysts under growth and reaction conditions. The focus will be on the most recent achievements in characterization of key functional components used in energy-conversion devices and ongoing efforts for development and implementing in-operando experimental set-ups.

Photocatalytic and energy-saving properties of stratified coatings for glass functionalization

Corrado Garlisi^{a,b}, Esra Trepçi^c, Elie Azar^c, **Giovanni Palmisano**^{a,b}

^a *Department of Chemical Engineering, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates*

^b *Research and Innovation on CO₂ and H₂ (RICH) Center, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates*

^c *Department of Industrial and Systems Engineering, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates*

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We propose here a new approach based on a combined study of the self-cleaning and energy-efficiency properties of stratified WO₃/Cu-TiO₂ coatings for glazing applications. The multifunctional performance was investigated by varying the number of layers deposited on the glass substrate (i.e., 1, 2, 4 layers). The photocatalytic activity was assessed by the oxidation of carbon monoxide (CO) and a model volatile organic compound (i.e., toluene) under simulated solar light. Results indicate that wettability and photoactivity can be boosted by a multilayer configuration due to the inhibited charge recombination, as showed by photoluminescence spectroscopy, and to a gradual rise in surface roughness and porosity with the increasing number of layers, as revealed by morphological analysis (i.e., SEM, AFM). The 4-layer configuration enabled us to achieve the highest wettability and degradation of toluene over the coating consisting of Cu-doped TiO₂ stacked with WO₃. On the other hand, the analogous sample, but in the 2-layer configuration, was the most active sample towards CO oxidation.

Using building energy modeling, it was also shown that the applied coatings lead to important energy savings, exceeding 9% in total energy consumption and 18% in cooling loads. The best energy efficiency was achieved with a single layer of WO₃. However, its low visible transmittance reduced the amount of natural daylight entering the studied buildings, unintentionally increasing the electric lighting loads. The results highlight the importance of alternative configurations, such as Cu-doped TiO₂ in a dual-layer arrangement with WO₃, which provide a better balance between energy efficiency and access to daylight, an important driver of occupant comfort and wellbeing. The presented approach may pave the way for the development of a new generation of glass for building applications that optimize both building-centric and occupant-centric metrics of performance.

Understanding the performance of hierarchical carbon electrodes for lithium-air batteries by molecular dynamics simulations

Lourdes F. Vega^{a,b}, Mostafa Elabyouki^a, Daniel Bahamon^{a,b}, Maryam Khaleel^{a,b}

^a Chemical Engineering Department, Khalifa University, PO Box 127788, Abu Dhabi, UAE.

^b Research and Innovation Center on CO₂ and H₂ (RICH), and Catalysis and Separation Center (CeCaS), Khalifa University, PO Box 127788, Abu Dhabi, UAE.

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Currently, lithium-air batteries can achieve specific energy densities in the range of 500 to 1000 Wh.kg⁻¹ which is very comparable to gasoline, making them very promising candidates for competitive electric vehicles (EVs).[1] During discharge, lithium is oxidized at the anode to form lithium ions and release electrons. However, the formation of Li₂O₂ within the cathode degrades the performance of such batteries and is the requirement for high overpotentials during charging.[2] The mechanism through which Li₂O₂ is formed is considered a major debating point among researchers and could vary depending on the conditions to which the battery is exposed.[3]

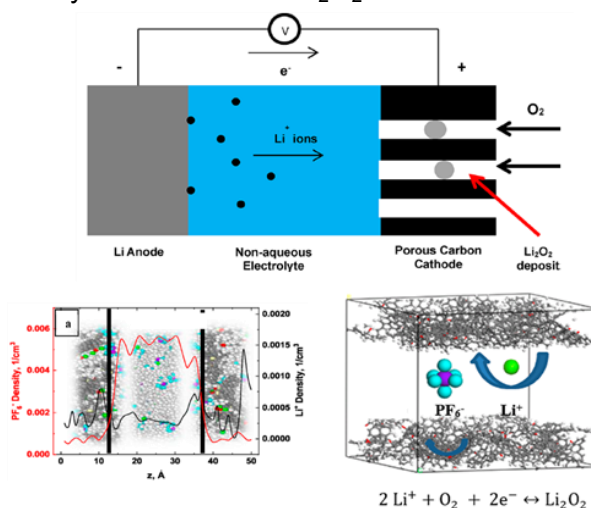
Tailoring the porosity of the carbon cathode has been shown to improve the discharge capacity of the lithium-air batteries.[4] Such tailored porosity can be achieved in hierarchical materials through the use of multiscale pores ranging from micropores (<2 nm) to mesopores (2–50 nm) and macropores (>50 nm). Understanding the mechanisms occurring at the electrochemical interface is key to explaining the improvement in performance provided by the hierarchical cathode. The ability to experimentally control structural features at the molecular level and recent progress made on modeling realistic carbon-structures, enable building predictive models from molecular simulations for novel applications.[5] In this regard, molecular simulations can be used as a robust, complementary tool to experiments, providing a direct route from the properties of interacting molecules to the thermodynamic properties of their bulk phases, and hence, they provide an alternative source of property data, while allow gaining insights into the physical phenomena of the adsorption process.

Hence, in this contribution, a hierarchical amorphous carbon structure synthesized from functionalized graphene was study using molecular dynamics (MD) simulations. Results show that the hierarchical carbon structure boosts the diffusivity of Li⁺ ions by several orders of magnitude compared to typical porous carbon structures.[6] Moreover, simulations provide insights into how the lower interface resistivity and higher energy storage capacity of a hierarchical cathode can guide the electrolyte to aid in the Li₂O₂ solvation within the meso/macropores, delaying the clogging of smaller pores.

We acknowledge the support of Khalifa University under the project CIRA-103 and the Research and Innovation Center on CO₂ and H₂ (RICH) RCII-2019-007.

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Design of carbon nanodots as photo-catalytic nanozyme for oxygen reduction reaction

Alexandre Loukanov*

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This research reports the generation of a novel phosphorescent “heavy carbon” nanodot via halogenation of the carbon nanodot structure. T_1 triplet character is introduced, and subsequently phosphorescence is observed in liquid media at room temperature. Phosphorescence and its pH-dependence were studied with aim to achieve photocatalytic oxygen reduction reaction of the carbon nanodots as an artificial nanozyme at neutral conditions.

