University of Jaffna
Sri Lanka

Western Norway
University of
Applied Sciences

Proceedings of the

International Conference on
Advanced **M**aterials for **C**lean **E**nergy and **H**ealth **A**pplications

February 6 - 8, 2019
University of Jaffna, Sri Lanka

AMCEHA - 2019

Conference Proceedings

International Conference on
Advanced Materials for Clean Energy and Health Applications

February 6 – 8, 2019

AMCEHA-2019

University of Jaffna, Sri Lanka

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Message from the Vice-Chancellor

It gives me great pleasure to give this message to the International Conference on **Advance Materials for Clean Energy and Health Applications (AMCEHA-2019)**, the First Conference of this nature at the University of Jaffna.

The international conferences are anticipated to extend an opportunity for scientists, academics and young researchers, both locally and internationally, to exchange their knowledge and experiences. Even though the University of Jaffna has its own history and fame for its academic activities, it was unable to hold international or national conferences until 2010 due to the unsettled situation prevailed in this region. Since 2010, the University is striving hard to regain its status by holding Workshops, Symposia and Conferences at National and International levels.

This conference is aimed at gathering suggestions, views, successes and experiences for the development of clean energy technologies and health applications utilizing nanomaterials while addressing the current progress in development processes of the same. These suggestions can provide ideas and thoughts for the modifications or changes which have to be brought into the current ongoing projects as well as the new projects which are in the developmental stages or at planning levels.

For this conference, 4 symposia, namely Symposia on Advanced Materials for Health Applications, Solar Energy Applications, Advanced Functional Materials and Bioenergy/Wind Energy/Hydrogen Energy and Storage/Environmental Applications, were identified and a total of 136 abstracts have been accepted out of 184 submissions. Another highlight of this conference is the keynote/plenary speeches by internationally recognized researchers from UK, USA, Japan, Australia, Norway, Sweden, Finland, India and Sri Lanka.

I would like to congratulate and thank the Conference Co-chairs, Prof. Dhayalan Velauthapillai and Prof. Punniamoorthy Ravirajan, and all other members of the organizing committee for their tireless effort to make this Conference a success. The University of Jaffna should make efforts to continue to hold such International Conferences.

Prof. Ratnam Vigneswaran

Vice-Chancellor, University of Jaffna

Message from Rector, HVL

The growing world population and the environmental challenges demand more focus on clean energy and health technologies.

As the demand for clean energy is going to be immense in the future and many countries consider transforming themselves into clean energy economies, it is of utmost interest for the research community to work on novel ideas and find solutions for the challenges faced by the clean energy sector.

Countries are also becoming more and more focused on efficient medical care and new innovative medical and healthcare technologies. Rapid progress in nanotechnology in the past decade and use of advanced nanomaterials have provided significant breakthroughs in the area of both energy and health sectors.

The UN's 2030 Agenda for sustainable development has identified 17 development goals, the SDGs. Goal number 7 is to ensure access to affordable, reliable, sustainable and modern energy for all. Goal number 3 is to ensure good health and well-being for the world population.

I am very happy that this conference directly deal with two important development goals. I hope that through new cooperation and networks created by this conference, we will address several of the SDG goals and contribute to achieve them.

It is of utmost importance that we create arenas across the globe to bring together academic scientists, leading engineers, industry researchers and research scholars to work on new technologies. Thus, I am very pleased to note that the international conference has created wide interest among the researchers in Sri Lanka, Norway, India and other countries with over 180 quality research presentations.

This international conference on Advanced Materials for Clean Energy and Health Applications (AMCEHA 2019) is another important milestone in the partnership between University of Jaffna, HVL and our partners.

I sincerely hope that the conference will provide a forum for exchange of technical and scientific information between international researchers, engineers and students. My best wishes to all the participants at AMCEHA 2019, and I hope that the proceedings published with the accepted abstracts will contribute positively to this important research field on advanced materials.

Prof. Berit Rokne

Rector, Western Norway University of Applied Sciences (HVL), Norway

Message from the Vice-Chairman, UGC

I am delighted to learn that the University of Jaffna is organizing an International Conference on Clean Energy Technologies through effective collaborations with several leading foreign universities under a vital research project titled “Higher Education and Research Collaboration on Nanomaterials for Clean Energy Technologies” (HRNCET). The University Grants Commission has always been appreciative of such collaborations with international partners by the Universities under its purview. Therefore, I congratulate the University of Jaffna for the initiative and express my sincere gratitude to one and all who involved in bringing this project to the University of Jaffna.

As a Head/Research and International Collaboration Unit of the University Grants Commission, I have been observing the tremendous progress of this substantial project, HRNCET since the signing the MOU between the University of Jaffna and Western Norway Universities of Applied Sciences in March 2017. Apart from international students - staff exchange and development of the MSc curriculum on Clean Energy Technologies, this initiative further strengthens and expands research collaboration between the partner institutions by carrying out collaborative research activities in the field of advanced materials for clean energy and health applications. Possibilities for sharing knowledge with fellow researchers and disseminating research findings in the area through international conferences and publications in reputed journals is an added advantage brought by the project.

I wish the organizing committee and participants to have a successful conference by way of sharing knowledge through useful deliberations and conference proceedings with high-quality abstracts. I am confident that this will lead to more active collaboration in the future.

Prof. P. S. M. Gunaratne

Vice-Chairman and Head/Research and International Collaboration Unit
University Grants Commission

Message from the Ambassador

Energy and health are two essential areas that need attention for safeguarding our future. No society can hope to achieve economic sustainability without adequate energy supplies; energy is needed in all aspects of life. Dependency on energy sources like coal, oil and gas pollute our air and water, which in turn harm the health of our communities. We therefore need to look towards a future where clean energy is more accessible and profitable than fossil fuels, not only to meet the energy demand, but also to make our surroundings healthier. We can live better lives while creating good jobs, making great neighbourhoods, and saving our green space.

With a growing population and global economic development the demand increases for both energy and more efficient healthcare technologies. Nanotechnology has paved the way for new ideas and innovations that will benefit both sectors. The progress made with advanced nanomaterials can be applied to both innovations in clean energy technologies and health applications. How do we make sure these technologies gain the attention and focus they need and deserve?

The international conference on Advanced Materials for Clean Energy and Health Applications (AMCEHA 2019), jointly arranged by University of Jaffna and Western Norway University of Applied Sciences, is hence a timely event and response. This conference gathers both national and international actors, researchers and scholars. It provides a platform where opportunities can be explored, where research and ideas can become ambitions and possibilities, where projects can be driven forward, and the industry promoted. I am pleased to learn that over 180 research articles have been submitted for publication, and hope that the wide participation will inspire and motivate the younger generation in Sri Lanka to get involved in high quality research in clean energy and health technologies.

I wish all the researchers, academics, students and participants a successful conference, and hope that the conference proceedings with high quality abstracts will lead to a more active collaboration.

Thorbjørn Gaustadsæther

Norwegian Ambassador to Sri Lanka and Maldives

Message from Co-Chairs

Universities are not merely institutions that only engage in teaching and learning. Engagement in research and dissemination of the research findings to society in productive ways is an important role for any university.

In this regard, Western Norway University of Applied Sciences (HVL) and University of Jaffna (UoJ) have jointly secured funds from Norwegian Centre for International Cooperation in Education (SIU) and Royal Norwegian Embassy in Sri Lanka over a period of five years (2017-2021) for projects on Higher education and Research collaboration on Nanomaterials for Clean Energy Technologies (HRNCET) and Capacity Building and Establishment of a Research Consortium, respectively (http://project.jfn.ac.lk/hrncet/) .

One of the objectives of these projects is to strengthen the collaboration between the partner institutions by carrying out collaborative research activities in the field of advanced materials for clean energy and health applications and sharing knowledge with fellow researchers and disseminating research findings in the field through international conferences.

The theme of this conference was born out of a desire to highlight the challenges in utilizing potential nanomaterials for clean energy and health applications and to provide an opportunity for the community of researchers to respond to the challenges identified. AMCEHA 2019 is held under six thematic areas, namely (1) Solar energy (2) Wind energy, (3) Hydrogen energy and storage, (4) Materials for health applications, (5) Bio energy and (6) Advanced Functional Materials. As part of the conference, workshops and meetings are also arranged for administrators of the Universities and private enterprises involved with clean energy technologies in order to encourage the private sector involvement in clean energy research.

About 320 participants, including more than 120 international participants from around the globe are attending the conference. Over 180 articles were submitted and up to 140 research publications have been selected after peer-review process for presentations. Selected quality papers will be published as full-scaled articles in renowned journals through another set of peer-review.

We thank our partners, University of Peradeniya and Sri Lankan Sustainable Energy Authority, Universities of Bergen and Agder and Institute for Energy Technology from Norway, the University of Exeter from the United Kingdom, Coimbatore Institute of Technology and PSG College of Technology from India. Special thanks go to for the Royal Norwegian Embassy in Colombo, the Norwegian Centre for International Cooperation in Higher Education (SIU), the Norwegian Research Council, Sri Lankan Sustainable Energy Authority and Ministry of Science, Technology and Research for funding the conference. We are obliged to render our sincere gratitude to the Chief-editor of the AMCEHA-2019 Conference Proceedings, Mr. S. Suthakar for his valuable and tireless efforts in establishing an efficient technical system for paper submissions, and in coordinating the reviewing process and the editorial committee.

Prof. Punniamoorthy Ravirajan and **Prof. Dhayalan Velauthapillai**
Conference Co-Chairs/AMCEHA 2019 and Coordinators/HRNCET project

Editor's Note

It is with great pleasure I have organized and put together the Proceedings of the International Conference on Advanced Materials for Clean Energy and Health Applications (AMCEHA-2019). This experience gives me an opportunity to read the studies and work of internationally well-known research scholars and makes me proud.

This Proceedings comprises of twenty-five abstracts of keynote/plenary speeches and 136 abstracts of research works carried out by researchers all around the world. We received a total of 184 abstracts. After a rigorous, double blind, review process, 103 were accepted for oral presentations and 33 for poster presentations. Thus the acceptance rate was about 70%.

On behalf of the editorial committee, I would like to take this opportunity to extend our sincere thanks to all our reviewers. For this AMCEHA-2019 conference, we recruited a team of 134 experienced reviewers from the broader research community. Each paper was reviewed by at least three reviewers and screened by symposium co-chairs and editors before a decision was made. The double-blind nature of the review process was strictly maintained throughout. While it was difficult to assign three reviewers for each submission, the selected reviewers distinguished themselves by both the number and quality of their reviews.

As the conference editor, I am deeply aware of how much I personally owe to our conference team. I would like to sincerely thank all the AMCEHA-2019 committee members, especially the conference chairs, symposium co-chairs, and our editorial committee for their continuous guidance, support, motivation, and valuable suggestions.

Finally, I wish all the attendees a highly stimulating, informative, and enjoyable conference.

S. Suthakar

Conference Editor / AMCEHA-2019

Our Speakers

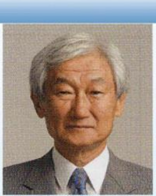
Symposium on Solar Energy Applications

Prof. Jenny Nelson
Professor
Imperial College London
United Kingdom

Prof.Kirthi Tennakone
Professor
Georgia State University
USA

Prof.MAKL Dissanayake
Professor
National Institute of Fundamental Studies
Sri Lanka

Prof.Satoshi UCHIDA
Professor
The University of Tokyo
Japan



Dr.Shoji Kaneko
Former Professor
Shizuoka University and SPD Laboratory
Japan

Symposium on Advanced Materials for Health Applications

Prof. Kamal Mustafa
Professor
University of Bergen
Norway

Prof. Anna Finne Wistrand
Professor
KTH Royal Institute of Technology
Sweden

Prof. Susanna Miettinen
Professor
University of Tampere
Finland

Prof.J. Annaraj
Professor
Madurai Kamaraj University
India

Dr.K. Ganeshan
Senior Research Fellow
University of Melbourne
Australia

Symposium on Bioenergy/Wind Energy/Hydrogen Energy and Storage/Environmental Applications

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Professor
University of Peradeniya
Sri Lanka

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Professor
University of Technology, Sydney
Australia

Prof. Aleksandar Matic
Professor
Chalmers University of Technology
Sweden

Prof. Kumudu Perera
Professor
Wayamba University of Sri Lanka

Eng. Namiz Musafer
Member of the board of directors of
Bio Energy Association and
Lanka Biogas Association

Symposium on Advanced Functional Materials

Dr.Smagul Karazhanov
Senior Scientist
Institute of Energy Technology (IFE)
Norway

Prof. K. M. Nalin de Silva
Professor
University of Colombo
Sri Lanka

Prof. S. Balakumar
Professor
University of Madras
India

Prof. P. Ravindran
Professor
Central University of Tamil Nadu
India

Symposium Co-Chairs

Solar Energy Applications

Prof.N. Muthukumarasamy
Coimbatore Institute of Technology
India

Advanced Materials for Health Applications

Prof. Kamal Mustafa
Professor
University of Bergen ,Norway

Advanced Functional Materials

Dr.Senthilarasu Sundaram
University of Exeter
United Kingdom

Bio, Wind, Hydrogen Energy & Environmental Applications

Prof.Alfred Christy
University of Agder
Norway

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Symposium on

Solar Energy Applications

Abstract of Keynote Speech – I

Molecular Electronic Materials for Solar Energy Conversion

Jenny Nelson

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Molecular electronic materials such as conjugated polymers and small molecules have attracted intense interest for applications in solar energy conversion as well as to light emission, thin-film electronics and other fields. Their appeal lies in the potential to tune material properties (electronic, optical, mechanical and thermal) through control of chemical structure and molecular packing, whilst using facile fabrication methods. Achieving this goal has been challenging, however, due to the intrinsic disorder and structural heterogeneity of the materials and the lack of appropriate device-physics models to relate structure to physical properties. Recent developments in materials design, computational modelling and experimental characterisation have led to the demonstration of improved molecular materials systems for photovoltaic energy conversion. We will discuss the factors that control photovoltaic efficiency in molecular materials, considering the impact of chemical and physical structure on properties such as phase behaviour, electronic transport, light harvesting, and charge recombination and consider the limits to conversion efficiency in such systems. We will briefly address the application of conjugated polymers to the challenge of energy storage, as functional materials for both electrochemical devices and photocatalytic energy conversion.

Abstract of Keynote Speech – II

Nanostructured Solar Cells: Problem of Hole Collector Materials

K. Tennakone [1], A.G.U. Perera [1], A. De Silva [2], G.R.A, Kamara [3]

[1]Department of Physics, Georgia State University, USA
[2]Department of Physics, University of West Georgia, USA
[3]Institute of Fundamental Studies, Sri Lanka

Dye-sensitized solid-state and perovskite solar cells are heterojunctions of the configuration n-type-semiconductor/light absorber/p-type semiconductor, where the optical transparency of both nanostructured semiconductor films, ensure optimum light harvesting. Generally one film (in most cases, the n-type substrate made of an oxide semiconductor) is designed nanostructured, so that the sandwiched light absorber layer acquire a high folded surface area, optimizing the light absorption cross-section. In the ideal situation, the hole collector subsequently deposited, acquire similar nanostructure maintaining a perfect physical contact. However, in reality, it is hard to achieve a perfect contact and even if such a contact is made, it may not establish the necessary electronic coupling- enabling hole transfer- directly or via exciton decomposition. Low efficiency and instability of thin absorber solar cells owes much to the nature of the absorber/hole-collector junction. Fundamental and practical issues related to use of hole collector materials in heterojunction devices will be discussed.

Abstract of Plenary Talk – I

The Role of "Mixed Cations" in Electrolytes of Dye Sensitized Solar Cells

M.A.K. Lakshman Dissanayake

National Institute of Fundamental Studies, Kandy, Sri Lanka
E-mail: makldis@yahoo.com

Dye sensitized solar cells (DSSCs) based on nanostructured titanium dioxide (TiO_2), offer a low cost alternative to conventional silicon and thin film solar core stable cells can be fabricated by replacing the liquid electrolyte by quasi-solid (gel) or solid electrolytes at the expense of their efficiency. The efficiency enhancement in these solar cells has therefore become an important research problem. In solar cells using iodide-tri-iodide as the redox couple, the iodide salt, particularly the cations, play a vital role in determining the short circuit current density (J_{sc}), open circuit voltage and hence the efficiency. Based on independent work on single cation iodide salts by several research groups, it is generally established that, small cations like K^+ and Li^+ can get easily adsorbed by the TiO_2 in the photoanode causing a positive shift in the conduction band of TiO_2 leading to an increase in the J_{sc} while at the same time decreasing the open circuit voltage (V_{oc}) of the cell. The J_{sc} increase is due to the increase in electron injection rate with increase in cation charge density. This positive shift caused by the intercalation of cations varies according to the type and the size of the cation used and the shift is generally higher for small size cations. On the other hand, the adsorption of bulky cations, such as Pr_4N^+ in tetrapropyl ammonium iodide (Pr_4NI), causes only a smaller positive shift in the TiO_2 conduction band favouring the open circuit voltage (V_{oc}).

The beneficial effect of both these mechanisms, the increase in J_{sc} due to smaller cations and the increase in V_{oc} due to bulky cations, can be optimized and harnessed by having a binary mixture of two iodide salts, one with a small cation and the other with a bulky cation. Examples for such systems are: $LiI+Pr_4NI$, $KI+ Hex_4NI$, $LiI + CsI$. These binary iodide salts have been incorporated in several different polymer hosts, such as polyacrylonitrile (PAN), polymethylmethacrylate (PMMA), poly(vinylidenefluoride (PVdF) and polyethylene oxide (PEO) do demonstrate this effect. This "*mixed cation effect*" reported by us several years ago can enhance the solar cell efficiencies by about 20-30% due to the synergetic effect of optimizing the J_{sc} and V_{oc} values. From these studies, it was also established that the variation of the power conversion efficiency with the concentration ratio of the two iodide salts follows the same trend as the short circuit current density (J_{sc}) and goes through a maximum at a particular salt concentration ratio. The observed efficiency enhancement has been explained on the basis of the electrode effects as well as electrolyte effects where the cations play a dominant role.

Abstract of Plenary Talk – II

Spray Pyrolysis Deposition for Thin Film Formation towards Next Generation Solar Cell Research

Shoji Kaneko, Shun-ichi Ohta, P.V. V. Jayaweera

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A spray pyrolysis deposition technology (SPD) is one of chemical processes for obtaining nano-sized thin film from liquid phase and is performed by spraying a solution with compressed air using a simple pneumatic system consisted of atomizer, air compressor, solution reservoir and substrate heater. A starting solution with raw materials is atomized toward a heated substrate not consecutively but intermittently to keep at a prescribed substrate temperature, because a mixture of solution and compressed air acts constantly as a coolant of substrate through the processing.

The progress of SPD thin film preparation process is as follows: (1) Innumerable mists from an atomizer wet the surface of substrate to make liquid film just after sprayed and the boiling temperature of solvent can be kept until its complete evaporation due to the Gibbs's Phase Rule, despite the substrate temperature is set much higher than that boiling temperature. (2) Then the temperature of solute dried on the substrate increases toward a preset value to yield metal clusters firast throughout thermal decomposition. (3) These metal clusters could be converted to compound clusters smoothly, if negative ions available in the starting solution. (4) Film deposition is occurred with the condensation and cohesion of these fuse metal or compound clusters on the substrate.