Photocatalytic $\text{Bi}_2\text{O}_3/\text{TiO}_2:\text{N}$ Thin Films with Enhanced Surface Area and Visible Light Activity

Carlos Jose Tavares*

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Bi_2O_3 nanocone films functionalized with an overlayer of TiO_2 were deposited by d.c. reactive magnetron sputtering. The aforementioned nanocone structures were formed via a vapour-liquid-solid (VLS) growth, starting from a catalytic bismuth seed layer. The resultant nanocones exhibit an improved surface area, measured by atomic force microscopy, when compared to non-VLS deposition of the same metal oxide. X-ray diffraction texture analysis enabled the determination of the crystallographic tetragonal b-phase of Bi_2O_3 . Through atomic force microscopy analysis scans the roughness and projected surface area parameters of the Bi_2O_3 layers were quantified, while X-ray photoelectron spectroscopy determined the binding energy, composition and valence states of the main ions. A very thin TiO_2 overlayer (6 nm thick), undoped and doped with nitrogen, was deposited onto the nanocones template, in order to functionalize these structures with a photocatalytic, self-cleaning, cap material. N-doped TiO_2 overlayers increased the selective absorption of visible light due to nitrogen doping in the anatase cell, thus, resulting in a concomitant increase in the overall photocatalytic efficiency.

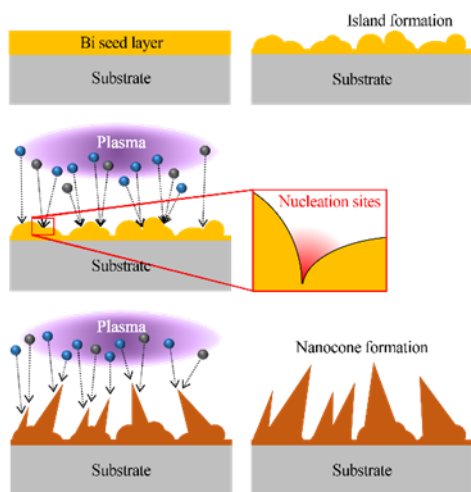


Figure 1 - Vapour-liquid-solid growth of Bi_2O_3 nanocone structures by reactive magnetron sputtering.

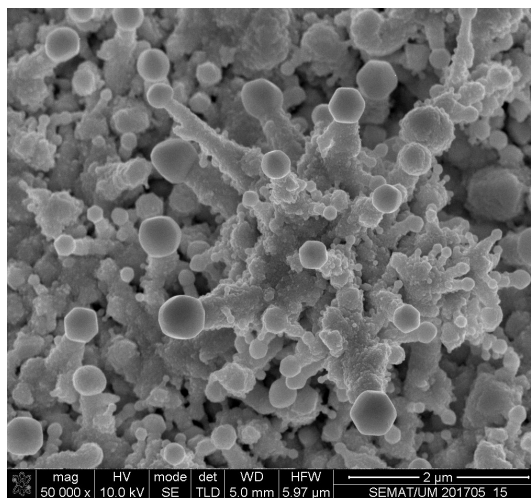


Figure 2 – SEM micrograph of the surface of Bi_2O_3 nanocone templates.

Ferrocatalysis: water splitting reactions on ferroelectric oxide surfaces

E. Pach,^{1,2} I. Spasojevic,¹ K. Cordero-Edwards,^{1,3} I. Gaponenko,³ P. Paruch,³ V. Pérez-Dieste,⁴ C. Escudero,⁴ A. Verdaguer^{1,2} and N. Domingo^{1,*}

¹ *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, 08193 Bellaterra, Barcelona, Spain*

² *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Barcelona, Spain*

³ *DQMP, University of Geneva, 1211 Geneva, Switzerland*

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It is well known that water molecules, either physisorbed or dissociated, play a major role in the stabilization of ferroelectric thin films and their polarization dynamics; water is a polar molecule sensitive to the stray electric fields on ferroelectric surfaces, can dissociate on the surface forming hydroxyls or providing ionic charges and moreover, under high relative humidity conditions, the deposited surface water layers enhance ionic movement and facilitate fast charge screening, having strong impact in polarization switching dynamics. But the entanglement between ferroelectricity and surface electrochemistry is two-fold, and as a counterpart, ferroelectric surfaces show specific electrochemical reactivity as a function of the ferroelectric polarization. This leads to a different composition of surface adsorbates as a function of ferroelectric polarization [1,2] as well as an irreversible imprint of the polarization on the native adsorbates layer [3]. On the other hand, this feature opens new opportunities such as *ferrocatalysis*, that is, to exploit ferroelectric surfaces in catalysis for water splitting since ferroelectric polarization becomes a switch to adjust surface catalytic properties.

Here, I will present a detailed analysis of the water splitting reactions (including oxygen and hydrogen evolution reactions) on ferroelectric surfaces as a function of polarization, obtained from the combination of near ambient pressure XPS analysis and Scanning Probe Microscopy techniques (essentially Piezoresponse Force Microscopy and Kelvin Probe Force Microscopy). We have studied surface electrochemical reactivity (and associated oxidation and reduction reactions) in Pb(Zr,Ti)O₃, BaTiO₃ and BiFeO₃ thin films, as compared to non-ferroelectric SrTiO₃ surfaces and BaTiO₃ single crystals in the paraelectric phase. I'll show how the surface redox activity is coupled to ferroelectricity by several different factors: the polarity of the stray electric fields, the coupling to screening mechanisms and the specific chemical active sites of each surface. The polarity of the surfaces determines their potential to reduce or oxidize, and tunes the surface chemistry by: i) altering molecular adsorption and changing the binding energies, ii) modifying the electronic band structure by internal screening mechanisms such as band bending near the surface, facilitating the concentration of electronic carriers close to the surface and iii) overall enabling the lowering of redox overpotentials. In this sense, the potential of ferroelectric materials for photocatalytic water splitting applications will be discussed.