It could be speculated that atomic diffusion or migration in newborn thin film occurs to advance the crystallization of fine particles and densification of texture while the atomizing is stopped to avoid the reduction of substrate temperature. This stopping operation could properly contribute to the qualification of deposited thin film.

Finally, the applications of this SPD technology to next generation solar cells (DSC and PSC) fabrication will be introduced in terms of fluorine-doped tin oxide (FTO), and porous or dense TiO_2.

Investigations of RF Magnetron Sputtered Cu_2ZnSnS_4 (CZTS) Absorber Layer Using X-ray Photoelectron Spectroscopy for Thin Film Solar Cell

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Abstract

Cu_2ZnSnS_4 (CZTS), a quaternary compound semiconductor, is an earth abundant and sustainable semiconductor material that is used as an absorber layer for thin film solar cells. In the present work, CZTS thin films were deposited onto soda lime glass (SLG) substrates by RF magnetron sputtering using the stacking sequence CuS / ZnS / SnS at a substrate temperature of 300^oC. The samples were then sulphurised at 400^oC in H_2S atmosphere for 60 min. A comparison of as-deposited and sulphurised CZTS thin films are discussed in this paper. The composition of the CZTS thin film samples were studied using X-ray photoelectron spectroscopy, which revealed the presence of Cu, Zn, Sn, S in 2:1:1:4 ratio respectively. The presence of O and C was also detected due to atmospheric contamination. It is evident from the atomic % calculation that the stoichiometry has improved for the sulphurised samples. The formation of stoichiometric CZTS is an important factor to use it as an absorber layer in a thin film solar cell. Thus, from the XPS results it is obvious that the sulphurised CZTS thin films can be used as absorber layer in a thin film solar cell.

Direct Absorption Solar Collectors with Magnetic Nanofluid

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Abstract

Direct absorption collectors (DASC) with nanofluids demonstrate superior thermal performance relative to conventional flat plate collectors. The volumetric absorption of heat by both the nanoparticles and the liquid in DASC becomes more efficient in case the extinction coefficient of the nanofluid is optimal. When the metal nanoparticles are used, the collector gains extra performance due to enhanced thermal conductivity and an excess heating originating from surface plasmon resonance. Even more, the magnetic nanoparticles may increase the collector efficiency, converting under the influence of an external magnetic field. In this contribution, we foremost demonstrate experimentally that a lab-scale DASC with an aqueous iron oxide nanofluid (184 nm) is up to 25% more efficient than the same collector with a carbon black nanofluid (51 nm) at equivalent particle concentration. We further develop a multiphase CFD-model for the solar heating of a magnetic nanofluid with 8nm MnZn ferrite particles. Enhancing the most standard approach to model nanofluids as single-phase liquids with altered thermal properties, we extended the two-fluid Eulerian-Eulerian method to account for such details of the process as: Brownian dispersion and sedimentation of nanoparticles, inter-phase slip, in-phase volumetric absorption of thermal radiation and magnetic forces, acting on nanoparticles. The model was validated against two independent experimental benchmarks, demonstrating discrepancies below 10%. As it followed from our simulations, the magnetic convection increases DASC efficiency up to 30% in a moderate magnetic field of 113 mT.

Effect of Annealing Temperature on Structural, Morphological and Optical Properties of Nanocrystalline TiO_2 Thin Films Synthesized by Sol-Gel Dip Coating Method

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Abstract

TiO_2 is one of the common materials used for solar cells, diodes, different types of gas sensors, optoelectronic devices, etc. TiO_2 is widely used in photovoltaic devices due to interesting optical and electrical properties. In this work, nanocrystalline TiO_2 thin films have been prepared by sol-gel dip coating method. X-ray diffraction results showed the formation of anatase phase of TiO_2. The SEM is used for analysis of morphology. The EDX analysis confirmed that Ti and O elements are present in the sample. PL and UV-Vis spectroscopy was used for investigation of TiO_2 optical properties.

Keywords: Nanocrystalline TiO_2, X-Ray Diffraction, Scanning Electron Microscopy, EDAX, UV-Vis spectroscopy, Photoluminance.

Effects of Physical Orientation of Dye Molecules and Molecular Orbitals on Performance of Solid-State Dye Sensitized Solar Cells

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Abstract

Studies on Dye-Sensitized devices (DSDs) were initiated around late 1960s. DSDs are studied as a low cost alternative for photovoltaic optoelectronic devices, notably as solar cells. Their performance depends on the photon absorption and carrier injection properties of the sensitizer (dye). In general, the charge transfer in the molecule is based on the Donor-*π-bridge*-Acceptor (D-π-A) mechanism. Additionally, the orientation of the dye molecule affects the photon-absorption-cross-section, the injection efficiency of the carriers from the sensitizer to the semiconductor-electrode. Three variants of cyanine dyes were identified to have different orientations with respect to the TiO_2 surface. The current-voltage variations of the three dyes as sensitizers were studied experimentally on an *n*-TiO_2/Dye/*p*-CuSCN configuration. The TiO_2 films were prepared on fluorine-doped tin oxide (FTO) glass plates (1×1.5 cm^2) by hydrolyzing titanium isopropoxide slurry mixed with Degussa P25 TiO_2 powder. The TiO_2 film thickness was ~10 µm. The I-V characteristics of the cells were recorded using a calibrated halogen lamp and a KEITHELY 2400 source meter; the photocurrent action spectra was measured using a SP-DK480 monochromator and a SR-850 lock-in-amplifier set-up calibrated with a standard silicon photodiode. The absorption spectra were obtained using Ocean Optics USB2000 UV-VIS spectrometer. Additionally, a theoretical study was conducted, using the inbuilt functions in ChemDraw®, to calculate the MM2 energy minimization, identify the molecule's orientation and the HOMO and LUMO positions. The results have shown a correlation between the orientation of the dye molecule and the photocurrent of the device. Furthermore, the orientation of the dye molecule appears to be influencing the photon-harvesting efficiency and the penetration of the hole-conductor into the device. Additionally, the photocurrent results imply the MO‘s positions affecting the carrier transport properties of the device.

Exploring Optoelectronic and Electrochemical Behavior of γ-CuI Thin films Prepared by Solid Iodination Process

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Abstract

A simple and efficient solid iodination method is reported for the fabrication of p-type γ-CuI thin films. The structural, morphological, optical, electrical and electrochemical properties are studied in order to utilize γ-CuI thin films as effective hole transporting layer in solid state solar cells. The fabricated films exhibited p-type conductivity with resistivity of 7.0×10^{-2} Ωcm, hole concentration of the film was around 10^{19} cm^{-3} and the mobility was found to be in the range of 15.07 to 18.34 cm^{-2} $V^{-1}s^{-1}$. The cyclic voltammetry result shows a maximum specific capacitance of 43 $mFcm^{-2}$ at scan rate of 10 mVs^{-1}. The cyclic stability and capacitance retention was found to be 99.7%. These findings would assist γ-CuI film as a potential candidate for multiple applications, such as hole transporting material for solid state solar cells and electrochemical supercapacitors.

Keywords: Copper Iodide, Solid Iodination, Hole mobility, Cyclic voltammetry

Online Monitoring of Rooftop SA-SPV System on Residential Building

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Abstract

The technologies involved in solar photovoltaic (SPV) conversion have been advancing rapidly. Since last decade, the costs of SPV panel and other subsystems have been regularly decreasing which resulted in increase in demand and competition in business. The future demand for the SPV systems, will largely depend on user's perception of successful performance of the SPV systems. Recognizing this fact, the SPV systems integrators and operators have started incorporating modern technology features such as net-metering, advanced/smart metering, data recording and acquisition facilities and web-based platform for online monitoring. These features are important to users of the system, as well as system operators, researchers and developers. In this work, we present results of online monitoring of performance of a stand-alone SPV (SA-SPV) system (3.7 kWp), installed on a residential building, located 25 km away from the monitoring station, with the objective of generating accurate performance records of SA-SPV systems in the region. The results are useful for setting benchmarks for enhancing performance of SA-SPV systems, for large number such systems to be installed in the region. The widely varying orientations of roof surfaces of existing residential buildings offer stiff challenges to system integrators in guaranteeing performance of the system. Also, the load matching for the installed system is a challenging task, particularly in residential buildings. The online monitoring also provides insights into the performance of the sub-systems during short interval of 10minutes. The performance is measured in terms of power output of PV array, state of charge (SoC) of battery, and energy supplied to load by the PV array or by the utility grid. The online monitoring also helps in predicting performance of the system. The challenges in using online monitoring system are due to limited access to internet and loss of performance data at SA-SPV end. It is suggested that the scope of online monitoring system may be enhanced by including web camera for live streaming of data for periodic visual inspection.

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Impact of TiO_2 Nanorods-Nanoparticles Bilayer Assembly in the Performance of Dye Sensitized Solar Cells

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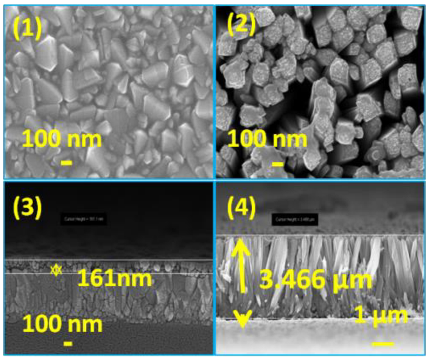
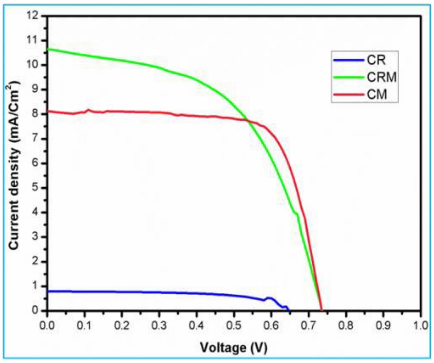
Abstract

The photo anodes in dye sensitized solar cells (DSSCs) with two different morphologies such as one dimensional nanorods and nanoparticles of TiO_2 were utilized for improving the short circuit current density of the device. The synergistic effect of both structures offer high Jsc by providing better pathway for the electron transportation through one dimensional nanorod morphology and efficient light absorption due to more dye adsorption on the mesoporous nanoparticles. The performance analysis of the dye sensitized solar cells were done by using photo anodes of three different combinations, such as compact layer with mesoporous nanoparticles (CM), compact layer with nanorod structure (CR) and finally compact layer with both the nanorods and mesoporous nanoparticle as a bilayer assembly (CRM).The FESEM images confirm the presence of vertically aligned nanorods and they are perpendicular to the substrate surface. XRD and RAMAN studies confirm the crystalline nature of synthesized bilayer film was a mixture of anatase and rutile phase of TiO_2. The absorption and emission properties for the synthesized samples were studied using UV-Vis and Photoluminescence (PL) spectroscopy. The efficiency of the solar cells with the photo anodes of CR, CM and CRM were found to be 0.30%, 4.41% and 4.23% respectively.





First figure shows the FESEM images of the top view of compact layer and TiO_2 nanorods (1&2), cross sectional view of compact layer and TiO_2 nanorods (3&4) and second figure represents J-V graph of CR, CM layers and CRM bilayer assembly.

Keywords: Anatase TiO_2, Rutile TiO_2, Nanorods, Bilayer assembly, DSSCs.

Plasmonic Effect on Photocurrent in PbS/CdS Quantum Dot-Sensitized Solar Cells with TiO_2 Nanofiber/Nanoparticle Photoanode

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Abstract

Semiconductor quantum dots have gained more attention due to their unique optoelectronic properties applicable in many important research fields such as fabrication of light emitting devices, photon detecting devices, medical equipment, spectrometers and photovoltaic cells. Quantum dot – sensitized solar cells (QDSSCs) are photovoltaic devices with low fabrication cost and high efficiency due to the ability of multiple exciton generation and tunable energy gab by quantum confinement effect. Ag plasmonic colloidal nanoparticles were synthesized using reduction method. PbS/CdS quantum dots were loaded on the TiO_2 electrode by successive ionic layer adsorption and reaction (SILAR) technique. Plasmonic Ag nanoparticle incorporated TiO_2 double layer (nanofiber/nanoparticle) nanostructured photoanodes have been prepared for solar cells sensitized with PbS/CdS core-shell structure quantum dots. Ag plasmonic PbS/CdS QDSSC shows a better power conversion efficiency of 4.09% with short-circuit density of 14.85 mA cm^{-2} and open-circuit voltage of 627.70 mV under the simulated light of 100 $mWcm^{-2}$ with Air Mass (AM) 1.5 spectral filter. The efficiency of the similar QDSSCs made without Ag nanoparticles under the same condition was 3.55%. The overall performance and short-circuit current density of the QDSSC are enhanced by 15% and 23% respectively. The enhanced performance of the QDSSC is clearly due to the enhanced optical absorption by localized surface plasmon resonance effect by the Ag nanoparticles in the TiO_2 photoanode and the resulting increase in the short-circuit photocurrent.

Electrodeposition of Bismuth Oxyiodide for Photoelectrochemical Applications

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Abstract

This study reports the electrodeposition of bismuth oxyiodide thin films on FTO substrates for the first time from aqueous nitrate baths. The electrodeposition process involves the reduction of Bi(lll) to Bi(l), elemental iodine to iodide and simultaneous oxidation of iodide to oxyiodide. The key to obtaining bismuth oxyiodide is the control of concentrations of Bi(l), iodide and oxyiodide ions at the electrode surface. This is in turn achieved by appropriate choices of Bi(lll) concentration, iodine concentration, the amount of a suitable polyol for complexing, bath pH and the potential of deposition of BiOI. It is shown that decreasing the Bi(lll) ion concentrations in the bath promotes the formation of bismuth oxyiodide over bismuth triiodide on FTO. Cactus-like microspheres of the oxyiodide, made of nanoplates, are formed. UV-Visible spectroscopy shows an indirect band gap of 2.19 eV for the deposited oxyiodide. These films are currently being used to examine photo- electrochemical degradation of pollutants in water.

Titanium Dioxide and Cadmium Sulfide Thin Films as the Electron Transporting Layer for P3HT:PCBM Bulk-Heterojunction Solar Cells

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Abstract

Poly (3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) bulk heterojunction solar cells are of immense interest due to their potential towards fabrication of flexible and low-cost solar cells using simple solution process techniques. The role of hole-blocking layer (HBL) is vital in the inverted device structure. In this work, we investigated the effect of Titanium dioxide (TiO_2) and Cadmium sulfide (CdS) thin films as the hole blocking layer on the performance of the P3HT:PCBM solar cells. TiO_2 and CdS thin films with same thickness were fabricated by using simple chemical bath deposition and spray pyrolysis respectively [1–4]. Solar cells were fabricated on the fabricated HBL by spin coating a chlorobenzene (CB) solution of P3HT: PCBM (1:1 by weight) containing 25 mg/ml P3HT and 25 mg/ml PCBM. Solar cells fabricated with TiO_2 as HBL showed better short circuit current density (Jsc) when compare to CdS devices. However, the overall power conversion efficiency (PCE) is higher for the devices with CdS as HBL predominantly due to higher Voc and fill factor. The increased Voc of the CdS devices was due to higher valence band position of CdS when compare to TiO_2 from the vacuum level. The detail results and the mechanism behind the improved PCE of the CdS based devices will be discussed in the presentation.

Divalent Metal Doped Absorbing layers for Perovskite Solar Cells

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Abstract

Perovskite solar cells (PSC) having a unique crystal structure of ABX_3 (A-Monovalent Cation, B-Divalent Cation, X-Halogen anion) that provides good power conversion efficiency (PCE) in cost-effective photovoltaic. The main reason for its crucial role in today's photovoltaic is its rapidly increased PCE up to 22.1% within a few years. This highest PCE obtained by only using lead (Pb) as light absorbing material; although, chemical instability and environmental hazards of lead are still a big challenge. Stability can be improved by modifying the halogen ions (Cl-, Br- and I-) and exchanging divalent cation (CH_3NH_3I). Even the percentage of lead consumption in perovskite is low, but it causes more harm to the environment and also acts as a carcinogenic agent for humans due to its water solubility and chemical instability. In the path of lead-free perovskite solar cells, we made a try of doping divalent metals with the Pb as an absorbing layer and analysed. The absorbance of the active layer is analysed by UV-Visible spectrophotometer. X-Ray Diffractometer result confirms the structure of perovskite. I-V characteristics of fabricated PSC device have been analysed by Keithley Source Meter-2450.

Synergistic Effect of Hybrid WS_2 Quantum Dots/Co-Fe Nanocubes, WS_2 Nanorods/Co-Fe Nanocubes: Towards Pt-Free Counter Electrode for Dye Sensitized Solar Cells

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Abstract

WS_2 (Transition-metal dichalcogenide) are known for their novel electro catalytic properties and have analogous structure with graphene. It is noted that catalytic performance of WS_2 can be further increased by doping either heteroatom or transition metal. Facile one-pot hydrothermal method was used for synthesis of WS_2 quantum dots and WS_2 nanorods, Nanocubes are prepared by simple chemical ageing method. The obtained WS_2 quantum dots, WS_2 nanorods show good transmittance in visible region (400 – 800 nm). The photoluminescence peak was obtained around 420 nm for WS_2 quantum dots, CoFe shows high intense peak at around 424 nm confirms the product quality. Raman active modes of CoFe around 501 cm^{-1} (T_{1g}) and 620 cm^{-1} (A_{1g}) reveals cubic structure formation. The structural features of the as prepared (0D/3D), (1D/3D) are characterized systematically by the X-ray diffraction, Field emission scanning electron microscopy, EDAX, High-resolution transmission electron microscopy, FTIR and Raman spectroscopy. Here we identified the synergistic effect of the prepared hybrid WS_2 quantum dots/Co-Fe nanocubes (0D/3D), WS_2 nanorods/ Co-Fe nanocubes (1D/3D) by appropriate doping composition shows more exposed edge sites, large specific surface area and outstanding catalytic activities, when compared with bare WS_2 and CoFe and it is a real substitute for Pt-counter electrode in Dye sensitized solar cells.

Keywords: WS_2 Quantum dots, WS_2 nanorods, Co-Fe nanocubes, Synergistic effect

Performance Enhancement of Dye Sensitized Solar Cells by Co-sensitization of Triple Layered Photoanode Consisting of TiO_2 Nanofibers

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Abstract

Morphology of the photoanode in Dye Sensitized Solar Cells (DSSCs) is one of the crucial factors determining their overall efficiencies. Despite the use of composites with other semiconductors or the modification of the morphology of the material, the efficiency enhancement of these devices can be achieved by increasing the light harvesting rate of the photoanode. On the other hand, harvesting of photon energies in full solar spectrum by co-sensitization of photoanodes is another approach towards the efficiency enhancement in these devices. Here we report the possibility of enhancing the efficiency of DSSC by employing a co-sensitized triple layered photoanode with electrospun nanofibres (NF) and nanoparticles (NP) of TiO_2. Performances of DSSCs comprising with TiO_2 NP/NF/NP triple layered structures were compared with the devices fabricated with conventional NP TiO_2 photoanodes under the identical conditions by using inexpensive Eosin-Y and Rose Bengal dyes. Dramatic enhancement in the efficiency of DSSC was obtained due to the incorporation of the NF layer. DSSCs fabricated with Eosin–Y dye sensitized triple layered structure showed 1.77% overall efficiency whilst the cells fabricated with the conventional photoanodes showed 0.89% efficiency thus giving an increase in efficiency by ~ 98% under the irradiance of 1000 W m^{-2}. DSSCs sensitized with Rose Bengal dye showed 0.25% and 0.76% efficiencies with conventional and triple layered photoanodes respectively. UV-Vis absorption measurements suggest that the main cause for this improvement could be due to the enhanced light harvesting by scattering effect within the electrospun TiO_2 NF layer. While the DSSC fabricated with co-sensitized TiO_2 NP/NF/NP photo anode showed energy conversion efficiency of 2.09%, the cells fabricated with co-sensitized conventional photoanode showed an efficiency of 1.04%. Incorporation of triple layered co-sensitized photoanode enhanced the efficiency of DSSCs by two fold.

Water Adsorption Properties of Titanium(IV) Oxide Embedded in Multiwalled Carbon Nanotubes (CNT)

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Abstract

Titanium(IV) oxide was embedded into carbon nanotubes through sonication. The water adsorption properties of the carbon nanotubes, titanium(IV) oxide and the titanium(IV) oxide embedded carbon nanotubes have been studied using near infrared spectroscopy and second derivative techniques. Each sample was evacuated, then exposed to 40% and 60% relative humidity to adsorb water molecules and the evolving adsorption near infrared spectra were studied. Adsorption properties were further studied by gravimetric analysis. Near infrared spectroscopy of titanium(IV) oxide showed a high water adsorption characterized by the presence of sharp peaks at 7169 cm^{-1} and 5282 cm^{-1} (first overtone of OH on the surface of titanium(IV) oxide and the combination frequency of the free water molecules respectively) . The CNT s showed no water adsorption. Titanium(IV) oxide embedded carbon nanotubes showed a peak at 5282cm^{-1} suggesting the inclusion of the titanium(IV) oxide in the CNT .Spectroscopic data and Scanning Electron Microscopic studies confirm that the titanium(IV) oxide has been embedded into the carbon nanotube samples. This conjugation can enhance the electronic and optical properties of TiO_2 which is advantageous in the water splitting and the solar cell applications. The water adsorption profiles show that the TiO_2 adsorbs more water at a relative humidity of 60% than at relative humidity of 40%. However, the titanium(IV) oxide embedded in CNTs loses its ability to adsorb water. Embedding of titanium(IV) oxide in CNT has altered the adsorption properties of pure TiO_2

Keywords: Carbon nano-tubes, Titanium(IV) oxide nanoparticles, Near Infrared Spectroscopy, Second derivative, Water adsorption

Ag Decorated TiO_2 Nanoparticles Synthesized by Rapid Photo Deposition Technique as Electron Transport Layer (ETL) for Dye-Sensitized and Perovskite Solar Cells

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Abstract

Electron transport layer is one of the important part in the dye-sensitized and perovskite solar cells which is responsible for the transport of photo-generated electrons to the outer circuit. Thus, selection of appropriate Electron transport layer (ETL) is important for attaining higher power conversion efficiency. Localised surface plasmon resonance can be used as a strategy to improve the total light absorption and it also has been reported that the metallic nanoparticles induce localized electric field, which can excite dye/perovskite molecules more effectively than far-field light which would lead to enhanced light absorption by the adsorbed dye/perovskite molecule which in turn would result in improved generation of photo-excited electrons. In this work TiO_2 nanoparticles were synthesized by a simple solvothermal method and the Ag nanoparticles were decorated over TiO_2 by photo deposition technique. The X-ray diffraction analysis of the sample showed characteristic peaks for anatase phase of TiO_2 and the Ag decorated TiO_2 showed peaks corresponding to (200) planes of Ag nanoparticles. Optical properties were studied using UV-visible absorption analysis and it showed strong absorption in the UV region for TiO_2 and the surface plasma resonance (SPR) effect is observed in Ag decorated samples. TEM analysis showed the presence of near-spherical shape Ag nanoparticles which were present uniformly over TiO_2 nanoparticles. XPS analysis revealed the chemical states of the prepared material. For the constructed DSSC using the prepared material, open circuit voltage (Voc) of 0.67 V and 0.69 V and efficiency (η) of 5.4 and 7.3 % were obtained for bare TiO_2 and Ag decorated TiO_2 based solar cells respectively. A similar trend of enhanced performance was observed for the Ag decorated TiO_2 when compared to bare TiO_2 when used as ETL layer in the case of perovskite solar cells as well.

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Investigation of PbS Quantum dot Sensitized ZnO Nanorods - Photo Anode for Solar Cell Applications

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Abstract

Sol gel dip coating method has been used for preparing ZnO nanorods (NRs). PbS quantum dots (QDs) have been synthesized by successive ionic layer adsorption and reaction (SILAR) method. The structural and optical characteristics of the ZnO NRs, PbS QDs and PbS QDs sensitized ZnO NRs films have been studied using X-ray diffraction method and UV absorption studies. From the x-ray diffraction analysis, it is observed that the ZnO NRs based sample exhibits hexagonal structure. The optical absorption peak was found to be around 365 nm for ZnO nanorods and the band gap value has been calculated and is 3.27 eV. PbS quantum dots thin film is found to exhibit good absorption of light in the visible region. The surface morphology of the prepared thin film has been analyzed by using FESEM. The image showed the presence of PbS QD in ZnO nanorods based sample. Further quantum dot sensitized solar cells were fabricated using the prepared material as photo anode and its performance has been studied.

Keywords: Quantum dot, SILAR method, XRD and FESEM.

Effect of Polyaniline on the Performance of Dye Sensitized Solar Cells Fabricated With Poly (Ethylene Oxide) Based Gel Polymer Electrolytes

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Abstract

Dye sensitized solar cells (DSSCs) mainly consists of a dye adsorbed photo-anode, a counter electrode and a redox electrolyte, in which the electrolyte plays an important role as the charge transport medium. DSSCs generally employ a liquid electrolyte based on I^-/I_3^- redox couple and have impressive energy conversion efficiencies. However, the lack of long-term stability due to liquid leakage, electrode corrosion and photodecomposition of the dye in the solvent medium due to the usage of volatile liquids are some of the major drawbacks preventing large scale practical applications of DSSCs. One solution to this is to introduce polymer gel electrolytes having fast charge transfer processes and low interfacial resistance. Ionically conducting gel electrolytes are promising in improving the power conversion efficiency and stability of quasi-solid-state DSSCs. In this work, polymer electrolytes containing polyethylene oxide (PEO), LiI and I_2 are used as the redox electrolyte and different amounts of polyaniline (PANI) conducting polymer is introduced to the PEO based electrolyte. The effect of incorporating PANI into the PEO based gel electrolyte on solar cell performance was studied. Ionic conductivity measurements and FTIR studies were done for the PANI incorporated gel electrolyte samples. The gel polymer electrolyte without PANI showed a conductivity of 1.32×10^{-2} Scm^{-1} at room temperature and with the incorporation of PANI, the conductivity increased and a maximum conductivity of 1.75×10^{-2} Scm^{-1} was obtained for 1.0 wt. % PANI added sample. PANI can form interconnected channels within the PEO polymer matrix. These conducting channels formed by PANI chains function as pathways for electron transfer and can improve the reduction reaction of triiodide ions in the DSSC. The resultant DSSC made with 1.5 wt % PANI incorporated PEO based gel electrolyte showed a maximum efficiency of 6.56% in comparison with the efficiency of 5.00% obtained for a PANI free gel electrolyte based DSSC.

Keywords: Dye sensitized solar cell, electrolyte, conducting polymer, polyaniline.

Bio-based Carbon Hole Transporting Material Obtained from the Extract of Invasive Species of Aagaya Thamarai Plant (*Eichhornia crassipes*) for Cost-Effective Carbon Based Perovskite Solar Cells

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Abstract

Herein, we report a novel and naturally extracted carbon based hole transporting material (HTM) for perovskite solar cells (PSCs) synthesized using an eco-friendly and cost-effective ancient Indian method. Also in this work, the low-cost and bio-based carbon suitable for PSCs have been prepared by a facile brush painting technique and their structural, morphological and electrical properties have been investigated at two different annealing temperatures 850 and 1000 °C. At these temperatures, the obtained carbon exhibited similar structural and morphological properties and are favourable for the PSCs as both HTM and top contact layer. The current density-voltage (J-V) characteristics of the fabricated perovskite device with structure FTO / c-TiO_2 / mp-TiO_2 / $CH_3NH_3PbI_{3-x}Cl_x$ / Methylammonium Iodide + Carbon / Carbon counter electrode has been studied and the device fabricated using the bio carbon annealed at 1000 °C achieved a higher power conversion efficiency (PCE) of 8.52% with current density (J_{SC}) of 23.49 $mAcm^{-2}$, open circuit voltage (V_{oc}) of 0.672 V and fill factor (FF) of 54.01%. Further, the J-V performance of the perovskite cell with aagaya thamarai plant processed carbon based HTMs annealed at 850 and 1000 °C have been compared with the solar cells fabricated using commercially available carbon paste HTMs. Although our invasive plant species-processed natural carbon HTM based solar cells show a moderate photovoltaic efficiency they exhibited higher air-stability and better long-term stability.

Keywords: Bio-based processed carbon, Perovskite solar cells, Carbon HTMs, Brush painting technique, Carbon electrodes

Effect of Annealing on Phase Transition and Its Impact on Second Harmonic Generation in Barium Titanate Nanopowder for DSSC Solar Cell Applications

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Abstract

Barium titanate ($BaTiO_3$) nanoparticles synthesized at 200 °C by sol- hydrothermal process demonstrated stabilization of orthorhombic and tetragonal phases. The influence of annealing at different temperatures (100, 200, 300, 400, 500 & 800 °C) on the phase separation/transition is investigated in this study. The annealing process had substantial impact on the structural and phase variation in $BaTiO_3$ nanopowder as observed from XRD analysis. An evident phase transition from the orthorhombic to the tetragonal phase is observed when the $BaTiO_3$ nanoparticles are annealed at 100°C and tetragonal phase along with orthorhombic phase is observed for all other annealed samples. Annealing at 800 °C resulted in stabilization of pure rhombohedral phase. Surprisingly, dominating XRD peaks (NP) were observed in annealed samples at 100 – 400 °C, often related to $BaCO_3$ in literature, even though barium (II) chloride, titanium (IV) chloride and NaOH were used as the precursors. The nanoparticles were further characterized by SEM and TEM, which showed uniform spherical shaped nanoparticles transformed to rod morphology with increase in agglomeration of particles. Raman Spectroscopy analysis showed the presence of characteristic tetragonal and orthorhombic Raman bands and the annealed materials exhibited similar characteristics as that of as-synthesized material, in addition, it shows an additional sharp peak around 690 cm^{-1}, identified as corresponding to hexagonal phase in literature, suggests new phase transition or phase separation in $BaTiO_3$. These results coincide well with UV and PL spectrum analysis. All the samples demonstrate non-linear optical properties demonstrating second harmonic generation. Identification of the NP-XRD peaks and influence of annealing on the second harmonic generation are presented in detail. Finally, Dye-sensitized solar cell with $BaTiO_3$ as photo anode will be fabricated and its IV characteristics will be studied.

Application and Characterization of Blueberry Fruit Pigment as the Photosensitizer for High Performance and Stable Natural Dye Sensitized Solid Solar Cells

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Abstract

The natural dye pigment of blueberry was extracted from its peals using our own acetonitrile assisted method and used in a liquid electrolyte free natural dye sensitized solid solar cell (NDSSSC) which exhibited he highest efficiency (ɳ) of 1.7% and short circuit current density (Jsc = 11 mA/cm^2) for the blueberry dye sensitized any type of solar cell. Natural dyes are always inexpensive, nontoxic and reliable sources that can be used in photovoltaic application as a cheap alternative for commercial expensive synthetic dyes. The typical problems of stability of natural pigments and the unreliability, expensiveness and the toxicity of the iodide / tri-iodide electrolyte were addressed by introducing a deposition of p-CuI on dye incorporated nanoporous TiO_2 films from a solution containing a crystal growth inhibitor Triethylammine Hydrothiocyanate (THT) by drop casting method in order to make a NDSSSC. I-V characteristics and impedance measurements were carried out to investigate the photovoltaic performance and further characterized by UV-Visible spectroscopy, FTIR spectroscopy and SEM. Stability measurements were carried out for a period of 30 days and promisingly showed a good stability

Keywords: Natural dye, DSSC, Blueberry dye, solid cells, Copper Iodide

The Effect of Incorporation of Mixture of TiO_2 Crystallites from P25 and P90 in Photoanode towards the Efficiency Enhancement in Dye Sensitized Solar Cells

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Abstract

Dye-sensitized solar cells (DSSCs) are emerging as promising candidates to replace expensive silicon solar cells because of reasonably high efficiency and lower production cost. Photoanodes of these DSSCs generally have TiO_2 particles having the diameters in the range of 15-25 nm, which facilitate the enhanced dye adsorption due to their large specific surface area. In this research work, mixtures of P25 TiO_2 powder (particle size ~22 nm) and P90 TiO_2 powder (~14 nm) with different weight percentages were used to prepare the photoanodes for DSSCs. Powder sample mixtures were analyzed by the XRD to identify the ratio of the anatase and rutile phases present in the above photoanodes. DSSCs fabricated with above photoanodes were characterized with I-V measurements. Electrical Impedance Spectroscopic measurements were used to characterize the interfacial resistance of the different interfaces in the DSSC. The DSSC with the highest power conversion efficiency of 7.0% was fabricated by using a photoanode fabricated with 70:30 ratios of P25:P90 composite. Factor of 10% efficiency enhancement is achieved by using this modified photoanode when compared with the conventional P25 photoanode. The best DSSC showed a short circuit current density of 13.91 $mAcm^{-2}$, open circuit voltage of 743.9 mV, and a fill factor of 68%. Observed enhancement in the dye adsorption of the best photoanode would have contributed to the increment in the photocurrent generation. Therefore, the occupation of the inter-grain spaces in the P25 matrix by smaller nanoparticles of P90 would have increased the surface area of the photoanode leading to this efficiency enhancement. Further, this occupation leads to lower the interfacial resistance between the TiO_2 nanocrystallites and the electrolyte from 13.5 Ω to 3.75 Ω. Possible reduction of trap states due to this occupation would also have contributed to this efficiency enhancement by lowering the electron recombination dynamics of DSSC.

Photoluminescence Studies of Stillwellite type Eu, Ho, Er co-doped Lanthanum Borosilicate Up Conversion Luminescent Materials for Solar Energy Applications

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Abstract

In the present study, a new luminescent stillwellite type lanthanum borosilicate (doped with Eu^{3+} and co- doped with either Er^{3+}/Ho^{3+} or both) up-conversion materials were synthesized and characterized by photoluminescence studies. Using Eu^{3+} luminescence as a local probe, the microscopic symmetry around it in the host matrix is studied. Two cationic sites were found to exist. Co-doping of Er^{3+} and /Ho^{3+}, has altered the PL line spectrum of Eu^{3+} into a broader one which could be explained based on carrier energy transfer model and this broadening is a proof for the existence of up conversion property in the new materials synthesized. Further, a blue shift is observed in the PL emission spectra by progressively increasing the excitation wavelength from 240 nm to 270 nm which, also infers the presence of successful up-conversion property in the newly developed material.

Keywords: Upconversion materials, Solar energy application, quantum efficiency enhancement, stillwellite type materials, photon up-conversion, luminescent materials, blue shift

Efficiency Enhancement in Dye-Sensitized Solar Cells Using Hierarchical TiO_2 Microspheres as a Scattering Layer

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Abstract

Dye-sensitized solar cells (DSCs) have emerged as a viable alternative to the conventional silicon-based solar cells due to simple fabrication, low cost and tunable aesthetic features, such as colour and transparency. The photoanode of DSCs, usually TiO_2 layer, plays a crucial role in the overall power conversion efficiency as it influences in both photon absorption and electron transport. The efficient photoanode should have large surface area, well-connected internal pores and efficient light scattering property. In order to further enhance the efficiencies of DSCs, different light scattering techniques are used. Typically, this is achieved by employing another layer of TiO_2 containing larger size spheres on top of the smaller size particle layer of TiO_2. In this work, we have succeeded in designing a hierarchically structured TiO_2 scattering layer consisting of sub-micron size TiO_2 spheres composed of aggregates of TiO_2 nanoparticles of size around 10 nm. The DSCs with hierarchical TiO_2 sphere scattering layer sensitized with N719 dye outperform the DSCs having TiO_2 nanofiber and TiO_2 nanotube scattering layers. The highest current density of 14.80 $mAcm^{-2}$ was achieved with TiO_2 sphere scattering layer compared with TiO_2 nanofiber and TiO_2 nanotube scattering layers. The power conversion efficiency of DSC with hierarchical TiO_2 sphere scattering layer was 7.38 % under standard AM 1.5 illumination conditions, whereas the efficiency of DSC without scattering layer was 6.68 % and the efficiency of DSC with TiO_2 nanofiber scattering layer and TiO_2 nanotube scattering layer was 6.47 % and 7.03 % respectively. The diffuse reflectance measurements reveals that the better performance of DSC with hierarchical TiO_2 sphere scattering layer is mainly due to the improved light harvesting by scattering of long wavelength radiation by the sub-micron size TiO_2 spheres.

Effect of Hole Transporting Materials on the Performance of Perovskite Solar Cells in Air

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Abstract

Perovskite solar cell (PSC) has been intensively studied for improving the efficiency and stability for the past few years. Various Hole Transporting Materials (HTMs) have been reported in optimizing the performance of the PSC and the best efficiencies have been obtained using 2,2′,7,7′-tetrakis (N,N′-di-p-methoxyphenylamine)-9,9′-spirobifluorene (Spiro-OMeTAD) as HTMs. However, Spiro-OMeTAD has several challenges related to cost, stability, handling and poor carrier mobility. In order to overcome these challenges, this study focuses on employing various organic / inorganic HTMs such as Spiro-OMeTAD, Poly -3-hexylthiophene (P3HT), Copper (I) iodide (CuI) and Poly(ethylenedioxythiophene):polystyrene sulphonate (PEDOT:PSS) in fabricating organic-inorganic hybrid PSC in air. A comparison study on several TiO_2 / $CH_3NH_3PbI_xCl_{3-x}$ / HTMs / Au PSCs with the above HTMs such as Spiro-OMeTAD, P3HT, CuI, PEDOT:PSS were carried out. The best efficiency of 8 % was obtained with CuI as HTM under Air Mass (AM) 1.5 conditions (100 mW cm^{-2}, 1 sun) in air separately. Here a novel pressing method was employed for incorporating CuI. An efficiency of 4.6 % was achieved with P3HT as HTM, whereas with Spiro-OMeTAD, the best efficiency of 5.6 % was achieved by doping Spiro-OMeTAD with lithium-bis-trifluoromethanesulfonyl-imide (LiTFSI) and tert-butylpyridine (TBP) under Air Mass (AM) 1.5 conditions (100 $mWcm^{-2}$, 1 sun) in air. Better efficiency achieved with CuI may be due to the novel method used for preparation, that leads to the efficient hole transport that minimizes the electron-hole recombination. In contrast, stability of P3HT based PSCs was observed to be superior than Spiro-OMeTAD based solar cells in air. PSCs with P3HT as HTM were air stable even after one month.