References

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Regular Talks

Contents

Photocatalytic Hydrogen sulfide splitting over noble metal-free CdS/TiO₂ Heterojunction	17
<i>Oladipo Habeebllah</i>	
Growth of transition-metal diselenides thin films and their application in electrocatalytic hydrogen evolution	18
<i>Saim Emin</i>	

Photocatalytic Hydrogen sulfide splitting over noble metal-free CdS/TiO₂ heterojunction

Oladipo Habeebllah^{1,2,3} Yusuf Ahmed,^{1,2,3} Al-Ali Khalid,^{1,2} Pagliaro Mario,⁴ Palmisano Giovanni,^{1,2,3}

Department of Chemical Engineering, (2) Research and Innovation Centre on CO₂ and H₂, and (3) Centre for Membrane and Advanced Water Technology, Khalifa University, P.O. Box 127788, Abu Dhabi, United Arab Emirates. (4) Institute for Scientific Methodology, and Istituto per lo Studio dei Materiali Nanostrutturati, CNR via Ugo La Malfa 153, 90146 Palermo (Italy).

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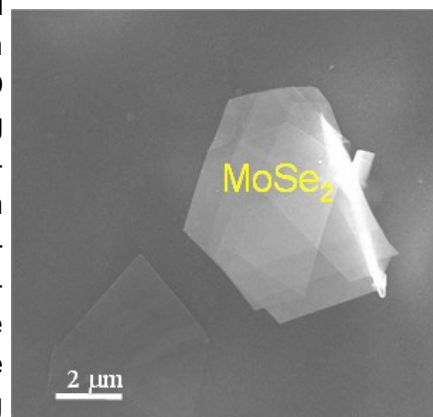
Cadmium sulfide (CdS) is considered one of the most efficient photocatalyst towards photocatalytic hydrogen sulfide splitting. However, due to its band positions, it suffers from recombination of photogenerated electrons and holes leading to a reduced photocatalytic activity. In this research, series of CdS-coupled nitrogen-doped titanium dioxide (N-TiO₂) was synthesized in order to reduce the recombination of electron-hole pairs. Evidence from UV-Vis DRS, XRD and SEM/EDS results show that under the catalyst preparation condition, a good contact is established between CdS and TiO₂ with CdS particle agglomerates grown on TiO₂ support. Reactivity study showed that the home-made composite CdS/N-TiO₂ outperformed bare CdS and N-TiO₂. This observation is attributed to Interparticle Electron Transfer (IPET) resulting from contact created by Ti – O – Cd bond connecting TiO₂ to CdS. Such electron transfer could reduce the recombination rate of photo-generated excitons. Thus, electrons and holes have longer life-span on the photocatalyst which consequently leads to improvement in the hydrogen production rate.

Growth of transition-metal diselenides thin films and their application in electrocatalytic hydrogen evolution

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Transition metal dichalcogenides (TMDs) with a general formula MX_2 (M- transition metal; X- chalcogen) have been demonstrated as promising catalysts for water splitting [1,2]. Especially, TMDs such as MoS_2 , MoSe_2 , WS_2 , WSe_2 , etc. in the form of two-dimensional (2D) layered materials have been studied for electrocatalytic hydrogen evolution reaction (HER) [3]. Here, we demonstrated for the first time the CVD growth of MoSe_2 and WSe_2 thin films onto graphite substrates starting from colloidal metallic (Mo,W) nanoparticles (NPs). The synthesis of metallic NPs has been achieved using a modified pyrolysis approach which involve molybdenum and tungsten hexacarbonyl precursors in 1-octadecene. The colloidal approach in combination with the CVD overcomes the disadvantages seen in other methods for achieving dense coatings with MoSe_2 and WSe_2 thin films. Electrocatalytic activities of the obtained MSe_2 (M- transition metal) films were evaluated for HER using linear sweep voltammetry (LSV). The best performing MoSe_2 film showed overpotential of 218 mV at 10 mA cm^{-2} in 0.5 M sulfuric acid (H_2SO_4). In conclusion, we have developed a procedure for the synthesis of metallic NPs which can be used for the preparation of different class of materials for water splitting studies. The colloidal approach combined with CVD is a promising route to produce carbon supported MSe_2 electrocatalyst for HER.



SEM image of MoSe_2 flakes.

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Posters

Contents

Photodegradation of Diclofenac Amide using N-TiO₂/Fe-TiO₂ in a recirculating Micro-slit photocatalytic reactor: Kinetic study and 3D simulation	20
<i>Ahmed Yusuf</i>	
Growth of Longest Cr doped Core-Shell Ge/GeO_x Nanowire	23
<i>Amar S. Katkar</i>	
Statistical mechanics of DNA adsorption on a carbon nanotube	24
<i>Artem Badasyan</i>	
Effect of Hafnium doping on photoelectrochemical properties of ZnO thin films	25
<i>Corrado Garlisi</i>	
Design of hybrid graphene oxide membranes via crown ether intercalation for water desalination	26
<i>Daniel Bahamon</i>	
Ruthenium Nanoparticle Immobilized on Mesoporous Silica Functionalised Ionic Liquid Catalyst for Selective Hydrogenation	28
<i>Hind Alshaikh</i>	
Synthesis of Cu₂O nanoparticles using wheat-grass (<i>Triticum aestivum</i> L.) and investigation of its optical properties	29
<i>Pramod V. Shelar</i>	
rGO-(Pt/Cu-TiO₂) composite for the photocatalytic conversion of CO₂ into fuel: Activity in gas and liquid state	30
<i>Samar Al Jitan</i>	
Controllable synthesis of ZnO floweret by facile chemical bath deposition	31
<i>Sonia Siwatch</i>	
Iron phosphide as an efficient electrocatalysts for hydrogen evolution	32
<i>Takwa Chouki</i>	

Photodegradation of Diclofenac Amide using N-TiO₂/Fe-TiO₂ in a recirculating Micro-slit photocatalytic reactor: Kinetic study and 3D simulation

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Abstract

The use of microfluidic reactors to study photocatalytic reactions such as pollutant degradation in wastewater are gaining tremendous attention. This is due to the remarkable properties of microreactors (such as high specific surface area, excellent mass and heat transfer rates, laminar flow, high spatial illumination homogeneity etc.), and the ease with which process variables can be precisely controlled and optimized. In this study, diclofenac amide (DCFA) was photodegraded in a recirculating micro-slit photocatalytic reactor with immobilized N-TiO₂/Fe-TiO₂. The conversion of DCFA was studied at varying initial concentration, recirculation flowrate and micro-channel height. A three-dimensional 3D computational fluid dynamics (CFD) simulation was carried out to simultaneously predict the DCFA degradation and estimate the observed intrinsic kinetics parameter.

Introduction

Heterogeneous photocatalysis (HPC) continue to attract great interest for decontamination of wastewater especially the recalcitrant pollutants pharmaceutical¹. One of the major research areas in HPC is in the design and operation of a photoreactor compatible with the photochemical reactions. Slurry reactors are the conventionally used and studied photochemical reactors operated in batch mode. These reactors are stymied with non-uniform distribution of light (be it UV or VIS) and mass transfer limitation as a result of slow diffusion². These setbacks are incompatible with heterogeneous photocatalytic reactions. In light of this, there have been surge in the amount of effort towards finding possible solutions³.

Of these possible solutions is process intensification, specifically the use of microfluidic photocatalytic reactors. Microreactors (MRs), with channel having at least one of its dimensions in few hundred microns, possess remarkable properties compatible with photochemical reactions. These properties include higher surface to volume ratio, better utilization of incident radiation, fast diffusion etc., compared to conventional reactors². Several studies have recently demonstrated the use of MRs in decontamination of water containing pollutants, in order to better study the effect and benefits of using such reaction environment. Charles et al.⁴ had recently investigated the degradation of salicylic acid in a MR by varying process parameters such as microchannel size, pollutant initial concentration, flow rate and UV light intensity. Corbel et al.⁵ had shown degradation of Ilos famide using ZnO-based quantum dots in a MR operating at low flow rate. Satuf et al.³ also degraded Clofibric acid, a pharmaceutical pollutant of concern, in a MR by varying flow rates, catalyst film thickness and UV illumination. The number of studies involving the use of MR for optimizing photochemical reactions is still insignificant and the benefits of this micro-systems is far from been fully leveraged and studied.

Therefore, in this work we present kinetics study and CFD simulation on the degradation of DCFA in a recirculating micro-slit photocatalytic reactor operating $N\text{-TiO}_2/\text{Fe-TiO}_2$. The conversion yield of DCFA was studied by varying initial pollutant concentration and recirculation flowrate.

Experimental

The experimental set up can be seen as shown in Fig. 1. The catalyst used was immobilized on the glass substrate through electron beam evaporation with thickness of about (350 nm). The conversion of DCFA was monitored using the UHPLC, DCFA showed maximum absorption at a wavelength of 200 nm. Before the light reactivity, the set up was Allowed to achieved adsorption equilibrium after about 4 h. Then the light was switched on for the photodegradation to commence. Degradation of DCFA was studied by varying the initial concentration (0.5, 1, 1.6 and 2ppm) and recirculation flowrate (2.5, 6.23 and 15 ml/min).

Results

Fig. 2 (dark) and Fig. 3 (light) show the effect of varying initial concentration of DCFA at recirculation flowrate of 6.23 ml/min. Fig. 4 and Fig. 5 depict the effect of changing flowrate in both dark and light at $C_o = 2\text{ppm}$.