Keywords: Perovskie solar cells, Hole transporting materials, Pressing method, Copper (I) iodide, Spiro-OMeTAD, P3HT, Airstable

Effect of Counter Ion in an Iodide Ion Conducting Gel-Polymer Electrolyte Intended for Dye Sensitized Solar Cells - A Comparative Study between Potassium Iodide and Tetrahexylammonium Iodide

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Abstract

Quasi-solid-state dye-sensitized solar cells (DSSCs) give higher stability and reasonably good efficiency compared to those of liquid electrolytes based solar cells. It was recently revealed that counter ions in electrolytes intended for DSSCs have an influence on solar cell performance. In this work, the effect of the counter ion is studied using an iodide ion conducting gel-polymer electrolyte based on host polymer, polyacrylonitrile (PAN) and plasticizers, ethylene carbonate (EC) and propylene carbonate (PC). Two electrolytes, one using potassium iodide (KI) and the other using tetrahexylammonium iodide (Hex_4NI), were prepared by hot press method. The electrolyte containing KI shows significantly higher conductivity compared to that of the tetrahexylammonium iodide. The room temperature conductivity of KI based electrolyte was found to be 3.74 $mScm^{-1}$. The temperature dependence of electrolytes shows VTF behaviour and data fitting revealed that the pre-exponential factor and activation energy of KI based electrolyte is higher and has values of 130.96 Sm^{-1} K1/2 and 0.032 eV respectively. In-depth analysis of the dielectric properties of the electrolytes was conducted to understand the charge transport behaviour. The energy conversion efficiencies of DSSCs containing Hex_4NI and KI are 5.06 and 6.05 %, respectively under the illumination of 1000 Wm^{-2} irradiation (1.5 AM). The Electrolytes and solar cells were characterized further by using electrochemical impedance analysis. The real and imaginary parts of the dielectric constant of the electrolyte samples were calculated at different temperatures. The frequency dependence of the dielectric function is analysed to understand the polarization behaviour of the species in the electrolyte.

Synthesis and Characterization of Electro-spin Deposited Perovskite Nanostructures for Solar Cell Application

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Abstract

Perovskite nanostructures have been prepared via electrospinning technique using polyvinyl alcohol and methylammonium lead iodide ($CH_3NH_3PbI_3$ – perovskite). In the electrospinning experiment, the formation of different nanostructures was observed for different applied voltages (0-D nanodots for 10 kV, 1-D nanofibers for 20 kV, and 3-D nanocubes for 30 kV). The X-ray diffraction pattern of the samples synthesized, revealed the existence of perovskite nanostructures with tetragonal phase. The energy dispersive X-ray analysis indicates the stoichiometric presence of lead, iodine, carbon and nitrogen in the synthesized perovskite materials. The absorbance spectra have been also recorded and consequently, the optical band gap energy was found to be in the range of 1.45 to 1.52 eV which is quite close to the optimum theoretical value (1.5 eV) required for solar cell application for interfacial absorber materials. The photoluminescence spectra of the prepared methylammonium lead iodide perovskites exhibited a broad band at 780 nm which corresponds to the band-to-band transition of the perovskite nanostructures. Hence, the perovskite nanostructures synthesized could be possibly used as an interfacial modifier in perovskite solar cells for enhancing the charge transport between the active absorber layer and the transporting layers.

Keywords: Perovskite nanostructures, lectro-spin deposition, Interfacial modifier, Absorbance layer, Energy bandgap

Experimental Study on Hybrid Natural Circulation Type Solar Air Heater with Thermal Storage

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Abstract

The hybrid natural circulation type solar air heater has the potential of preserving the agricultural produces and it saves conventional fuels and reducing environmental destruction. A new type of V-trough solar collector has been proposed, designed and tested. The proposed hybrid system consists of absorber plate, insulation materials, glass covers, Phase Change Materials (PCM), V trough reflectors with thermal energy storage and a drying chamber. The dimension of the hybrid solar air heater is 1 m long, 0.27 m wide and 0.025 m thick and incorporates absorber and thermal energy storage unit. Air flows through pipe by natural circulation for 3 m length as 3 passes and excess thermal energy stored in PCM. The experiments are conducted for drying half kilo capsicum and the results show that considerable improvement in moisture removal. It is concluded that the design is compact, sufficiently simple and gives a high thermal performance. The fabricated system is tested at outdoor condition on sunny days in Kengeri, Mysuru Road, Bengaluru (Latitude :12.96° North,Longitude:77.63° East). It is found from the experimental results, the thermal efficiency of the solar air heater is varies from 12 % to 65 % in a day.

Keywords: Phase Change Material (PCM), V-Trough Solar Collector, Solar Air Heaters, Absorber plate, Free Convection

A Comparative Study of CZTS Thin Films Deposited By Different Non Vacuum Techniques

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Abstract

Thin-film solar cells technology is one of the solutions for expensive silicon solar cells. The kesterite-structured Cu_2ZnSnS_4 (CZTS) semiconductor has been considered as a promising light-harvesting material and a great progress on CZTS based solar cells has been achieved during the past few years. For the fabrication of CZTS solar cells, vacuum and non-vacuum deposition techniques have been reported. Among these methods, non-vacuum techniques such as spray pyrolysis, spin coating, and electrodeposition are widely being used owing to their simplicity and the low cost. In this study, CZTS thin films were prepared on Florine doped tin oxide (FTO) by spray pyrolysis, spin coating, and electrodeposition methods and their properties were compared. The Cu–Zn–Sn (CZT) containing precursor solution for spray pyrolysis and spin coating was prepared by solution-based sol-gel method. In the spray pyrolysis method, the precursor solution was sprayed on to the heated FTO substrate at 150 ^{0}C using compressed Nitrogen as a carrier gas. In the spin coating method, the precursor solution was spin coated on the FTO at 2500 rpm and dried at 150^{0}C on the hot plate. The co-electrodeposited Cu-Zn-Sn film was grown by using a metallic precursor solution and the deposition was carried out potentiostatically using a 3-electrode cell with a platinum counter electrode and Ag/AgCl reference electrode. The stacked metals layer which prepared by three different technics were sulfurized by annealing in a sulfur-nitrogen environment for 15 minutes at 280 ^{0}C. The photoelectrochemical response during chopped illumination was studied comparatively for each deposition techniques. The electrodeposited films were observed to be shown well with good photocurrent response, compared with the CZTS films made by spray pyrolysis and spin coating techniques. All prepared CZTS films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), UV- visible spectroscopy to obtained detail of the crystal structure, surface morphology, atomic composition and optical properties of the CZTS thin films respectively.

Keywords: CZTS, spray pyrolysis, spin coating, electrodeposition, thin film solar cell

Cupric Oxide Thin Films Grown by DC Magnetron Sputtering for Photovoltaic Applications

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Abstract

Solar energy has been considered as one of the cleanest forms of energy. Though conventional silicon solar cells are leading the market, recently, there are many alternative materials found attractive in the solar photovoltaic research in order to replace the silicon. Among them, metal oxides are also in the competition to prove themselves as solar materials. Copper oxide (Cu_xO) system is selected as an absorber in the present study because of its abundance and its high absorption coefficient. Thin films of Cu_xO were grown by dc magnetron reactive sputtering by using copper targets of high purity (99.99%). Argon and oxygen gases serve as the sputter and reactive gases, respectively. The films were prepared by varying the deposition parameters such as $Ar:O_2$ ratio and sputter power. The phase transformation in the Cu_xO thin films was analysed by varying the $Ar:O_2$ ratio during deposition through x-ray diffraction and x-ray photoelectron spectroscopy analysis. It was found that the films deposited at lower $Ar:O_2$ ratio crystallizes in Cu_2O phase (for e.g. 8:1) and CuO phase predominated in the films deposited at higher $Ar:O_2$ ratio such as 8:6. We have observed that there is an optimum sputter power range (50-80W) in which a CuO phase with low band gap value and comparatively high absorption coefficient values could be achieved which is desired for photovoltaic applications. The electrical resistivity has shown a decreasing trend with increase in sputter power during deposition. At high sputter powers of 80W, the electrical resistivity showed a low value due to the better crystallinity of the films. The structural, optical and electrical properties of the studied films suggested that these films could be used as absorber layer for oxide based solar cells.

Mk-2 dye for Dye-Sensitized Solid-State Solar Cells with Copper Iodide as a Hole Transport Material.

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Abstract

Dye-sensitized Solid-state Solar Cell (DSSC) has been received great deal of attention due to its attractive features over the wet type Dye-sensitized Solar Cells (DSCs). However the configuration of DSSC, n-type semiconductor/ dye/ p-type semiconductor susceptible to have charge recombination and that would lead to have low photovoltaic performance than liquid DSCs. The metal-free organic dye, which comprises of Donor–π spacer–Acceptor (D–π –A) configuration is identical dye structure for diminish the recombination and consists several advantages as a sensitizer. Alkyl-functionalized carbazole dye MK-2 comprises (D–π –A) architecture, where carbazole and cyanoacrylic acid act as a donor and acceptor group respectively. The long alkyl chain is susceptible to decline the charge recombination by providing long distance for charge separation and suppress the dye aggregation due to steric hindrance. DSSC was prepared by deposition of ~15μm thickness of nanoporous layer of hydrolysis TiO_2 with P25 Dugessa powder on FTO substrate and dyed with MK-2 dissolved in acetonitrile / tert-butyl alcohol (1:1 by volume) and also in toluene. Inorganic hole conductor CuI was used as a p-type semiconductor with adding Triethylaminethiocyanate (TAT) as crystal inhibitor. UV-visible absorption data has shown MK-2 is capable of absorb boarder wavelength 400-700 nm in visible range. MK-2 dissolved in acetonitrile / tert-butyl alcohol has shown higher photovolatic performance, 0.496 V open circuit voltage, 16.14 $mAcm^{-2}$ current density, 0.42 fill factor with overall efficiency 3.33% under 1.5 AM illumination than MK-2 in toluene. Photon-to-current Conversion Efficiency(IPCE) results has indicated more than 55% of photon converted into current in the range of 400-650 nm for DSSC based on MK-2 dye. SEM images of CuI films reveal the crystal inhibition ability of TAT. Alkyl-functionalized organic dye can be successfully use to sensitize DSSCs.

Keywords: Dye-sensitized Solid-state Sola Cell, Alkyl-functionalized carbazole dye, Copper iodide

Effect of Ligand Attached to Fluorescein on the Photocurrent of Solid-state Dye-sensitized Solar Cells

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Abstract

Organic dyes have received much attention due to environmental compatibility. Fluorescein is one of the environmental friendly dyes. The effect of ligands attached to fluorescein on the photo-performance of TiO_2|dye|p-semiconductor type solar cells was examined. CuI and CuSCN were used as the p-type semiconductor. A relatively higher photocurrent was observed for TiO_2|dye|CuI cells than TiO_2|dye|CuCNS cells. The Maximum photocurrent was observed for mercurochrome among the dyes used from fluorescein family. Our results give an idea that not only the chromophore but also the ligands attached to the chromophore influences the absorption properties of the dyes and thereby dye- sensitized solar cells.

Keywords: organic dyes, solid-state cells, effect of the ligands

V_2O_5 Incorporated Nano-Structured TiO_2 Photo-Anodes for Solar Cells and Sensor

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Abstract

Many studies have been conducted to increase the effectiveness and efficiency of solar cells using low cost materials. This field of research is highly important due to the increasing demand for energy and environmental pollution caused by energy resources used today. In an attempt to replace dye in photo-electrodes of DSSCs by other materials, organic inorganic perovskite solar cells emerged. Recently, such organic- inorganic perovskite solar cells obtained revolutionary advancement. However, the use of organic compounds causes stability issues, though such cells exhibited efficiencies above 20%. Therefore, search for new stable completely inorganic photo-electrode capable of harvesting sunlight is highly important. The present study is focused on improving light harvesting properties of TiO_2 based electrode by incorporating V_2O_5 nanoparticles. The photo-electrodes were prepared by adding 0, 5, 10, 15, 20% mass fractions of V_2O_5. The fabricated photo-electrodes are characterized by analysing XRD, SEM, UV visible absorption spectrum, Mott-Schottky plots and Tauc plots. The peaks in the XRD spectrum are used to calculate the crystallite size and dislocation density. For the TiO_2 film the crystallite size and dislocation density are about 31.6 nm and 9.98×10^{14} m^{-2} while those of V_2O_5 are about 52.6 nm and 3.62×10^{14} m^{-2} respectively. Table 1 shows the bandgap values obtained using Tauc plots for all the photo-electrodes investigated.

Table 1 Bandgap and Flat band potential for the photo electrodes the photoelectrodes

Sample	V_2O_5 mass fraction/%	Band gap (eV)	Flat-band potential *(V)
a	0	3.49	-0.69
b	5	3.11	-0.54
c	10	3.06	-0.64
d	15	2.84	-0.66
e	20	2.75	-0.71

* Relative to Pt electrode

Photo-electrochemical cells are assembled by sandwiching a gel polymer electrolyte between TiO_2/V_2O_5 photo-anode and Pt counter electrode. The energy conversion efficiency of these dye free solar cells improved from 0.006 to 0.083 % with increasing amount of V_2O_5. .

Poly(Methyl Methacrylate) (PMMA) Based Gel Polymer Electrolytes for Possible Application in Dye Sensitized Solar Cells

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Abstract

Solar cells are considered as an economical and environmental friendly solution for the global energy demand. Dye-sensitized solar cells (DSCs) offer low production cost and many possibilities for further development. In general, a DSC composed of a dye-sensitized photo-electrode, a counter electrode and an electrolyte. The intention of this work is to prepare new gel polymer electrolyte (GPE) in order to address the issues of poor chemical and physical stability in DSCs. The efficiency drop originates from the lower ionic conductivity in GPEs is attempted to solve using mixed salts and performance enhancers. Under this study, Poly(methyl methacrylate), PMMA, based series of GPEs with a mixture of two salts, LiI and Pr_4NI (Tetrapropylammonium Iodide), were prepared by changing the salt mass fractions. Ethylene carbonate and propylene carbonate were incorporated to the electrolyte to enhance the ionic conductivity and 4-tert-butylpyridine and 1-butyl-3-methyl imidazolium iodide were added to enhance DSC performance. In addition to the characterization of electrolytes, a set of DSCs were assembled by employing the series of electrolytes investigated. The temperature dependence of conductivity in the electrolytes showed Vogel–Tammann–Fulcher (VTF) behaviour with the activation energy in the range of 0.07-0.09 eV. The highest conductivity in the temperature range from 30 °C to 75 °C was given by the electrolyte containing 60% of LiI and 40% of Pr_4NI with respect to the total salt weight and the ionic conductivity of the electrolyte at 30 °C was 3.20×10^{-3} Scm^{-1}. The frequency dependence of the real and imaginary parts of the dielectric constant at different temperatures were investigated to understand the electrical properties of the GPEs. Highlighting the positive effects of using PMMA based GPEs, the investigated DSCs showed very good short-term stability. Highest efficient cells showed energy conversion efficiencies above 5%.

Keywords: Dye-sensitized solar cells, gel polymer electrolytes, Poly(methyl methacrylate), binary salts

Nano Structured Silicon as Antireflection and Emitter for Terrestrial Solar Cells

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Abstract

The demand for renewable energy has increased in the last few years due to the limited availability of the widely used fossil fuel. Solar energy is by far the most abundant renewable energy source available, but the levelized cost of solar energy is still not competitive with that of fossil fuels. Therefore, there is a need to improve the power conversion efficiency of solar cells without increasing the production cost. A big challenge is to reduce the cost via utilizing the cheapest materials with high thorough put is essential. The lecture will cover the main objective to develop nanostructured silicon (Si) solar cells with higher power conversion efficiency using scalable and cost-efficient production methods. The nanostructures are fabricated by simple maskless single-step electrochemical and two-step metal assisted chemical etching (MACE). Currently, electronic grade silicon wafers has been widely used for the preparation of porous silicon (PS) layers in decades. In our work, we have made an attempt to employ cheaper upgraded metallurgical grade (UMG) wafers replacing the expensive electronic grade and fabricated the PS layers with Si nanostructure as observed from the SEM images shown in Fig 1. In general, the optimization was done through varying the parameters like etching time, electrolyte concentration, current density for the electrochemical etching and the metal concentration & etching time for MACE process. For the first time, in-house low temperature and high pressure setup was utilized to passivate the active PS layer. The details of the optical and structural properties shall be elaborately discussed with the necessary experimental methods. Finally, a solar cell device was fabricated using the PS layer and subjected to solar cell testing.

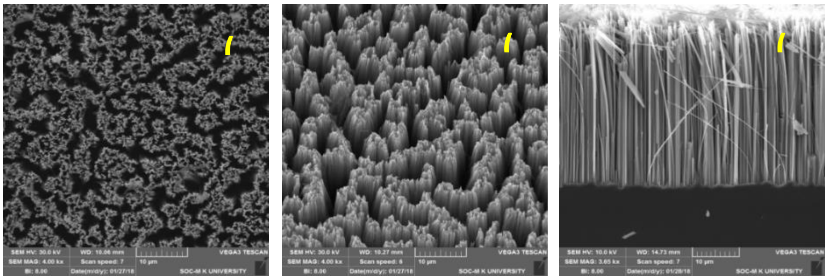

Fig. 1: SEM images of Si nanostructure by MACE a) top view, b) 20^o tilted view, c) cross section.

Comparative Study of ZnO, ZnS and Zn (O, S) Thin Films Grown by Chemical Bath Deposition for Buffer Layer Application in Solar Cells

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Abstract

Zinc Oxide (ZnO), Zinc Sulphide (ZnS) and Zinc Oxide Sulphide (Zn (O, S)) thin films were deposited on a clear soda lime glass substrates using chemical bath deposition at room temperature. The structure of ZnO, ZnS and Zn (O, S) thin films was found to be hexagonal Wurtzite with <100> and <111> orientations for ZnO and ZnS thin films respectively based on XRD measurements. Field Emission Scanning Electron Microscopy images revealed smooth surface for the films with the formation of flakes. Transmission spectra of the films were studied by UV-Vis-NIR Spectrophotometer and the transparency was found to be above 80% for ZnO, ZnS and Zn (O, S) thin films. The optical band gap was found to be around 3.3 eV for ZnO film, 3.5 eV for ZnS and 3.0 eV for Zn (O, S) film which is in accordance with the reported values. The results show that the quality ZnO, ZnS and Zn (O, S) buffers layers can be deposited using Chemical bath deposition.

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Effect of Annealing Temperature on Earth Abundant Cu_2ZnSnS_4 Thin Film for Photovoltaic Application Synthesized by Low Cost Sol-Gel Spin Coating

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Abstract

Copper Zinc Tin Sulfide (Cu_2ZnSnS_4 or CZTS) thin film have been deposited on Soda lime glass substrates by a spin coater and annealed in air with different temperature varied from 300 – 500 °C. The effect of annealing temperature on structural, optical, electrical, morphological and compositional properties has been studied. The XRD study depicts that sharpness of the peak increases with annealing temperature. The major peaks are observed at 28.74^{o}, 33.2^{o}, 47.7^{o} and 56.6^{o} with (112), (200), (220) and (312) plane. Optical studies show relatively high absorption co-efficient within 10^4 - 10^5 cm^{-1}. The band gap energy (Eg) varies from 1.42 to 1.49 eV for CZTS thin film. Hall measurements show p type conductivity. Further, SEM analysis revealed the surface texture of CZTS film. The EDX measurement for CZTS thin films confirms the formation of CZTS which is Cu rich and Zn poor.