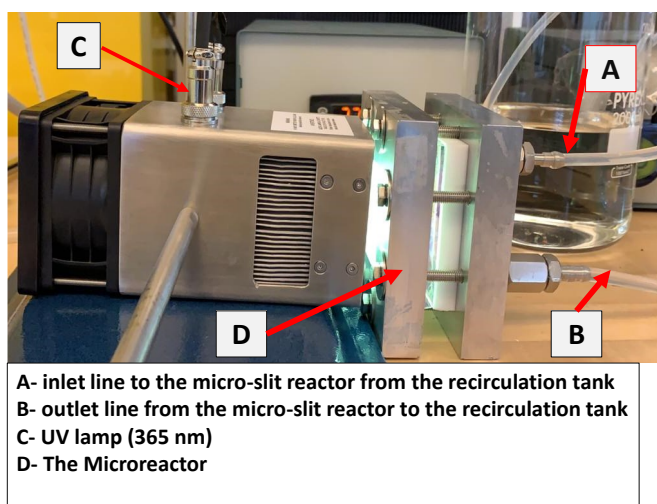


Fig. 1. Experimental setup for DCFA degradation

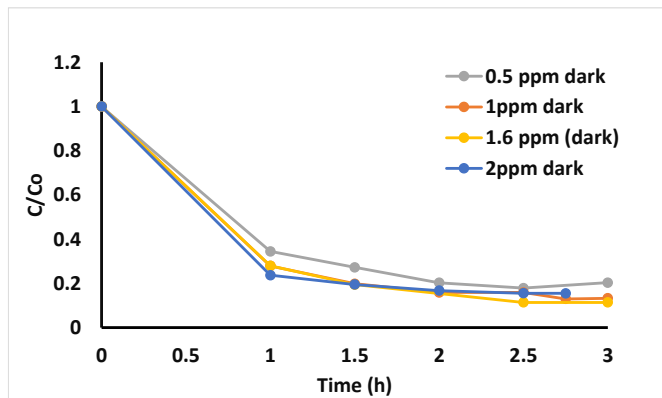


Fig. 2 effect of changing initial concentration in the dark at 6.23 ml/min

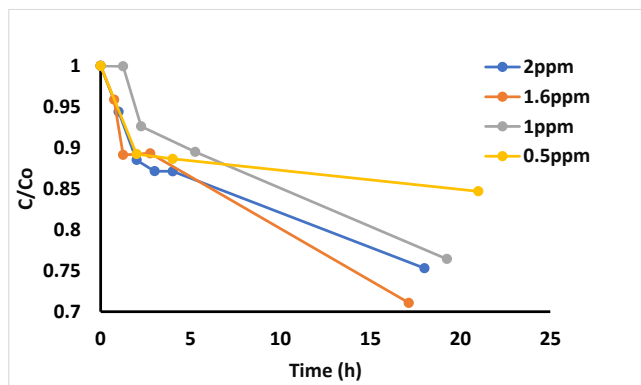


Fig. 3 effect of changing initial concentration in the light at 6.23 ml/min

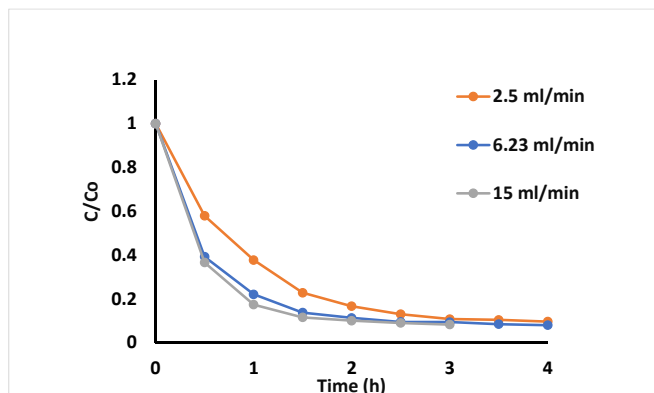


Fig. 4 effect of changing flowrate in dark at $C_o = 2\text{ppm}$

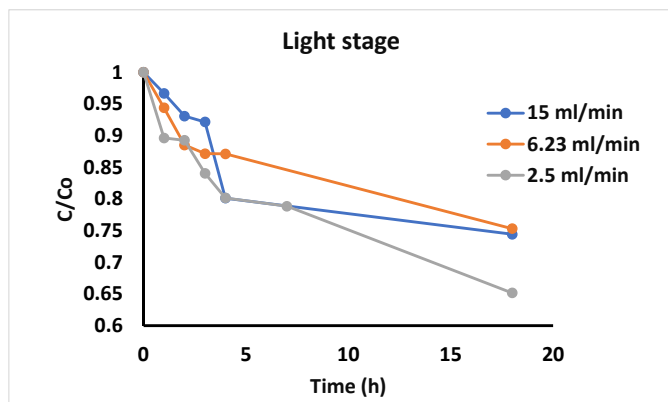


Fig. 5 effect of changing flow rate in the light for $C_o = 2\text{ppm}$

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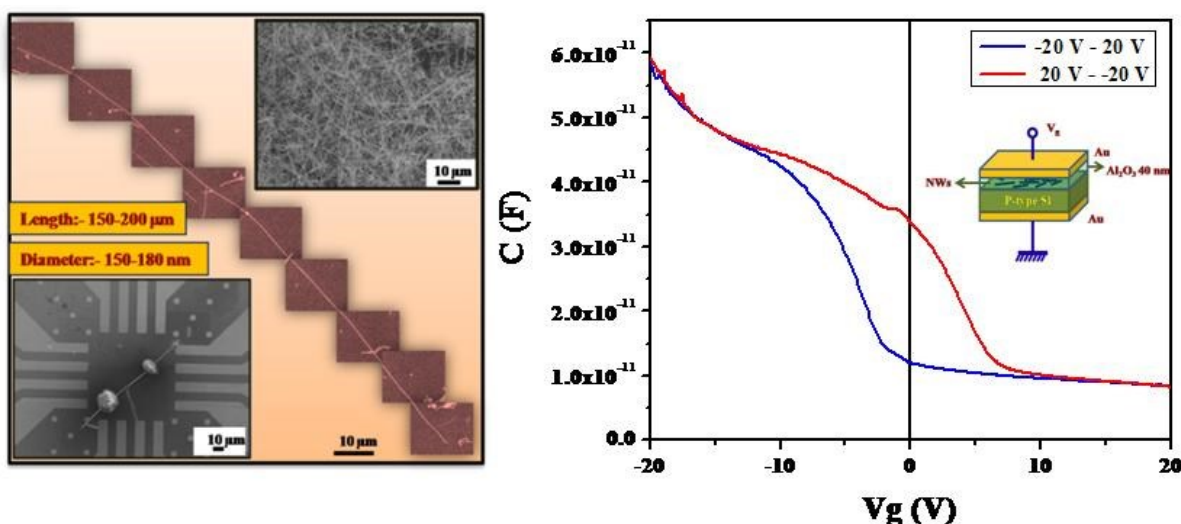
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Growth of Longest Cr doped Core-Shell Ge/GeO_x Nanowire

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Synthesis of ultralong, low diameter (High aspect ratio) and uniform nanowires could be useful for integration of multiple devices using one nanowire. In the present work simple vapor transport method was used to synthesize ultralong Cr-doped core-shell Ge/GeO_x nanowires. The conditions such as substrate temperature, precursors and required dopants were optimized for the growth of uniform ultralong Germanium nanowires. After characterizations the as prepared samples were utilized to investigate electrical and biological applications. The ultralong Cr-doped Ge/GeO_x nanowires could be very useful in future for the fabrication of electronic and biological devices.



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Statistical mechanics of DNA adsorption on a carbon nanotube

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The attraction between the polycyclic aromatic surface elements of carbon nanotubes (CNT) and the aromatic nucleotides of deoxyribonucleic acid (DNA) leads to reversible adsorption (physisorption) between them. With the goal to provide the theoretical support to numerous technologies on the basis of DNA-CNT hybrids [1], we propose a Hamiltonian formulation for the zipper model that accounts for relevant interactions and allows for the processing of experimental data, which has awaited an available theory for a decade.

We start by using the analogy between ssDNA adsorption on CNT and DNA melting: both can be considered as adsorption (desorption) of two 1D objects on each other. Following Ref.[2] we employ spin Hamiltonian formulation of Zimm-Bragg model, and take a short chain limit to derive expressions for zipper model [3]. We arrive at theoretical formulas for the degree of adsorption that are ready for the comparison with experiment.