A Study on $CdCl_2$ Activation of CBD-CdS Thin Films

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Abstract

"$CdCl_2$ treatment" on CdTe absorber is known to be a key step for a drastic improvement of the CdS / CdTe solar cell conversion efficiency. However, $CdCl_2$ treatment on the CdS window layer has not extensively studied in the literature. In this work, a detailed study is reported on $CdCl_2$ solution treatment on chemical bath deposited of CdS (CBD-CdS). The CBD-CdS thin films were grown using 0.001 mol dm^{-3} $CdSO_4$ ($3CdSO_4.8H_2O$, 99%, Sigma Aldrich, USA), 0.002 $moldm^{-3}$ $CS(NH_2)_2$ (99%, Sigma Aldrich, USA) and 1.1 ml of NH_4OH (NH_3, 35% w/w, Sigma Aldrich, USA) at a bath temperature of 80 °C for one hour on FTO glass substrates (~10 Ω /□, TEC 10, Sigma-Aldrich, USA). For the $CdCl_2$ treatment, deposited CBD-CdS thin films were dip-coated in a saturated methanol (99.8%, ACS reagent, Sigma Aldrich, USA) solution of $CdCl_2$ (99%, Fluka, USA). Later the $CdCl_2$ treated samples were cleaned with DI water and annealed at 200 °C for one hour. The dipping duration was varied from 0 to 20 minutes. The $CdCl_2$ treatment was found to increase the cluster size of CdS thin films and the formation of clusters was identified to be due to coalescence of small clusters. Higher V_{OC} and I_{SC} parameters in the photoelectrochemical cell (CdS/0.1 M $Na_2S_2O_3$/Pt) were observed for $CdCl_2$ treated CBD-CdS thin films, compared to untreated CBD-CdS thin films. The improved, V_{OC} and I_{SC} parameters found may be due to high effective area as well as grain boundary passivation. The flat band potential (V_{fb}) value was found to be tunable with $CdCl_2$ treatment duration. The photo efficiency was found to be almost doubled for CdS films which underwent $CdCl_2$ treatment for 10 minutes, compared to the untreated ones.

Keywords: CBD, CdS, $CdCl_2$, activation

Fault Ride-Through of Grid Connected Photovoltaic Solar System

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Abstract

Contribution from the photovoltaic solar power plants has significantly increased in supplying the power demand to the power system. The occurrence of a short time fault in the power system trips the solar power plant from the grid and it takes a long time to reconnect. This outage time causes a big loss to the solar power generating industries while disturbing the power system. This paper presents a Fault Ride-Through (FRT) operational technique, based on the switching control of the Insulated Gate Bipolar Transistors (IGBTs) of the Voltage Source Inverter (VSI). This will minimize the outage time. The solar system is designed in such a way that it will detect the fault, by measuring the grid voltage. If grid voltage is getting significantly low (for example <50%) due to a fault, the DC link voltage is set to the open circuit voltage of the solar module. This is achieved by controlling the pulse to the IGBTs. This makes sure that the power supplied by the solar cells, during the fault time, is kept to zero. In other word, the power blocking operational mode is achieved by the VSI control. After the fault is cleared, the VSI control technique is set in such a way that the solar system gets back to the Maximum Power Point Tracking (MPPT) operational mode. The voltage control of the system was designed using Sine-triangle Pulse Width Modulation (SPWM). A comprehensive system includes (i) solar cells, (ii) VSI, (iii) power system grid and (iv) proposed control technique, is modelled using PSCAD software. Performance of the system is studied by applying a short time ground fault for 150 ms period. The voltage and current wave forms of the system were analysed. In normal manual control operations, it takes more than 10 minutes to recover. With the proposed automated control technique, it is proven in simulations that it reduces the outage period to be less than 0.3 seconds.

Alternative Back Contact Materials for CdS/CdTe Thin Film Solar Cells

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Abstract

CdS/CdTe thin film solar cells have become matured photovoltaic technology, next to silicon solar cells technology due to ideal band gap, low manufacturing cost, and scalability of CdTe deposition. Although CdS/CdTe solar cells with copper based back contact have shown the best efficiencies by reducing roll-over effect and enhancing the electrical properties of CdTe, it is well known that their performance reduces with time, mainly due to diffusion of Cu through the CdTe absorber. This study focuses on finding a suitable alternative back contact namely, spiro/Au, MoO_3 / Ag, CuI / Au and Poly(ethylenedioxythiophene): polystyrene sulphonate(PEDOT:PSS) /Au in which Au and Ag contacts were deposited through thermal evaporation under high vacuum together with MoO_3 as a hole transporter while spiro, CuI and PEDOT:PSS hole transporters were deposited using spin coating technique. Performance of the device with PEDOT:PSS/Au exhibited the highest short-circuit current density over 24 $mAcm^{-2}$ together with an open circuit voltage of 0.39V and a fill factor of 0.32 which resulted an efficiency of 3.04% at solar simulator intensity of 100 mW/cm^2 among the studied material combinations. However, fill factor of this device was poor in comparison with device with Cu/Au contact, probably due to poor compatibility between inorganic and organic interface. These solar cell structures were subjected to stability checking for a period up to 8 months from their fabrication. Device with Cu/Au lost about 5 % of its initial efficiency while efficiency of device with PEDOT:PSS/Au remained the same over the period of 8 months.

Keywords: Back contact, thermal evaporation, hole transporter, thin film solar cell

Multifunctionality of Novel Ruthenium Dye (RuC) as an Interface Modifier for Nanocrystalline Titanium dioxide / Poly (3-hexylthiophene) Hybrid Solar Cells

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Abstract

This work reports the multifunctionality of a novel Ru based dye (RuC) in enhancing the performance of nanocrystalline Titanium dioxide (TiO_2) / Poly (3-hexylthiophene) (P3HT) hybrid solar cells. TiO_2 / P3HT nanocomposite films were fabricated with and without the RuC dye as the interface modifier and their optical properties were tested using UV-Vis and photoluminescence (PL) spectroscopies. UV-Vis spectra of TiO_2 / RuC and TiO_2/RuC/P3HT films ensure that the absorption spectra is broadened in the UV region due to the addition of the RuC dye. The PL measurements were carried out by pumping with laser at wavelength corresponds to maximum absorption of P3HT. The PL of TiO_2 / P3HT nanocomposite films were significantly quenched when the RuC dye was introduced at the TiO_2 / RuC interface. The PL quenching ensure the efficient exciton dissociation in P3HT when RuC is introduced. The corresponding solar cells were then fabricated using successive evaporation of MoO_3 and silver on top of the films and characterised under monochromatic and under Air Mass (AM) 1.5 conditions (100 mW cm^{-2}, 1 sun). The insertion of the RuC dye suppresses the dark current while extends external quantum efficiency spectra. As such, device with dye shows improved open circuit voltage and more than a factor of two times higher short circuit current density in comparison with the corresponding control. Hence, RuC dye improves the power conversion efficiency by a factor of two. This study concludes that, RuC dye has dual role; extending the spectral response and suppressing the dark current.

Keywords: Solar Cells, Ruthenium Dye, Titanium dioxide, Poly(3-hexylthiophene), co-sensitizers, photovoltaic, absorption, photoluminescence, polymers, efficiency

Silver Nanoparticles-Decorated Visible Light Responsive Titania Nano-Rods for Dye Sensitized Solar Cells

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Abstract

Dye-sensitized solar cells (DSSCs) based on nanocrystalline metal oxides are cost-efficient photovoltaic devices and work better even during darker conditions, such as in cloudy weather. Although higher efficiencies have been reported for DSSCs made with TiO_2 nanoparticles and Ru – based dye, their performance is apparently limited by both charge transport and charge separation efficiencies. This may be overcome by using templated porous structures, tetrapods, or vertically aligned nanorods. This work focuses on synthesizing TiO_2 nanorods using hydrothermal method which requires low operating temperature and short growth time. When the particles are made from multi-materials, it does not only improve the property of the main material but also develops their multifunctionality. As such, Ag nanoparticles were synthesized using chemical reduction method and deposited on the synthesized TiO_2 nanorods to enhance the efficiency of DSSCs. The surface morphology of the TiO_2 nanorod samples with and without Ag nanoparticles were compared using SEM images. The effect of silver deposition was investigated by UV-Visible spectroscopy while the particle size of the synthesized Ag nanoparticles was determined by the particle size analyser. Then the liquid state DSSCs were fabricated with N719 dye and photovoltaic performance of the fabricated solar cells were tested under simulated irradiation of 100 $mWcm^{-2}$ with AM 1.5 filter. DSSCs fabricated with Ag nanoparticles deposited TiO_2 nanorod arrays yielded about 60 % higher power conversion efficiency than its control device mainly due to the increment of short circuit current density which is consistent with broad spectrum of the TiO_2 nanorods with Ag.

Keywords: Dye sensitized solar cells, TiO_2 nanorods, hydrothermal method, power conversion efficiency

Optimizing the Performance of Perovskite Solar Cells by Varying Active Layer Thickness

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Abstract

Perovskite solar cells (PSCs) have been emerged as a strong contender for the next generation of photovoltaic technologies due to their promising power conversion efficiency (PCE) along with high absorbance, low-cost of production and facile fabrication process of absorber and Nanocrystalline TiO_2 layers. This study focuses on optimizing the performance of PSCs by modifying the active layers by varying the thickness of the active layers and the reaction time for the perovskite precursor solution. The corresponding ITO /compact TiO_2 / mesoporous TiO_2 / $CH_3NH_3PbI_xCl_{3-x}$ / P3HT / Au devices were fabricated. Mesoporous TiO_2 (mp-TiO_2) layer was deposited by solution processed spin coating method. Various spin rates and different concentrations of transparent Titania (18NR-T) nanocolloidal paste dissolved in Tetrahydrofuran (THF) were investigated for optimizing mp-TiO_2 layer with five different thickness of 400 nm, 500 nm, 600 nm, 750 nm and 950 nm. The best efficiency of 8.6 % was achieved with mp-TiO_2 thickness of 400 nm. Two different reaction times were investigated to identify the optimum reaction time for the perovskite precursor solution, and the device with reaction a time of 8 hours exhibited efficiency of over 3%, whereas the best efficiency of 6.4 % was achieved for the one fabricated with the reaction time of 2 hours. Furthermore, thin layers of perovskite with 400 nm thickness of TiO_2 exhibited better performance than the devices fabricated with the TiO_2 layer thickness of 550 nm. All the measurements were carried out under Air Mass (AM) 1.5 conditions (100 mW cm^{-2}, 1 sun) in air.

Keywords: Perovskite solar cells, thickness of active layers, Mesoporous TiO_2 layer, Titania (18NR-T) nanocolloidal paste

Enhancing the Performance of Dye Sensitized Solar Cells Using Ru-Doped TiO_2 Electrode

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Abstract

During the past few decades, the dye sensitized solar cells (DSSCs) have intensively been focused as an alternative energy source due to their low cost, easy fabrication and environment friendly operation. However, relaxation and recombination processes connected to the charge carriers hinder the performance of DSSCs. One of the alternatives extensively studied to improve the mobility of charge carriers in DSSCs is the use of doped TiO_2 electrode. In this study, Ruthenium (Ru) was selected as the dopant as Ru-based dyes have been reported to give better photovoltaic performance. TiO_2 was doped with $RuCl_3$ and the performance of the DSSC using Ru- doped TiO_2 electrode was investigated systematically varying the Ru content (0.002 to 0.04 wt%). The synthesised Ru-doped TiO_2 nanomaterials were characterised by X-ray diffraction (XRD), UV–Visible spectroscopy (UV–Vis), Fourier-transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM) techniques. The XRD pattern confirms the presence of mixed anatase and rutile phases of TiO_2; the optical absorption spectra of undoped and Ru doped TiO_2 revealed red shift in the absorption peak with Ru doping. The undoped and Ru-doped TiO_2 thin films were separately deposited on dense TiO_2 coated FTO using doctor-blading method and subsequently liquid state DSSCs were fabricated with commercially available N719 dye, $\mathrm{I}^- / \mathrm{I}_3^-$ electrolyte and FTO/Pt electrodes and photovoltaic performance of the devices were studied using Keithley-2420 source meter under simulated irradiation of intensity 100 $mWcm^{-2}$ with AM 1.5 filter. The 0.004 wt% Ru-doped TiO_2 electrode showed the best power conversion efficiency (PCE) of 7.34% with a 25% enhancement in the PCE relative to undoped TiO_2 based DSSC (PCE= 5.88%) mainly due to the increment of short circuit current density.

Efficient Hybrid Titanium Dioxide / Poly-3-Hexylthiophene Solar Cells Using an Oligothiophene Dye as an Interface Modifier

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Abstract

Hybrid metal oxide-polymer nanocomposites are promising material combination for cost efficient solar cells. However, the power conversion efficiency (PCE) of these hybrid solar cells are limited due to several reasons, including poor chemical compatibility of inorganic acceptor and organic donor. Our group recently reported that hole mobility of the polymer can be increased up to two order of magnitude when an oligothiophene dye is introduced at TiO_2 / P3HT interface modifier. This work focuses on studying the influence of dyes, including a 3-hexylthiophene derivative dye with a cyanoacrylic acid group ((E)-2-cyano-3-(3′,3′′,3′′′-trihexyl-[2,2′:5′,2′′:5′′,2′′′-quaterthiophene]-5-yl) acrylicacid) (4T), on the photovoltaic (PV) performance of TiO_2 / P3HT solar cells. The insertion of dye at the interface improves the efficiency regardless of the dye used. However, 4T dye significantly improved the efficiency by a factor of three when compared to the corresponding TiO_2/P3HT solar cells. This improvement is mainly due to increase in short circuit current density, which is consistent with higher hole mobility value of the polymer reported in TiO_2/P3HT nanocomposite with 4T dye. Optical absorption data further reveals that 4T extends spectral response of TiO_2/P3HT nanocomposite which could also enhance the short circuit current density. The reduced dark currents upon dye insertion ensure that the carrier recombination is controlled at the interface and this in turn increased the open circuit voltage. Optimised TiO_2/P3HT device with 4T dye showed average efficiency of about 2.0 % under simulated irradiation of 100 $mWcm^{-2}$ (1 sun) with AM 1.5 filter.

Keywords: Hybrid solar cells, Titanium dioxide, Poly (3-heylthiophene), oligothiophene dye, interface modifier, photovoltaic, absorption, quantum efficiency, polymers, efficiency.

Polarization-Controlled Interface Charges for Generation of Open-Circuit Voltage Higher than the Band Gap Towards "Polarization Photovoltaic" Solar Cell

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Abstract

Recently, solar cells have gained significant interest due to renewed attention to sustainability. The energy harvesting effectiveness of a solar cell centres are critically influenced by surface and interface properties inherent in the manufacturing of these devices. Conversion efficiencies over 40% have been achieved using conventional III–V semiconductor compounds as photovoltaic materials. The fundamental bandgap of the group III-nitride alloy system covers over a wider spectral region (from 0.64 to 6.2 eV) with tunable bandgap and strong absorption coefficient. However, bottleneck limiting the performance of such device arises from the potential barrier at the hetero interface due to the electron affinity difference. Another important factor is the existence of significant interface charges induced by spontaneous and piezoelectric polarizations due to non-centrosymmetric crystal structure. In turn, results in surface band bending depending on the interaction with surrounding atmosphere. Heterojunction (HJ) between n-ZnO and p-Si has a potential to perform as efficient and inexpensive solar cell. However, the relation between the polarization bound charges and the electronic properties of the HJ interfaces is not yet well understood. Calculated work function, φZnO (or barrier height) for ZnO varied from 5.02 to 0.33 eV as a function of Zn/O molar ratios. Surprisingly, a non-centrosymmetric crystal structure can develop a giant photovoltage. Specifically, the electron processes: photo-excitation, scattering, and relaxation occur with different probabilities. Considering a hetero-structure with cubic and non-centrosymmetric material, each non-centrosymmetric layer can act as a photovoltaic, so that the overall open-circuit voltage across the multi-junction is large, potentially much larger than the bandgap. Fundamental issues considering wurtzite-GaN/cubic GaN and wurtzite-ZnO/cubic-CdO hetero-structures will be discussed towards next-generation solar cells.

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Characterization Techniques in the Field of the Solar Energy Storage Device

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Abstract

Energy storage devices, such as batteries and supercapacitors play important role in both solar and wind energy applications. Amount of electrical energy produced by the solar cell directly depends on the incident amount of sunlight and only work in the daytime. Wind energy production depends on the available speed of the wind. Usually, the peaks of energy production and consumption times are different in a day. Therefore, storage of energy is essential for non-grid-tied solar and wind energy systems. Thousands of research groups have been working on battery and supercapacitor development to invent a storage device with the highest possible energy density. Almost all researchers are spending more than half of their valuable time for measuring their samples and plotting graphs. In this study, we have developed an instrument and control software to automate characterization procedure of supercapacitor and battery. This instrument will allow researchers to focus on their material development work rather than spending most of the time for characterization work. This newly developed instrument is capable of measuring capacitance, energy density, internal resistance, leakage current and plotting all the stranded curves, such as charge-discharge, cyclic voltammetry, and self-discharge individually. The heart of the instrument consists of computer controllable power source and electronic load with potentiostat / galvanostat capability. It can charge and discharge capacitors up to 8 amperes of constant currents and up to 20 volts. The working principle of this instrument based on high power operational amplifier with two error-amplifies in the feedback loop to limit the current and voltage to given values. This work will discuss the working principle of the newly developed characterizing instrument and how it helps to resolve challenges researches faced during supercapacitor and battery characterization.

Plasma Assisted Chemical Vapour Deposition of Hydrogenated Carbons (a-C:H) as Recombination Barrier Layer in Dye-Sensitized Solar Cells

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Abstract

One of the common hindrance to the higher power conversion efficiencies in any kind of solar cells is the charge recombination. In the case of dye-sensitized solar cells, porous electrode (typically TiO_2 or other wide bandgap semiconducting oxides) / dye interface is a hot recombination centre, where the electrons recombine either with the oxidized dye or the electrolyte. The above-said process inhibits the power conversion efficiency as it decreases the photo-generated current and the open circuit potential of the cell. Generally, to overcome this, wide band gap insulating oxide coating of few nanometre thicknesses is employed. Some of the important parameters for the choice of the coating material includes the Position of bands, the oxidation state, and the structural modifications in the TiO_2 layer induced by coating. In this work, hydrogenated carbon (a-C:H) layer were coated over the TiO_2 thin films by Plasma assisted chemical vapour deposition technique. Acetylene and argon mixture was used as precursor. Hydrogenated carbon coated TiO_2 were analysed using X-ray diffraction analysis, and the sample showed characteristic anatase phase of TiO_2, peaks corresponding to the carbon coating were not observed owing to its insulating nature. Optical properties were studied using UV-visible absorption analysis, and it showed strong absorption in the UV region. TEM analysis was done by scratching out the coating from the films, and it reveals a thin amorphous carbon layer deposited over the TiO_2 nanoparticles. XPS analysis revealed the chemical states of the prepared material. Further, Mott-Schottky Measurements were carried out for the coated TiO_2 layer to study the flat band potential of the material. The dye-sensitized solar cells were constructed using the prepared material and its power conversion efficiencies were studied. Further, to study the charge recombination, transport properties and electron life time of the cells, electrochemical impedance measurements were carried out.

Symposium on

Advanced Materials for Health Applications

Abstract of Keynote Speech – I

Designing Three Dimensional Porous Degradable Scaffolds Using Rheology, Surface Functionalization and Structure-Processing Relationship

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Degradable aliphatic polyesters are largely used in biomedical applications, as for example when designing scaffolds for tissue engineering. Successful results in tissue engineering are indeed dependent upon the interaction between the medical device and the biological environment. There are many ways to optimize this interaction and one option is to understand and design the production process, generate the most beneficial material properties. Another option is to focus on the surface, optimize the interaction using functionalization. Examples from both approaches will be discussed.

We have assessed the rheological properties and melt stability of the most commonly used degradable polymers, produced fibres with different diameters (1,75 mm – 20 µm) in order to understand the structure-processing relationship. We have defined the important material changes that take place during the process from polymer melt to fibre formation and following post treatment. This knowledge has subsequently been used to design fibres that resorb fast when the mechanical properties are lost. The results give important understanding in how to produce successful fiber based degradable medical device for tissue engineering.

The second approach, surface functionalization, is of interest because of the lack of functional groups or biological cues in the most commonly used aliphatic polyesters. Optimized functionalization would enable the interactions with cells and proteins. We recently succeed in the synthesis of a lactide-type monomer carrying a pendant thiol group, and used it in controlled ring-opening copolymerization with other cyclic esters. The obtained thiol-functionalized aliphatic polyesters have been used for preparation of porous scaffolds, which were subsequently covalently linked to RGD oligopeptides sequences by exploiting a disulphide exchange reaction.

Abstract of Plenary talk – I

Biodegradable ZnO/Polymer Core-Shell Nanocarriers: pH-Triggered Curcumin Release Towards Human Gastric Cancer

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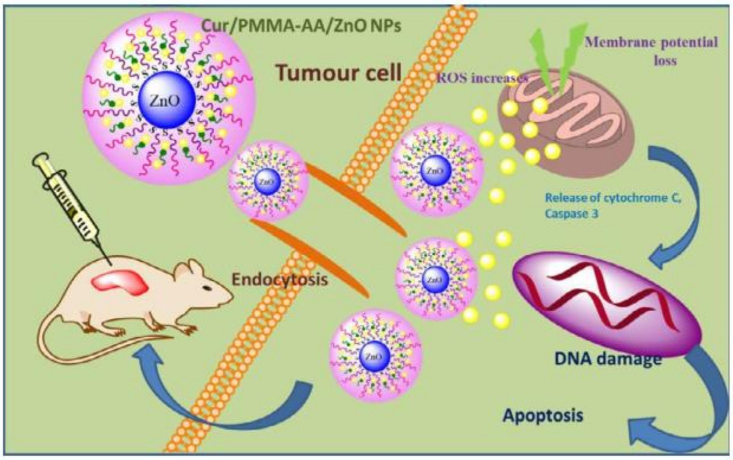
The co-polymer PMMA-AA encapsulated curcumin loaded ZnO bio-nanocomposite materials (Cur/PMMA-AA/ZnO bio-nanocomposite) of particle size 42 nm have been synthesized and magnificently utilized as good cargo materials to carry the well-known hydrophobic drug, curcumin by surface functionalization. Most importantly, the pH-responsive release of curcumin from the nano-vehicle ensures safer, more controlled delivery of the drug at physiological pH gradients. Their potential toxicity was studied by using AGS gastric cancer cell lines via MTT assay. These results revealed that these nanocomposites induce a remarkable cell death in in-vitro models. The curcumin loaded PMMA-AA/ZnO nanocomposite also potentially inhibited the growth of AGS cancer tumour in male Swiss albino mouse, which showed a promising targeted cancer therapy. Interestingly the given bio-nanocomposite was rapidly cleared from the organs with negligible exhibition of toxicity. From the obtained results it is understood that the apoptosis has been occurred through mitochondrial disruption-mediated pathway. Also these nanomaterials could efficiently hinder the Go/G1 transition along with cycle progression at S-phase transition due to the radiation-induced DNA damage. These findings declared that the auspicious candidate, curcumin could be efficaciously delivered into the target by the polymer encapsulated ZnO nanocomposites and exhibited a potent activity against gastric cancer cells at molecular and cellular levels as well as cell proliferation in a panel of tumour cells.



Abstract of Keynote speech - II

From Bench to Bedside, Stem Cells in Bone Augmentation

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Bone defects due to ablative surgery, injuries and to pathological and physiological bone resorption still represent a major challenge for oral/maxillofacial surgeons. Due to the complicated anatomy and physiology of bone tissue, as well as the limitations in the current medical technology, clinical treatments to repair bone defects are problematic and often yield poor healing. Tissue engineering has emerged as an interdisciplinary field for regenerative therapy of bone defects with tremendous potential to improve and replace the current classic strategies. Significant growth opportunities exist for synthetic bone grafts in association with mesenchymal stem cells from autologous or allogenic sources as alternatives to biological bone grafts.

This lecture covers research areas of central importance for bone tissue repair, including mesenchymal stem cells, biomaterial scaffolds for tissue engineering, osteogenesis and its molecular markers. A variety of cells in addition to stem cells, as well as advances in materials science to meet specific requirements for bone tissue regeneration by addition of bioactive molecules, will be discussed.

Abstract of Plenary talk – II

Use of Autologous Adipose Stem Cells to Reconstruct Cranio-Maxillofacial Defects

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We have used autologous adipose tissue derived stem/stromal cells (ASC) to reconstruct cranio-maxillofacial defects in 27 cases. For reconstructions, subcutaneous adipose tissue was collected and the ASC were extracted, expanded for 3-5 weeks, and then seeded onto porous resorbable scaffolds for subsequent implantation into hard-tissue defects. The defects were reconstructed with bioactive glass, β-tricalcium phosphate (β-TCP) or β-TCP/ε-polycaprolactone scaffolds seeded with ASC with or without human bone morphogenetic protein-2. Multilineage differentiation potential (adipogenic, osteogenic and chondrogenic differentiation) and surface marker profile (CD14, CD19, CD34, CD45, CD73, CD90, CD105, HLA-ABC-PE, and HLA-DR) of ASC was analyzed. Furthermore, chromosomal integrity, sterility, endotoxins and mycoplasma were analyzed before using cells for transplantations. Follow-up time has varied from 12 to 76 months. Successful bone formation and integration of the bone regenerate to the surrounding skeleton occurred in 18 of the 27 cases. In unsuccessful cases, 1 patient developed infection, 1 nasal septum transplant was lost due to recipient-related reasons and 7 patients did not produce sufficient volume of bone or the implant was resorbed. This study shows that the use of autologous ASC combined with biomaterial scaffolds is a viable option for reconstruction of cranio-maxillofacial hard-tissue defects. However, sufficient vascularization of the recipient site is an important factor in determining the outcome of the autologous ASC based therapy.

Abstract of Plenary talk – III

Diamond for Application in Retinal prostheses

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Starting with the introduction of the first implantable pacemaker five decades ago, implantable electronic medical devices have achieved remarkable success in the treatment of the most challenging conditions, such as deafness (cochlear implants) and heart conditions (pacemakers). Implantable electronic devices must necessarily adhere to a very strict set of standards before they can be approved for clinical use. Some of these standards are (i) the requirement that devices are manufactured from inert, bio non-toxic materials and (ii) the electronically active components such as microprocessors are encapsulated hermetically to protect the body from the toxicity of conventional electronic components and as well as to protect the components from the harsh environment inside the body which leads to accelerated device failure. We have developed a retinal implant fabricated using synthetic diamond. Retinal implants restore a sense of vision, for a growing number of users worldwide. Nevertheless, visual acuities provided by the current generation of devices are low. The quantity of information transferable to the retina using existing implant technologies is limited, far below receptor cells' capabilities. Many agree that increasing the information density deliverable by a retinal prosthesis requires devices with stimulation electrodes that are both dense and numerous. This work describes a new generation of retinal prostheses capable of upscaling the information density that can be provided to the brain via the retina. Fabricated from engineered diamond materials, the implant is very well tolerated in the body and shows long-term stability in the eye's unique physiological environment. The device is capable of delivering highly versatile stimulation waveforms – a key attribute in providing useful vision. Delivery of high-density information, close to the retina with the flexibility to alter stimulation parameters in situ provides the best chance for success in providing high acuity prosthetic vision. The Australia-developed Diamond Eye™ technology, supported by a made-in-Canada wireless solution for implantable bionic devices, will return partial vision to the blind.

Corrosion Resistance of Zinc Incorporated and Magnesium Incorporated Hydroxyapatite Coating on Surgical Grade Titanium Alloy

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Abstract

The present study is about the corrosion resistance behaviour of zinc incorporated and magnesium incorporated hydroxyapatite coated titanium alloy. Zinc incorporated and magnesium incorporated hydroxyapatite coatings were obtained on titanium alloy by the hydrothermal method. The formation and the morphology of the coating have been characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction analysis (XRD) and field emission scanning electron spectroscopy (FESEM- EDAX) techniques. The corrosion resistance of the coated titanium alloy substrate was investigated in Ringer's solution by electrochemical techniques. R_t values obtained for the Zn-HAp coated on titanium alloy is found to be greater as 233.3 ohm cm^2 than that of the uncoated titanium alloy (11.32 ohm cm^2).

Keywords: Hydrothermal deposition, Hydroxyapatite, Zn incorporated HAp, Mg incorporated HAp, corrosion resistance.

Cuttlefish Bone Derived Hybrid Composite Scaffolds for Bone Tissue Engineering

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Abstract

In recent years, there is a drastic increase in the demand of biomaterials for bone defects which results in newer research on the development of smart biomaterials with enhanced osteogenesis. The controlled and rapid healing of bone repair process is seemingly a matter of interest for biomaterials research. Notably, hydroxyapatite (HAp) and its polymer/metal oxide composites play a significant role in the field of biomaterials research for orthopedics treatment procedures. In this study, hybrid composite scaffolds derived from cuttlefish bone (CFB) for hard tissue engineering has been successfully demonstrated under hydrothermal process. The final cuttlefish bone scaffold product was completely transformed into biomimetic hydroxyapatite crystal structure under optimized hydrothermal condition without any change in the natural channelled structural arrangements. The X-ray diffraction pattern reveals the characteristic hydroxyapatite formation without the presence of any other calcium phosphate/carbonate derivatives. Further, to enhance its biological response, the developed scaffolds were coated with the polymeric mixture of sodium alginate and alumina/zirconia nanoparticles. The elemental analysis of the prepared scaffolds confirms the presence of respective elements such as Ca, P, O and Al/Zr. The *in vitro* biocompatibility study on these composite scaffolds shows excellent biocompatibility against MG63 osteoblasts like cells and cell attachment/proliferation. Therefore, the porous and channelled arrangement of cuttlefish bone derived hydroxyapatite-(alumina/zirconia)-sodium alginate based hybrid composite scaffolds should enhance cell attachment, bone tissue ingrowth that results in rapid healing of bone tissue damage.

Keywords: Cuttlefish bone, hydrothermal, scaffolds, biocompatibility, hydroxyapatite

A Pragmatic Review on the Property, Role and Significance of Polymers in Treating Diabetic Foot Ulcer

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Abstract

Diabetic Foot Ulcer is one of the traumatic complications that develop due to impaired glycemic control and increased plantar pressure. Addressing the issues of necrosis, ischemia, inflammation, infection and peripheral arterial disease is important to attain a wholesome treatment, depending on the prognostic stage in DFU. PAD leading to uneven plantar pressure can be better treated by off-loading techniques. It is essential to arrest further aggravation of the ulcer, attain ideal wound closure and prevent recurrence. Though various treatment methods have been employed from the past, search for novel dressings are still on the rise, since prevalence of ulcer varies between individual patients and their adapted life style. This review emphasizes the contribution of various natural and synthetic polymeric materials, composite forms and the role of incorporating signalling molecules such as growth factors, cytokines, chemokines, their properties and delivery mechanisms as standard wound dressing in diabetic ulcers. Through extensive study on the occurrence, prognosis, severity and the cellular responses observed at the site, strategic management to alleviate the conditions of the challenging DFU could be made possible.

Keywords: Diabetic Foot Ulcer, ischemia, infection, peripheral arterial disease, signalling molecules, delivery mechanisms

Extraction of Collagen from Fresh Water Pygocentrus Brachypomus (Red-bellied Piranha) and Its Physical, Biochemical and Morphological Characterization

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Abstract

Collagen is the most common structural protein constituting the skin and many other tissues in humans. The market for collagen extends from cosmetics to therapeutics and is estimated to be $ 6.63 billion by 2025. Owing to the increased demand and unbound religious restrictions, corollary parts of fish are extensively sought for as the source of collagen. *Pygocentrus brachypomus* (Red-bellied Piranha) is one of the largely consumed fish varieties in South India and the extraction of collagen from its scales is reported for the first time through this study. The yield of the Acid Soluble Collagen (ASC) extracted based on dry weight was 0.5 ± 0.08%. The Ultraviolet absorption spectrum exhibited the maximum absorption at 230 nm. The peaks from the Infrared spectrum, X-Ray Diffraction analysis confirmed that the extracted collagen retained the triple helical native conformation. The results of Differential

Scanning Calorimetry revealed that the thermal stability of the extracted collagen was higher with T_d – 38.94 ˚C and T_m – 92.5 ˚C and was comparable to bovine and porcine sources. The average particle size of the extracted collagen was calculated to be 517.2 nm. Electron micrograph of the extracted collagen presented loose, parallel oriented long fibres with interconnected fibrils. Hence, the collagen extracted and characterized is a safe alternative for various biomedical applications.

Keywords: *Pygocentrus brachypomus*, Acid Soluble Collagen, thermal properties, native conformation, interconnected fibrils

Synthesis of Acidity Triggered Cisplatin Encapsulated Slow Release Zinc Oxide Targeted Drug Delivery Nano Composite for Cancer Treatment

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Abstract

Cisplatin is a frequently used anticancer drug with a cis configuration that facilitates the covalently binding of the coordination complex to DNA strands and thus crosslinking the DNA strands triggering the cells to die in a programmed manner. However, cisplatin is associated with several side effects which can be either reduced or overcome if cisplatin could be encapsulated in a suitable host material and directed towards cancer cells in a targeted manner. To achieve these targets, we have prepared porous nanoparticles of zinc oxide (ZnO) and encapsulated cisplatin in them and studied their release kinetics in buffered solutions of defined pH values. Since cancerous cells are more acidic compared to normal cells and that ZnO is stable in neutral pH media while decompose slowly in low acidic conditions, it can be a highly suitable host to release drug slowly only at the vicinity of the cancer cells. We developed a novel surfactant-assisted method to synthesize porous nanoparticles of ZnO. The encapsulation of cisplatin was characterised by XRF, SEM, FT-IR and XRD studies. The release kinetics of cisplatin at different pH values was investigated by measuring the amount of Pt released as a function of time using ICP-AES. It shows the release of cisplatin is pH dependent and there is hardly any release of cisplatin at neutral and basic pH values. As such, at physiological pH of blood and that of healthy cells cisplatin is not released while at mildly acidic pH values of cancer cells cisplatin is slowly released.

Single Layer Carbon Loaded Polyethylene Film for Foot Pressure Monitoring

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Abstract

Arthritis is an intense or unremitting irritation ailment that influences the joints, connective tissues, muscle, ligaments, and stringy tissue. It is a main cause of inability among individuals more than 50 years old in developed country, also it tends to strike amid the most beneficial long periods of adulthood regularly causing torment and deformation. It offers ascend to tremendous healthcare expenditures and loss of work. With the existing system, there are different size of FSR sensors used for foot pressure analysis. A sole with major pressure points (2 - 9) was designed to analyse the foot pressure but unfortunately, the foot size differs from one person to another person. So, the single sole design setup cannot be used for all the persons. In the proposed method, a sensor array designed with single layer carbon loaded polyethylene film was designed and each sensor with sides 21 mm x 21 mm to form the 7x3 array pattern of foot pressure pad. By using the array foot pressure pad, we can analyse the pressure points throughout the pad. Each of the sensors in the array is having the gap of 5mm. The output analog signal acquired and this electrical signal may result in pre-emptive of the knee problem.

Keywords: Piezo resistive, Foot pressure monitoring, velostat, pressure pad

A Comparative Study of Chitosan and Glucosamine Isolated from Local Mushroom 'Lenahathu' (Schizophyllum Commune) and Oyster Mushroom (Pleurotus Ostreatus)

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Abstract

The use of mushroom as a raw material to obtain chitosan and glucosamine was investigated at laboratory level. Properties of chitosan extracted from local mushroom "lenahathu" (*Schizophyllum commune)* and common oyster mushroom (*Pleurotus ostreatus*) were compared. Isolation process of chitosan involved de-mineralization, de-proteinization, de-acetylation and de-coloration steps. The physico-chemical properties of chitosan such as solubility, moisture content, ash content, N content, fat binding capacity (FBC), water binding capacity (WBC) and degree of de-acetylation (DD) of chitosan samples extracted from *Schizophyllum commune* and *Pleurotus ostreatus* were analysed. The purity of two glucosamine samples were analysed by spectrophotometrically and scan electron microscope (SEM). The values for percentage yield, solubility, moisture content, ash content, N content, WBC were 1.73 ± 0.05% and 1.22 ± 0.01%, 7.38 ± 0.10% and 3.41 ± 0.14%, 6.39 ± 0.20% and 8.16 ± 0.42%, 8.19 ± 0.04% and 1.63 ± 0.05%, 11.31% and 3.02%, 387.13 ± 15.57% and 402.57 ± 12.78% respectively for chitosan samples from *Schizophyllum commune* and *Pleurotus ostreatus.* FBC were varied approximately 250% - 350% in coconut oil, soy bean oil and sunflower oil. Chitosan and glucosamine were characterized using Fourier Transformed Infra-Red (FT-IR) spectroscopy. DD% of chitosan using FT-IR and conductometric titration were 53.10% and 60.68% respectively for two species. The yield and purity of glucosamine sample of *Schizophyllum commune* were 95.70% and 0.97 ± 0.08%. However the yield and purity of glucosamine sample of *Pleurotus ostreatus* were 58.14% and 0.52 ± 0.04% respectively. According to results *Schizophyllum commune* could be a good alternative to extract chitosan and an important drug glucosamine.

Keywords: Chitosan, glucosamine, mushroom, Schizophyllum commune, Pleurotus ostreatus

A Review of Mechanical 3D Printed Upper Limb Prosthesis

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Abstract

Conventional passive upper extremities used by amputee's lack in hand control and grasp meanwhile their advanced substitute are expensive, unaffordable and less realistic. In recent years, affordable, functional and customizable upper limb alternatives, made using 3D printing technology, have increased in demand. This article reviews the available technologies to fabricate 3D printed upper limb prosthesis, different levels of upper limb amputations and materials used for fabrications. This also gives an overview about the mechanisms used in 3D printed mechanical upper limb prosthesis and cost factors affecting the popularity of the prosthesis in detail. A main reason for 3D printing to be used in prosthesis fabrication is the convenience and the efficiency in the process of customizing prosthesis according to user's requirements. Acrylonitrile Butadiene Styrene (ABS) or Poly Lactic Acid (PLA) are considered as the most suitable material for 3D printing of prosthesis, focusing on the factors of cost and availability, toxicity, biodegradability and comfortability. Most of the affordable prosthetic arms are operated using string networks or using lever mechanisms which limits the functionalities of prosthetic arms due to its inability of fingers to operate independently. Therefore, moving on to an improved operating mechanism to facilitate independent motion of fingers is suggested as the future outlook for mechanical 3D printed upper limb prosthesis.