While applications of DNA-CNT hybrids are very intense, the number of experimental studies of the phenomenon itself is surprisingly low. One of a few is the study of Albertorio et al. [4], where a solution of 12-base-long single stranded DNA oligomers was mixed with single-wall carbon nanotubes (SWNT). The thermal stability of the obtained hybrids was quantified indirectly by measuring the extent to which ssDNA dissociated from the nanotubes after incubation in an aqueous buffer solution at different temperatures by the detection of optical absorption at 815 nm.

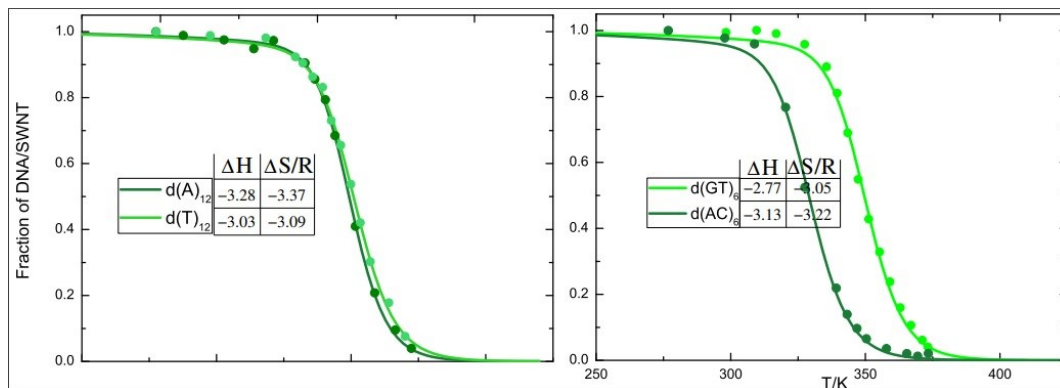


Figure 1. Fit results. Points are experimental points, lines are fitted theory. Parameters of fit shown in tables; enthalpy in kcal/(mol base) units. Errors of fit (not shown) in the range of several percents

We find that our theoretical formula nicely fits the data of Albertorio et al [4], with the enthalpy and entropy of adsorption about -3 kcal/(mol base), in agreement with previously reported values. Thus we illustrate the strength of simple spin models of Statistical Mechanics in describing systems, relevant for NanoBioTechnologies.

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Effect of Hafnium doping on photoelectrochemical properties of ZnO thin films

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Photoelectrochemical (PEC) water splitting is increasingly regarded as a very promising route to generate hydrogen gas using sunlight. Up to now, various semiconductor oxides such as TiO₂, ZnO, WO₃, Fe₂O₃ have been investigated as photoanodes for PEC hydrogen generation from water. Among these materials, zinc oxide ZnO is one of the best candidates due to its low cost, favourable band-edge position and non-toxicity. Unfortunately, the poor visible light-harvesting and fast recombination of the photogenerated carriers are severe limitations which undermine the activity of ZnO-based photoanodes. An increased performance of these materials is thus of utmost importance to make water splitting an efficient and cost-effective technology able to underpin a hydrogen economy. Doping with metal impurities is considered as being one of the most effective method for tuning the electronic structure of ZnO and overcome the intrinsic limitations. A wide range of metals such as aluminium, copper, vanadium, cerium and chromium have been used for this purpose. In this work, the effect of hafnium (Hf) doping on the PEC performance of ZnO thin films has been investigated for the first time. It was found that Hf-doping increased the donor density and caused a negative of the flat bend potential. Moreover, photocurrent transients and electrochemical impedance spectroscopy (EIS) confirmed how moderate doping improves the charge separation, allowing faster kinetics of the redox reaction at the thin-film surface and high PEC activity. Results showed that Hf-doping suppresses the formation of surface states, which act as recombination centers for the photogenerated carriers and determine a more inefficient water oxidation by the holes in pure and lightly doped ZnO. However, high doping levels preclude a further improvement of the PEC performance probably due to the emergence of new surface states in the materials introduced by superfluous Hf atoms.

Design of hybrid graphene oxide membranes via crown ether intercalation for water desalination

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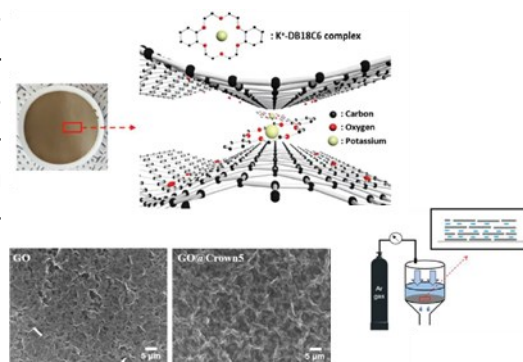
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Due to rapid population growth and climate change, the demand for fresh and clean water has increased over time. Membrane filtration has attracted much attention as a promising technique to secure clean water in an energy efficient manner.[1] As a result, various kinds of membrane materials, especially polymers, have been widely studied for desalination and water purification.[2,3] However, the availability of such polymer membranes in a large scale process is unsuitable due to a poor chemical stability, along with fouling issues.[4]

Graphene derivatives are emerging candidates for efficient water treatment membranes, attributed to their unique nanochannel network as well as the robust chemical and mechanical stability.[5] In particular, graphene oxide (GO) is regarded as a versatile platform for separating ions or contaminants due to its tunability and scalability. The characteristic nanochannels of GO membranes can be manipulated via intercalation of cations, inhibiting the transport of other ions in diffusion process. To maintain the tailored nanochannel during a pressure-assisted filtration procedure, it is essential to retain such inserted cations.

In this work, dibenzo-18-Crown-6 molecules (DB18C6) tightly binding to potassium ions were intercalated into GO nanosheets for an efficient desalination process.[6] The complex between potassium ion and DB18C6 forged sub-nanochannels between GO nanochannels, controlling the salt rejection rate as well as the permeation of water molecules, and selectively inhibiting the transport of Na⁺ ions compared to the untreated GO membrane. The as-prepared GO@Crown composite membranes exhibited excellent NaCl rejection rates (up to 60%) and water permeances (3.11–8.86 LMH.bar⁻¹) in the dead-end filtration process. In addition, molecular dynamics simulations were used to compute the tunable interlayer spacing of GO@Crown composite membranes and the possible configuration of crown ethers between GO layers, supporting the experimental results. Furthermore, it was found that the complex of crown ether and potassium ions can be further adjusted by varying the concentration and type of inserted crown ether molecules and cations.