Keywords: extremities, 3D printing, grasp, mechanical, amputation, Acrylonitrile Butadiene Styrene (ABS), Poly Lactic Acid (PLA)

Design and Optimization of a Wrist Powered Upper Limb Prosthesis

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Abstract

The primary function of a prosthetic device is to provide assistive support for patients with upper or lower limb amputation. Among the upper limb amputations, most of the patients with trans-metacarpal amputation avoids the use of prosthetics due to the high cost and complex nature of the commercially available prosthetics. These commercially available prostheses lack certain features, like adaptive grasp and comfort. In order to overcome these problems, 3D printing has shown a promising path in developing quick and customizable solutions using modern technology. Despite the importance of adaptive grasp in a prosthesis, literature shows that studies related to improving adaptive grasp seems to be limited. The purpose of this study is to improve the adaptive grasp mechanism used in mechanical prosthesis to effectively utilize the limited angle of the wrist to produce enough gripping force for better functionality. The typical angle of motion of the healthy person, the limitations and complications occurring were found and the effects of trans-metacarpal amputation to the motion of the wrist were analysed. According to the findings the design of the prosthesis was started using Computer Aided Designing (CAD) software and necessary improvements needed were taken into consideration during the design phase of the new prosthesis and the mechanism. The proper material was selected to be used in the 3D printer and the prosthesis was printed and tested for adaptive grasp and comfort. Whipple Tree mechanism was used to improve the adaptive grasp through proper force distribution. It was found that this kind of prosthetic hands will help the amputee to grasp complex shaped objects which cannot be grasped by commercially available prosthetic devices. Moreover, the 'Flexi' material will give enough comfort to the amputee during operation.

Keywords: Trans-Metacarpal Amputation, 3D Printing, Adaptive Grasp, Mechanical, CAD

A Study of Three-Dimensional (3D) Printed Prosthetic Upper Limb Models in Local Context

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Abstract

Northern Sri Lanka is recovering from a civil war that has left a large number with amputations. The centre for prosthetics initiated the production of four different widely available models of 3D printed prosthetic upper limbs and compared the pros and cons in local context. Flexy, Shira, LimbForge and a simple bionic hand were produced at the centre and they were analysed in this aspect. Manipulations, shape, weight, comfort and cost is accounted for during the selection of prostheses. LimbForge, an aesthetic nonfunctional solution is preferred by economically disadvantaged groups for its low cost and realistic look. But lacking basic requirements of functionality makes it a less effective choice. While a bionic hand opens to a wide range of possibilities for performance enhancement, in contrast with the high cost involved, the Flexy or Shira prosthesis seems to be much more promising as they offer essential functionality at low cost. A set of experiments were carried out with the Shira and Flexy prostheses to compare performance analysing parameters such as the maximum grasp strength, angle of wrist flexion required and types of grips attainable by the prosthesis. Based on these experiments regarding proper manipulation of day to day objects, the 3D printed Flexy showed high grip strength and increased dexterity compared to the Shira hand. Moreover, the 35 degrees angle of flexion required for a proper grip exhibited by the Flexy hand, compared to the 46 degrees of the Shira hand reflects a clear superiority of the former in the context of simplicity of manipulation. This study concludes that the Flexy hand is the most suitable among the four models developed by considering production cost and minimal functionality requirements, for low or middle-income amputees.

Wearable Piezoresistive Nanocomposite Sensing Mechanism for Non-Invasive Knee Pain Monitoring

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Abstract

Arthritis, an informal way of referring to joint pain or joint disease, is common among elderly people in industrialized countries. Epidemiology studies have reported that 19% of people at the age of 45 have radiographic evidence of knee arthritis, which increases to 27% for people aged 63 to 69 years and to 44% for people older than 80 years. Presently, diagnosis of arthritis is based basically on physical examination, followed by laboratory tests and imaging test, which are prohibitively costlier. Hence, this paper proposes a cost effective method to acquire stress and strain values from the knee joints by using light weight flexible piezo-resistive nano-composite sensor placed in suitable patella package. It is obvious that the stress and strain exerted by an arthritis affected knee will be different from its normal counterpart. The proposed biocompatible flexible piezo-resistive nano-composite is made up of conducting polymer composites. Conducting polymer composites consist of thermoplastic urethane (TPU) with uniformly distributed conductive filler carbon nano-fiber (CNF). Deformation due to stress and strain on the conducting polymer composite changes the mean particle distance of the conductive filler, which in turn results changes in surface or bulk resistivity of the material. This change in resistivity can easily be converted into equivalent electrical signals which are proportional to movements of knee joints. A meticulous analysis on these electrical signals may reveal the problem spectrum from which the nature of the knee problem can be analysed for subsequent treatment. The signals obtained through the prototype developed with the aforesaid materials are presented here which clearly distinct the variations between the normal knee movements and strained knee movements.

Keywords: Nanocomposites, Piezoresistive, Non-invasive sensors, Arthritis, Knee Pain Monitoring

Hydroxyapatite Reinforced Natural Polymer Scaffold for Bone Tissue Regeneration

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Abstract

Medical Advances had led to an increase in life expectancy. However, one of the challenges confronted by the orthopaedic surgeon is the repair and restoration of large skeletal bone defects resulting from resection of a malignant bone neoplasms and trauma. Nano hydroxyapatite is a naturally occurring mineral form of calcium apatite. Hydroxyapatite is the main component of bone which is constantly synthesized and degraded naturally by living bone and hence effectively used as a bio implant. Hydroxyapatite combined with starch can be used as a biomaterial for making scaffolds for bone tissue regeneration since starch is a natural polymer that is used for load bearing applications. This is used to improve the biocompatibility of scaffold for living cells. The materials are synthesized by Wet Chemical Method in liquid phase, dried to obtain solid particles and solvent casting technique is used for making scaffold in the ratio 1:1. Prepared materials are characterized using DLS, FTIR, XRD, and SEM. The size of prepared Hydroxyapatite particle is found to be 174.2 nm. Cytotoxicity test reveals highly compatible and non-toxic to the body.

Keywords: *Biomaterials, Hydroxyapatite, Polymers, Scaffold, Biocompatible, Cytotoxicity, SEM*

Latent Fingerprint Analysis using Bioconjugated Fluorescent Nanoparticle

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Abstract

Fingerprints are the direct unique patterns for identification of individuals. These fingerprint patterns of latent (not visible) nature are very challenging to investigators. Normal powder dusting methods have high background interference due to its chemical contamination. To enhance the contrast, sensitivity, selectivity, efficiency and to lower the background emission properties, fluorescent nanoparticles can be doped with bioconjugated adhesive polymers. These polymers can be favourable candidates for latent fingerprint detection. Europium has excellent physical and chemical properties. The narrow band emission of europium allows good filtering of undesired background interference. This rare earth metal nanoparticle when doped with bio-adhesive polymer forms a conjugate that would act as an excellent fluorescent material. In this work, the bio-adhesive polymer is extracted from marine mussel as mussel adhesive protein (MAP). This adhesive protein anchors itself to the solid support; it is highly stable and transparent. It can easily immobilize nanomaterials with its stable adsorption. This bioadhesive material has high adsorption with biomolecules which forms the fingerprint constituents (proteins, sweat glands, amino acids, carbonyl groups, etc.). The adsorption properties are characterized using Langmuir and freundlich models. Characterization studies are performed by XRD, SEM and FTIR. Photoluminescence activity is studied by photoluminescence spectroscopy. This study shows a pathway for improvement in latent fingerprint analysis through fluorescent nanoparticle doped bioadhesive polymer.

Design Framework for TPMS Bone Tissue Engineering Scaffolds Based on Multi-Field Model

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Abstract

Apart from the biomaterial selection, the geometrical & pore structure of bone scaffolds, their mechanical and bio-fluid properties play important criteria in the design of 3D porous scaffolds for bone tissue regeneration. The joint multi-fields such as computer aided design (CAD), finite element analysis (FEA) and computational fluid dynamics (CFD) will be applied for the design of bone scaffolds. The motivation of this research is to predict the mechanical and fluid properties of triply periodic minimal surface (TPMS) based bone scaffolds for different geometrical and material parameters. TPMS scaffold structure using CAD provides high surface to volume ratio, high permeability and interconnections with merits of aiding cell migration. The FEA and CFD help to improve the design of bone scaffolds and predict the behaviour of complex structures for efficient bone tissue formation in mechanical loading, compression and fluid perfusion. Further, an integrated model (Mechanical & Monte Carlo models) will be applied for simulation of scaffolds degradation and a model to simulate angiogenesis & tissue regeneration in the scaffolds will also be created.

Keywords: bone scaffolds, finite element analysis, computational fluid dynamics, triply periodic minimal surfaces

Biocompatible Spherical-Shaped Calcined Hydroxyapatite Nano Particles Synthesized Via Calcium Sucrets Method.

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Abstract

Recently, throughout the world, biocompatible hydroxyapatite (HA) nanomaterials have been widely used in a broad range of biomedical applications. However, current synthesis techniques of biocompatible HA nanomaterials are very expensive. Therefore, we have developed a simple and cost-effective method to synthesize HA having spherical porous structures with chemical compositions closely related to the mineral phase of the human bone so as to impart osteo-conductive properties. These products may be used in biomedical applications at low-cost.

These nanoparticles were prepared by precipitating from a precursor solution containing calcium sucrate and ammonium dihydrogen orthophosphate, at a Ca:P mole ratio of 1.67:1, at room temperature. The obtained product was analysed for its crystallinity, crystallite size, morphology, and composition, by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FT-IR) spectroscopic techniques. Analyses were also done after calcining the respective products, soon after their synthesis, for 3 h, at 700 °C. The calcined samples always produced spherical nanoparticles of essentially the same diameter, between 90 nm and 100 nm, which does not change due to aging or by changing preparative-temperature in the range from 20-90 °C.

Biocompatibility, cytotoxicity and bio-functionality of these materials are currently being under investigation to make sure their suitability for biomedical application. HA nanoparticles are nontoxic according to the cytotoxicity results which confirm their potential usage in biomedical applications. MTT (3-(4,5-dimethyl thiazol-2-yl)-2,5-diphenyl tetrazolium bromide) assay, Alamarblue assay for cell proliferation, Alkaline phosphatase (ALP) activity assay for cell differentiation and SEM analysis for the cell morphology studies confirmed that the synthesized HA nanoparticles are nontoxic

Carbohydrate Lyotropic Liquid Crystals Materials as Stabilizer and Permeation Enhancer for Microemulsion Based Drug Delivery System

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Abstract

Lyotropic liquid crystals (LC) having amphiphilic properties are promising materials as co-surfactants in emulsion formulations. A carbohydrate lyotropic liquid crystal, hexadecyl-β-D-glucopyranoside, was synthesized by linking D-glucose to cetyl alcohol via acetylated glucoside and its ability to stabilize microemulsions was investigated. The synthesized compound was characterized by using Nuclear Magnetic Resonance Spectroscopy (NMR) and Fourier Transform Infrared Spectroscopy (FTIR). Both acetylated and deacetylated compounds were found to exhibit thermotropic and lyotropic liquid crystal behaviour. The critical micelle concentration (CMC) value of 1.53×10^{-5} mol dm^{-3} obtained for hexadecyl-β-D-glucopyranoside from both UV-visible spectroscopic and turbidity methods suggests its non-ionic surfactant properties. Calculated HLB value of 8.86 indicates that it is suitable for making self-emulsifying oils and water in oil (W/O) emulsions.

ME systems were prepared using Olive oil, water and the nonionic lipophilic surfactant Sorbitan monooleate (Span 80) by selecting suitable compositions of both W/O (water in oil) and O/W (Oil in Water) emulsion systems from the phase diagram constructed at 70 °C. By introducing optimum amount of 0.05 wt.% of synthesized glycolipid, macro emulsions formulated was successfully converted into microemulsions. Then, hydrophilic drug, Diclofenac sodium (DS) (1.00% (w/w)) was introduced to the selected W/O and O/W emulsions separately and in vitro release of drugs through a pig ear (ear epidermis) fitted to a Franz diffusion cell system was observed with and without glycolipid (hexadecyl-β-D-glucopyranoside) (0.05% (w/w)) as permeation enhancer. Aqueous solution of DS (1% (w/w)) was used as the control.

The optimized ME formulations which contain DS as model drug show higher amount of release of 76.35% and 63.52% for W/O and O/W respectively. Those systems exhibit 6-10 nm nano-scaled aggregates which improve the permeation and its large surface area enhances the quick release of both sparingly soluble and highly soluble drugs in water. Finally, it is clearly understand that incorporating hexadecyl-β-D glucopyranoside in ME formulations shows significant potential as a delivery vehicle in the cosmetics and pharmaceutical industry.

Toxicity of CuO, ZnO, TiO_2 and MWCNT Nanoparticles on Human Pathogenic Bacteria

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Abstract

Toxicities of CuO, ZnO, TiO_2 and MWCNT nanoparticles towards human pathogenic bacteria *Bacillus cereus* (Gram - negative) and *Salmonella typhi* (Gram - positive) were determined using serial dilution method on Luria Bertani (LB) agar plate method. The structural and morphological properties of the nanoparticles were characterized using XRD, SEM, EDAX and TEM analysis. The above said human pathogens were inoculated in 20 ml of sterile nutrient broth and it was incubated at 37°C for 12 h. After incubation, the bacterial cultures were treated with nanoparticles (100 µg/ml) and the culture was incubated for 6 hrs. After incubation, 100 µl of culture test tubes was diluted (10^1 to 10^7 numbers of colonies) and each dilution were taken on LB agar plates using with spreader. The plates were incubated for 24 hours at 37°C. After incubation, the results were observed plates and colonies were counted. *S.typhi*: MTCC733 showed the uncountable colonies for all the nanoparticles. However, a countable bacterial colony for each dilution was observed for *Bacillus cereus*, when treated with ZnO nanoparticles. The CuO demonstrate countable colonies for 10^3 - 10^7 dilution, while TiO_2 & MWCNT demonstrate countable colonies for 10^5 - 10^7 dilution plates.

Keywords: Toxicity, nanoparticles, pathogenic bacteria and antibacterial activity

Design of Healthcare System Using IoT Enabled Application

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Abstract

Increase in the usage of wearable sensor nodes and advanced communication helps to progress diagnostic methodology in improving the quality of human life. Virtual monitoring of patients through wearable sensors nodes can avail the services of experts to the region with scarcity of medical facility hence medical services in those areas can be enhanced. The medical facility available to rural India is considerably lacking certain amenities. The Conventional practice of medicine and healthcare is mostly heuristic driven Knowledge of regular monitoring of vital health parameter helps the patients to take precautionary measure at the early stage. Medical App is necessary to avail quality services of IoT. The proposed system has three major basic blocks. The first being body sensor sensing the data from the body, second is sending data to cloud and the last part is to provide the data to an expert using designed APIs. The placement of sensor nodes on human body and selection of communication protocol plays an important role in designing the system. Sensors placed on the body are noninvasive sensors they collect the vital parameters. Sensors used in this research are body temperature sensor, blood glucose sensor, blood pressure and Electrocardiogram sensor (ECG) Sensor node records the data and transmits it to the cloud using coordinator node. The communication between body coordinator node and the cloud is established using ESP-8266 Wi-Fi Module. Data received is stored in Thing speak Cloud. The user friendly application programming interfaces (APIs) helps to provide early assistance of the doctor. The APP designed at the destination point can view the parameter of the patient and communicate message to the patient or user about the status of the health parameter, prescribe the medicine, sends an alert message during critical condition and provides with assistance. Research finds to develop low cost user friendly health monitoring application to receive the information from the patients and recommend appropriate service at the early stage of diagnosis.

Evaluation of Anticancer Activities of Gold - Chitosan Nanocomposite

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Abstract

The optical features of metal nanoparticles are due to their unique interaction with light, which give bright intense colours. In the presence of the oscillating electromagnetic field of light, the free electrons of the metal nanoparticle undergo a collective coherent oscillation. This motion is resonant at a particular light frequency and is termed as Localized Surface Plasmon Resonance (LSPR) oscillation. The electric field intensity and the scattering and absorption characteristics of the nanoparticles are all strongly enhanced at the LSPR frequency, which for silver, gold and copper show distinct and well-defined plasmon absorption in the visible region. The plasmon absorption frequency for silver, gold and copper nanoparticles were 390-400 nm, 500-550 nm and 565-570 nm respectively.

Moreover, due to the absence of band gap and the continuum of electronic states in the noble metal structures, the photogenerated electron-hole pairs can be readily recombined, which leads to deactivation of the active sites and a reduction in photocatalytic efficiency. Hence, active supports are more suitable to be used in various applications. Chitosan is a biopolymer, deacetylated derivative of chitin. Chitosan has been widely used due to its various properties such as microbial resistance, non-toxicity, biodegradability and metal ion absorptivity. The interactions of chitosan with metal ions described by three ways, i) metal chelation ii) electrostatic attraction and iii) formation of ion pairs. The use of natural biomaterials in the synthesis of nano-sized material provides an interface for the charge transfer resulting in the increase of bactericidal property. The development and application of biomaterials have been significantly influenced by advances in the field of medicine, surgery, biotechnology and materials science. The present work deals with the synthesis of bio-composite using bio polymer like chitosan. Chitosan can be used as binder to the metal. It will be very interesting to investigate the effect of anticancer activity of metal based bio-composite.

Nano Carbon Implanted Ag Doped Medical Cotton Fabrics by Plasma Implantation Technique for Health Applications

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Abstract

Cotton fabrics are well known for its textile usages. In addition to this, its role in medical applications such as surgical, wound dressing and sport wearables are also inevitable. In this favour, our research focuses on the incorporation of nano carbon-based materials over cotton fabrics found to be a promising technology for the medical applications. Incorporation of nano carbons over cotton fabric was done by using plasma implantation technique. Further, we have extended our plasma implanted nano carbons to make it anti-microbial by incorporation of silver nanoparticle (Ag-NPs) on the plasma treated cotton fabrics. These resultant nano carbon implanted Ag-NPs deposited cotton fabrics show admirable biomedical results. The processed cotton fabric samples were analysed by using various studies such as FTIR to identify the presence of its functional groups, surface morphology was carried out using electron microscopes (SEM & TEM). Further its biological activities were analysed to identify its antimicrobial behaviour, cell adhesion property and anti-cancer activity.

Keywords: Cotton fabric; Plasma implantation technique; nano carbon; Silver nanoparticles; antibacterial activity.

Waste Driven Hydroxyapatite

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Abstract

Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$) (HA) is widely used in the medical applications due to its superior bio-friendly properties. In this work we report simple technique to fabricate HA from waste materials. We fabricated HA using three different raw materials; (1) egg shell, (2) coral reefs, (3) sea shells as calcium sources. The materials were cleaned in water and dried under direct sun for a day. Then the raw materials were calcinated using a muffle furnace at 900°C for 2 hours. Calcinated powder was grounded and added into deionised (DI) water. Then the required amount of orthophosphoric acid (H_3PO_4) is added into the mixture and kept under stirring for 15 hours. The precipitate were then collected and washed twice in DI water to remove the excess solvents added. The resultant precipitate is dried at 60°C in an electric oven for 12 hours and dye pressed into pellets. The pellets were characterised by FESEM and XRD. As prepared samples show the nano HA and they agglomerated and spherical shape after sintering at 900°C. XRD pattern showed peaks for crystalline HA, regardless of the raw material used. The increased peaks after sintering indicated that the crystallinity increased after sintering.

Keywords: Hydroxyapatite, Biomaterial, Egg shell, Coral reefs.