This work was developed in the framework of a collaborative bilateral project between the Korea Advanced Institute of Science and Technology and Khalifa University of Science and Technology. This research was supported by the KAI-NEET Institute, KAIST, Korea. Additional partial support of this work was provided by Khalifa University of Science and Technology through project RCII-2019-007. Computational resources from the Research and Innovation Center on CO₂ and H₂ at Khalifa University are also acknowledged.



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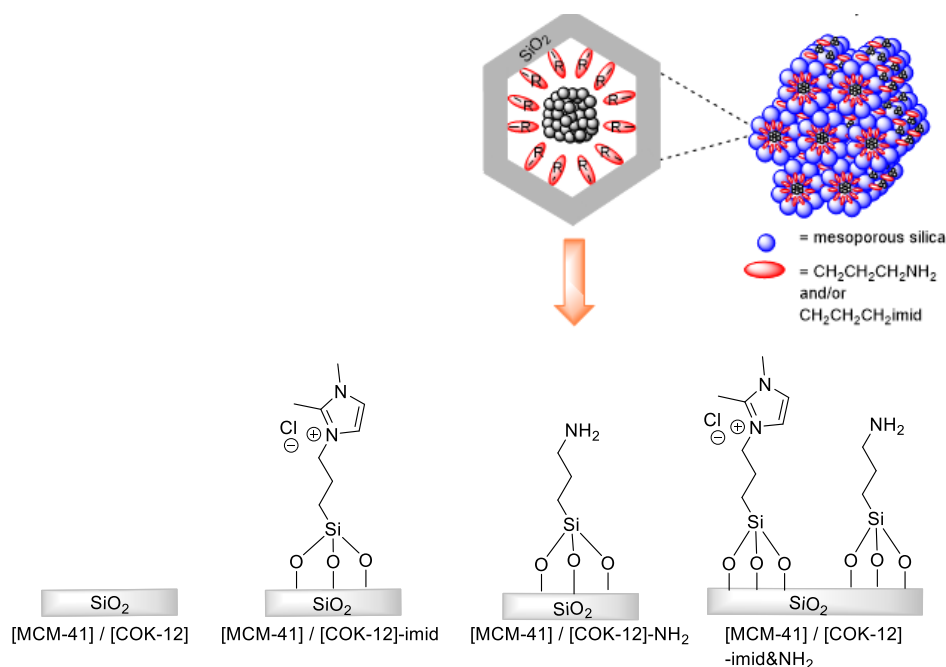
Ruthenium Nanoparticle Immobilized on Mesoporous Silica Functionalised Ionic Liquid Catalyst for Selective Hydrogenation

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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 A series of functionalized surfactant-templated mesoporous silicas were prepared by direct synthesis using a silica source such as sodium silicate (for COK-12 silica) in the presence of imidazolium-functionalized triethoxy silane and/or aminopropyltriethoxy silane.² The resulting mesoporous silicas carrying charged imidazolium and neutral amine functionality were loaded with Ru (0) nanoparticles by treatment with RuCl₃ followed by NaBH₄ reduction Figure 1. Solid-State NMR indicated that removal of the CTAB surfactant template from COK-12 by Soxhlet extraction was effective. The Ru (0) NPs immobilised on COK-12-based mesoporous support was shown to be an effective catalyst for reduction of a range of nitro aromatic compounds to the corresponding anilines using Me₂NHBH₃ as the stoichiometric hydrogen source. The material carrying both ionic imidazolium and neutral amine functionality outperformed the corresponding materials lacking either or both of these groups. The materials were characterized by HTEM, microanalysis, ICP-OES, XPS, XRD, SEM, and TGA-DSC.



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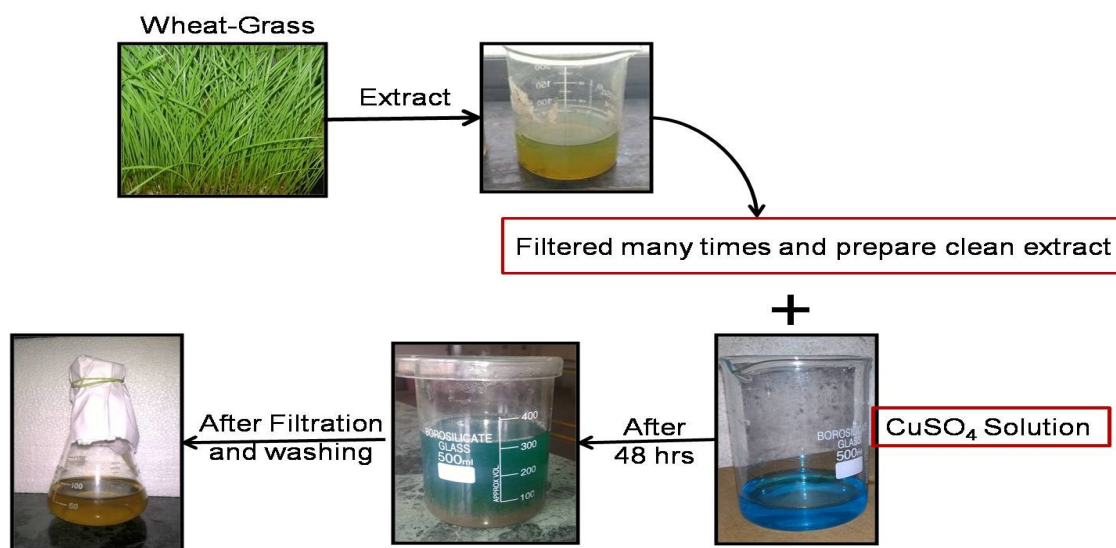
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Synthesis of Cu₂O nanoparticles using wheat-grass (*Triticum aestivum* L.) and investigation of its optical properties

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The Cu₂O nanoparticles has been synthesized successfully by using a simple biological synthesis method. Wheat-grass (*Triticum aestivum* L.) which can be easily grown, was used for the synthesis of Cu₂O nanoparticles. Due to required functional group for reducing and stabilizing the nanoparticles, wheat-grass extract was selected for the synthesis of Cu₂O NPs. The experimental conditions for synthesis of Cu₂O nanoparticles was optimized by variation in the ratio of extract solution and CuSO₄ solution. After filtration, the brown color residue the Cu₂O thin film was prepared using doctor blade method. The as prepared sample was characterized by XRD, FESEM and TEM. The optical properties of the sample was done using UV-VIS spectroscopy and Photo Luminescence. As wheat-grass is herbal medium and having pharmacological and medicinal properties, by investigation of functional group attached to Cu₂O nanoparticles the antimicrobial activity of the sample will be useful in future.



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rGO-(Pt/Cu-TiO₂) composite for the photocatalytic conversion of CO₂ into fuel: Activity in gas and liquid state

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The rising level of global CO₂ emissions is an ever-growing environmental concern. Although carbon capture and sequestration (CCS) technologies may appear to be very promising in removing excess CO₂ from the atmosphere, in most cases they are expensive and energy intensive. To make CCS technologies more economically feasible, carbon capture and utilization (CCU) technologies have emerged. Atmospheric CO₂ may be utilized by converting it into different value-added products, such as methane, methanol, ethanol and heavier hydrocarbons. Unlike other CO₂ conversion techniques, photocatalysis takes place at mild reaction conditions, utilizes a renewable and sustainable form of energy and most importantly doesn't increase net CO₂ emissions¹. Despite the extensive amount of studies performed in the area of CO₂ photoreduction, researchers have yet to discover an efficient photocatalyst that can reduce CO₂ to yield economical amounts of value-added products under the irradiation of solar light.

Hence, in this study, an attempt in enhancing the performance of TiO₂-based photocatalysts for application in CO₂ conversion was made. Surface modifications to help enhance the visible light absorption and the charge separation of TiO₂ photocatalysts were pursued. The end photocatalytic composite consisted of a (Pt/Cu-TiO₂) core and an (rGO) shell. To investigate the intrinsic and enhanced properties of the photocatalytic composite developed for this project, several advanced material characterization tools were employed and they include XRD, Raman, DRS, PL, TEM, STEM-EDX, BET, and FT-IR. A custom-built reactor was used to test the photocatalytic activity of (Pt/Cu-TiO₂)-rGO in reducing CO₂ under different reaction conditions. More specifically, the photocatalyst was tested for the photoreduction of gaseous CO₂ (P = 9.5 bar) and liquid CO₂ (P = 62 bar) under UV light irradiation. Gas-phase and liquid-phase products from the different photoreactivity tests were analysed using GC-FID and HPLC, respectively.

Results from this study show a significant enhancement in product yield with the photoreduction of liquid CO₂ when compared to that of gaseous CO₂. A variety of different catalysts have already been tested in numerous studies for the photocatalytic reduction of gaseous CO₂². The photocatalytic reduction of liquid CO₂, however, has been rarely investigated³.

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Controllable synthesis of ZnO floweret by facile chemical bath deposition

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Using facile chemical bath deposition process, the ZnO floweret were grown on ITO substrate. Synthesis process consists two steps, first step includes the formation of the ZnO seed layer on ITO substrate by spin coating method, second step which involves formation of ZnO floweret on seed layer by chemical bath deposition process. We demonstrate structural, optical and morphological characteristics of ZnO floweret by X ray diffractometer (XRD), UV-Vis spectrometer and Field emission scanning electron microscope (FESEM). Role of hexamethylenetetramine in the formation of ZnO floweret has been studied. The XRD results show the pure wurtzite phase with high crystallinity. The FESEM reveals that synthesized ZnO floweret is an assembly of nanopetals. Growth mechanism of ZnO floweret exhibits that tremendous amount of ZnO kernel clumps with each other and appears as a broad root for the growing of floweret like structure.

Iron phosphide as an efficient electrocatalysts for hydrogen evolution

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We report the solvothermal synthesis of iron phosphide electrocatalysts using a low-cost phosphorus precursor. The synthetic protocol allows for the preparation of a Fe_2P 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) Fe_2P provided a pure Fe_3P phase ($\text{Fe}_3\text{P}-500^\circ\text{C}$) and (ii) FeP transformed into a mixture of iron phosphide phases ($\text{Fe}_2\text{P}/\text{FeP}-500^\circ\text{C}$). The electrocatalytic activities of heat-treated $\text{Fe}_2\text{P}-450^\circ\text{C}$, $\text{Fe}_3\text{P}-500^\circ\text{C}$, and $\text{Fe}_2\text{P}/\text{FeP}-500^\circ\text{C}$ catalysts were studied for hydrogen evolution reaction (HER) in 0.5 M sulfuric acid (H_2SO_4). The lowest recorded overpotential of 110 mV at 10 mA cm^{-2} vs. a reversible hydrogen electrode was achieved with $\text{Fe}_2\text{P}/\text{FeP}-500^\circ\text{C}$ 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.

AUTHORS INDEX

Alshaikh, H.— p. 5, 19, 27
Badasyan, A.— p. 6, 19, 24
Bahamon, D.— p. 6, 19, 26
Chouki, T.— p. 6, 19, 31
Domingo, N.— p. 5, 7, 9, 15
Emin, S.— p. 2, 4, 5, 16, 17, 18, 31
Garlisi, C.— p. 5, 19, 25
Jitan, S.— p. 6, 19, 29
Katkar, A.— p. 6, 19, 23
Kiskinova, M.— p. 5, 7, 9, 10
Loukanov, A.— p. 5, 8, 9, 13
Oladipo, H.— p. 5, 16, 17
Palmisano, G.— p. 2, 4, 5, 8, 9, 11, 20, 25, 29
Shelar, P.— p. 6, 19, 28
Siwatch, S.— p. 6, 19, 30
Tavares, C. — p. 5, 7, 9, 14
Vega, L.— p. 5, 8, 9, 12, 26
Yusuf, A.— p. 5, 19, 20

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