Extraction and Characterization of Starch from Sri Lankan *Cassava*

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Abstract

The worldwide market for polymers is rapidly on the rise due to the high demand for consumer as well as technological applications. Bio-based polymers are considered as a potential replacement for petroleum-based polymers to minimize harmful environmental impact. Bio-based polymers are defined as polymers originated from biological sources. Most of the bio-based polymers are produced from bio-based monomers. Starch is one example of a simple bio-based polymer, that has been known and widely used for centuries. Starch can be used in packaging, textiles and construction applications. Starch can be extracted from different types of plant based materials such as cassava tubers. Cassava is cultivated in Sri Lanka in most of the districts for local and export market. Annual production of Cassava in Yala and Maha season in 2016 was about 300,000 MT.

The objective of this research was to extract and characterize starch from Cassava tubers. In this study, Sri Lankan cassava (*Manihot esculenta*) was selected as the main raw material for starch extraction. The cassava tubers were sourced from the Kalutara district in Sri Lanka for this study. Starch was extracted from cassavas tubers by crushing, blending and sedimentation. First, the cassava tubers were washed, peeled and chopped into small pieces. Then, they were ground in a high speed blender for 5 minutes. The blended pulp was then suspended in 10 times its volume of water and stirred for 5minutes. This product was filtered using a muslin cloth and the filtrate was allowed to stand for two hours. Then the product was kept for sedimentation. Finally, it was completely dried in the sun light to convert the starch in to dry powder. The extracted product was characterized by Fourier transform infrared spectroscopic technique (FTIR). Experimental results showed that 20 wt.% of starch could be extracted from the cassava that was tested. The extracted starch can be used for different applications as a bio- based polymer.

3D Printed Gelatin Scaffolds for Fibrocartilage Regeneration

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Abstract

The temporomandibular joint (TMJ) is bilateral synovial joint with an interpositional fibrocartilage disc connecting the mandible to the temporal bones. Unlike conventional treatment strategies, tissue engineering seems promising to regenerate lost/damaged TMJ structures. Gelatin type A were 3D printed, cross-linked with genipin, freeze-dried and sterilized. The scaffolds were characterized in terms of structure, swelling and stability. Interactions of the scaffolds with mesenchymal stem cells (MSCs) in terms of seeding efficacy, attachment and chondrogenic differentiation were conducted. The chondrogenic differentiation of the cells on scaffolds were compared to standard pellet culture and microspheres. The scaffolds demonstrated good shape fidelity. Structural characterization by SEM and µCT showed open porosity of 93%. The freeze-drying resulted in 38% shrinkage. However, the printed scaffolds had high swelling capacity (500%) after 1h and showed stability over 21 days in culture medium. With respect to the biological performance, the printed scaffolds supported cell attachment and differentiation. Compared with pellets and spheres, the 3D printed scaffolds had a similar trend of upregulation of the chondrogenic gene markers, i.e. SOX9, aggrecan, collagen I and II and a downregulation of the hypertrophy marker collagen X over 21 days. Gelatin is suitable for 3D printing fabrication and genipin successfully prevented rapid degradation of the scaffolds. Gelatin scaffolds supported cell attachment and chondrogenic differentiation *in vitro*. 3D printed gelatin scaffolds hold great potential for fibrocartilage tissue engineering applications.

Synthesis, Characterization and Biological Properties of Ruthenium(III) Complexes

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Abstract

The ruthenium complexes were synthesized from ruthenium(III) metal precursors and thiosemicarbazone ligands by ligand exchange reactions. The structural features of the synthesized complexes were studied by various physico-chemical and spectroscopic techniques. In all the complexes studied, the Schiff bases act as bidentate ligands. The efficiency of the ruthenium(III) complexes towards the biomolecules, the interaction between DNA/BSA was studied. In addition, the cytotoxic properties of the complexes were evaluated against a panel of bacteria and the efficiency of complexes to arrest the growth of HeLa and MCF-7 tumour cell lines have been studied along with cell viability test under *in vitro* conditions. The results showed a dose dependent anti-proliferative effect, thus indicating the biological significance of the complexes. Moreover, the complexes were examined the oxidation inhibition property against the DPPH and OH radicals.

Surface Modification of Polymeric Scaffolds for Bone Regeneration

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Abstract

Poly(L-lactide-co-ε-caprolactone) (poly(LLA-co-CL)) meets many of the requirements of a scaffolding material for bone tissue engineering, such as adequate biocompatibility, degradability, and tunable properties. However, poly(LLA-co-CL) scaffolding tends to be hydrophobic and does not favor cellular attachment and differentiation. The overall purpose of this research project was to improve the physical and chemical properties of poly(LLA-co-CL) scaffolds to enhance biological responses. The modifying effects were evaluated and characterized in vitro and in vivo. The hydrophilicity of the surfaces of poly(LLA-co-CL) scaffolding was increased, either by blending with Tween 80, or coating with nanodiamond particles (nDPs). Compared with pristine scaffolds, the modified poly(LLA-co-CL) scaffolds exhibited reduced albumin adsorption and significantly increased the seeding efficiency of bone marrow stromal stem cells (BMSC). Poly(LLA-co-CL)/3% Tween 80 scaffolds implanted subcutaneously in rats exhibited significantly increased mRNA expression of Runx2 and de novo bone formation. BMSC-seeded into poly(LLA-co-CL)/nDPs scaffolds were implanted into rat calvarial defects and live imaging at 12 weeks disclosed significantly increased osteogenic metabolic activity. Micro-computed tomography, confirmed by histological data, revealed a substantial increase in bone volume. Modifying the surface of poly(LLA-co-CL) scaffolds to improve hydrophilicity promotes osteoconductivity and bone regeneration. Further studies are needed to understand the immunogenic responses, because implantation of a biomaterial always initiates an inflammatory foreign body reaction. Moreover, the next generation scaffolding technique (3DF) may customize bio-inspired artificial extracellular matrices, incorporating optimal physical and chemical surface properties to improve stem cell support.

3-Dimensional Poly(LLA-co-TMC) Scaffolds Functionalized with Hyaluronic Acid Enhanced Cell-Material Interactions

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Abstract

Synthetic degradable polymers such as poly (L-Lactide) (PLLA) and poly trimethylene carbonate (PTMC) and their copolymers have been used to fabricate scaffolds in tissue engineering applications. However, they present with major drawbacks, including inherent hydrophobicity and acidic by-products. These drawbacks could affect the cell-scaffolds' interactions and host responses post-transplantation. Hyaluronic acid (HA), a non-sulfated glycosaminoglycan, has excellent hydrophilic properties and is known to play important roles in the extracellular matrix particularly during wound healing. In the current study, the effect of HA coating to improve the cell-scaffold interactions was investigated. Human bone marrow stem cells (hBMSC) were isolated and characterized based on multi-lineage differentiation as well as immunophenotype using flow cytometry. hBMSC were seeded onto 3-dimensional poly(LLA-co-TMC) scaffolds coated with three different concentrations of HA solution (0.1%, 0.25% and 0.5%). Non-coated scaffolds were used as control. Cellular responses were evaluated by studying cell attachment, viability and proliferation. Chemical analysis for the release and degradation of HA in cell culture medium was also quantified using cetyltrimethylammonium bromide turbidimetric method (CTM). DNA quantification exhibited higher cell number at all timepoints in 0.5% HA group than the other groups, while Live/Dead staining indicated that scaffolds coated with 0.5% HA promoted cellular infiltration into the pores of the scaffold. Western blotting showed phosphorylated focal adhesion kinase (FAK) CTM showed that HA was released into medium immediately, and that residual HA could be detected for a longer time in 0.5% HA group. Collectively, the data indicate that poly(LLA-co-TMC) scaffolds coated with 0.5% HA can significantly enhance the cellular interactions, which in return can improve the efficacy of tissue-engineered constructs.

Biomimetic Matrices Delivering Growth Factors

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Abstract

Current research focuses on developing potent bone substitutes or biomimetic 3D matrices/scaffolds for restoring the function and structure of tissue, not only by osteoconduction but also to deliver growth factors (GF) to synergistically instruct the body’s own mechanism for regeneration. A dose of 1 µg bone morphogenetic protein -2 (BMP-2), was physisorbed on nanodiamond particles (nDP) modified poly(LLA-co-CL) scaffolds and compared to BMP-2 physisorption on unmodified scaffolds. Release kinetics of BMP-2 was quantified for up to 70 days using mass spectrometry (MS) and their osteogenic potential was evaluated. Unmodified poly(LLA-co-CL) scaffolds were also functionalised by physisorption of a cocktail of GFs using human demineralised dentin matrix (DDM) and compared to control scaffolds. Release kinetics up to 21 days was studied and their efficacy on the osteogenic differentiation of human bone marrow mesenchymal stem cells (hBMSC) up to 21 days was evaluated. MS revealed a sustained release of low levels of BMP-2 from nanodiamond modified scaffolds (nDP-PHY) for up to 70 days compared to unmodified scaffolds plus BMP-2 (PHY). nDP-PHY and PHY scaffolds promoted bone regeneration in a rat mandible critical-sized defect after 4 weeks, however nDP-PHY scaffolds demonstrated osteogenic potential in vivo as well as in hBMSC cultures. When delivering cocktail of GFs, 390 proteins were identified by MS to be released from the DDM modified scaffolds, and the proteins involved in bone regeneration showed comparable release trends. Cells grown in DDM modified scaffolds showed the highest expression of inflammatory markers while also expressing higher mRNA expression of osteogenic markers. Poly(LLA-co-CL) scaffolds were successfully rendered biomimetic by physisorbing BMP-2 alone or a cocktail of GFs. In addition, nDP provide copolymer scaffolds with a platform for strongly binding a GFs, yet maintaining its bioactivity.

pH Tunable Curcumin Release from PMMA-AA Coated ZnO Nanoparticles for Excellent Anti-Gastric Cancer Therapy

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Abstract

PMMA-AA encapsulated ZnO bionanoconjugate (Cur/PMMA-AA/ZnO) was successfully synthesised and utilized as good cargo materials to carry the well-known hydrophobic drug curcumin by surface functionalization. Physical characteristics of this novel bioconjugate has been studied with transmission electron microscopy (TEM) and powder X-ray diffraction (XRD) in conjunction with spectral techniques. A narrow particle size distribution with an average value of 42 nm was found via TEM. Most importantly, the pH-responsive curcumin release from this nano-vehicle ensures safer, much controlled delivery towards gastric cancer cell lines at physiological pH gradients. The efficient curcumin entrapment and loading were evaluated along with its in vitro efficacy with mice model, which showed a potent inhibition on the growth of AGS cancer tumour in male Swiss albino mouse, and acts as a promising targeted cancer agent. Interestingly the given bio-nanocomposite was rapidly cleared from the organs with negligible exhibition of toxicity. From the obtained results it is understood that the apoptosis has been occurred through mitochondrial disruption-mediated pathway. Also these nanomaterials could efficiently hinder the Go/G1 transition along with cycle progression at S-phase transition due to the radiation-induced DNA damage. These findings declared that the auspicious candidate, curcumin could be successfully delivered into the specific target by the polymer encapsulated ZnO NPs and exhibited a potent activity against gastric cancer cells at molecular and cellular levels as well as cell proliferation in a panel of tumour cells. The multifunctional properties of the studied bionanoconjugate system may open up new avenues in cancer therapy through overcoming the limitations of conventional cancer therapy.

Symposium on

Advanced Functional Materials

Abstract of Keynote Speech – I

Design Multifunctional Materials from Ab initio Calculations

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Identifying advanced functional materials with efficiency higher than current level is one of the key areas of research. Studying materials with multiple functionalities attract much attention in recent years to resolve important issues such as energy crisis, environmental degradation etc. Also, by controlling various order parameters involved in magnetic, electric and lattice coupling one can tune the properties of functional materials to the desired level. So, using state-of-the-art ab initio methods we have studied magnetic, electric, optical, magnetoelectric, magneto-optic, photoelectric, photocatalytic, thermoelectric, and electro-chemical properties of materials useful for energy and environmental technologies.

Converting solar energy into fuel via photocatalytic water splitting to generate hydrogen is an attractive scientific and technological goal to address the increasing global energy demand. In this talk I will focus in detail on modelling and tailoring the band gaps and band edge positions of carbon-nitride based 2D nanostructures carbon nitrides suitable for water splitting applications. Specifically, the influence of iso-electronic substitutions and molecular adsorption on photocatalytic water splitting activity will be discussed.

Storage of hydrogen in chemical compounds offers a much wider range of possibilities to meet the transportation requirements, but no single material investigated to date exhibits all the necessary properties. I will show how one can weaken strong ionic bonding in the potential hydrogen storage material MgH_2 by ternary addition and also their nanophase aspects. Further, I will demonstrate that it is possible to keep hydrogen in amphoteric state within the same structural unit and this will break the mental barrier put forth by the rule-of-2A to design hydrogen storage materials with high volumetric density.

The magnetic multiferroic materials exhibit the coupling between the two distinct phenomena of (anti)ferroelectricity and (anti)ferromagnetism, which allow them to be useful for novel devices. I will show how one can introduce giant magnetoelectric coupling in multiferroics and in extreme case by varying electric field one can change materials from magnetic to nonmagnetic. Also, I will show how one can tune the magnetoelectric coupling in composite magnetoelectrics. Our results show that one can bring giant magnetoelectric coupling in materials those possess magnetic instability or metamagnetism. Further, I will discuss about some ideas to design new multiferroic using theoretical techniques and some of our recent works on composite magnetoelectrics. I will show how one can design semiconductors purely from metals and also their usefulness in thermoelectric applications. Further I will show how one can design higher efficient TE materials based on half Heusler alloys with multinary alloying using 18 valance electron count rule. I will show some of our recent work dealing with general trends in the variation of band gap as well

as electronic structure along with introduction of additional phonon scattering centers by multinary alloying which are essential in increasing the electrical conductivity and reducing the thermal conductivity of the crystal and hence increasing the ZT value. If time permit I will give results from other functional materials investigated in our lab.

Abstract of Plenary talk – I

Microscopical Understanding of Growth Mechanism, Doping, Alloying on 2D Materials

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Recent research of two-dimensional (2D) transition metal dichalcogenides (TMDC) materials, and its successful integration into the devices opens a new direction. The basic crystal structure of 2D TMDC materials consists of hexagonally packed atomic layers, with chalcogenide–metal–chalcogenide arrangements in the trigonal prismatic or octahedral coordination. Molybdenum (Mo) and tungsten (W) based dichalcogenides are two such representatives of well-defined family of structurally and chemically ordered 2D compounds.

Our knowledge on the microscopic process during the growth including nucleation and growth kinetics seems to be still limited, partly due to the few practical difficulties, i.e., the challenge in transferring ultra-fine clusters formed at an early stage of growth and possible loss of intermediate/by-products (some of them are aqueous soluble). As such, comprehensive studies to reveal the microscopic growth mechanism of 2D materials are needed.

In addition, alloying is widely used due to its ability to accurately controlling doping concentrations which determines the physical and chemical properties of 2D materials and hence comparatively better than other band gap engineering processes (such as strain, chemical functionalization, etc.,). Isoelectronic doping can be also useful in suppressing the detrimental effect of defects created during the growth of 2D monolayers which paves the way to find its valuable representation in opto-electronic devices. Direct observation of such alloy structure at the atomic scale is essential to understand and to further control the wide range of its behavior.

In the current paper, recent advances in atomic resolution imaging of 2D materials using aberration corrected transmission electron microscopy is reported. Growth mechanism of 2D materials is explained together with the theoretical calculations and metal-chalcogenide alloying into 2D structure is widely studied and reported. Spherical aberration-corrected scanning transmission electron microscopes (STEMs) are now able to form intense electron probes as small as 0.5 Å in diameter provide image resolution to well below 1 Å. The STEM works on the same principle as the normal scanning electron microscope (SEM), by forming a focused beam of electrons that is scanned over the sample while some desired signal is collected to form an image.

Abstract of Plenary talk – II

MedeA: Atomistic Simulations as an Accelerator in Innovations

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Analytical methods can provide a detailed picture of several materials properties. However, using this information to predict thermophysical properties is still limited by two main factors, namely (i) scarcity of experimental data on pure compounds and (ii) limited predictive capability of correlative methods (group contributions, equations of state). The development of new materials opens up exciting and often unimagined possibilities in many areas of life, from communication, information processing, mobility and medicine to energy conversion and storage. Of course, we expect long-term reliability as well as high safety, sustainability and environmental compatibility, but rarely do we envision the challenges of modern materials research in order to guarantee precisely those properties. In this field of tension, atomistic simulations have proven to be an indispensable component. Without them, neither the systematic search for materials with tailor-made properties nor comprehensive quality assurance would be conceivable. The talk describes the possibilities of atomistic simulations in an industrial context and gives an insight into current developments. The combination of powerful theoretical concepts, advanced computational software and today's extraordinary computational capabilities opens unprecedented opportunities for the industrial and R&D application of computational chemistry and materials science.

Abstract of Keynote Speech – II

Zinc Antimonate: An Advanced Functional Nanomaterial for Supercapacitors

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The current focus of research is mainly based on supercapacitors, which is the emerging field for future energy storage applications. To the best, nanostructured ruthenium oxide hydrate is a well renowned material for supercapacitors owing to their superior electrochemical properties. However, commercial practice of ruthenium oxide hydrate is hindered, due to its higher cost, relatively less abundance and toxic nature. In order to explore a material with supercapacitor qualities extensive research contributions is necessary. In addition, exploring an inexpensive electrode material for supercapacitors is also highly essential. Recently, a novel functional material, zinc antimonate (ZnSb2O6), a tetragonal crystal structured nanomaterial with an optical band gap of ~3.36 eV was reported as an electrode material for supercapacitors. ZnSb2O6 with nanorod morphology delivered a maximum specific capacitance of 53.3 F g-1 at a current density of 1.0 A g-1 with capacitance retention of 103.5% while the same material with particle morphology delivered a maximum specific capacitance of 47.5 F g-1 at a current density of 0.04 A g-1 with capacitance retention of 100.0%, respectively. The superior electrochemical properties of zinc antimonate nanostructures are attributable to the inclusion of two heterovalent metal cations such as Zn2+ and Sb5+. Furthermore, zinc antimonate has been utilized for the preparation of hybrid nanocomposites as electrode candidates for supercapacitors. The structural and electrochemical properties of zinc antimonate and its nanocomposites will be presented in detail.

Abstract of Plenary Talk – III

Functional Materials for Energy Conversion and Energy Saving Applications

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Materials research is important for many applications related to, e.g., energy conversion and energy saving. In the present talk some of the latest key developments will be reported. Preliminary results will be reported about applications of Si nanomaterials in energy conversion devices such as the emerging organic/Si solar cells and heterojunction Si/CZTS cells. Functionalization of the organic component with inorganic nanomaterials might help to extend durability of the organic/inorganic hybrid material and Si surface passivation. Applications of such organic/inorganic hybrid material will be discussed for applications in electrochromic and energy storage devices. Stability of the hybrid material will be discussed with respect to thermal processing and to influence of ultraviolet irradiation.

Si absorbs about 36 % of sunlight, which about five times exceeds that of the well-known photocatalytic material TiO_2. The composite of Si with TiO2 is expected to absorb more sunlight than pure TiO_2. In the presentation synthesis and characterization of such a composite nanomaterial, potential of their applications in photocatalysis, and in decomposition of methylene blue will be discussed.

Transition metal and rare-earth metal oxyhydrides are emerging class of materials with mixed hydride and oxide anions sharing the same sites in the lattice. One of the examples of the class of materials is the so-called black TiO_2 and yttrium oxyhydride. The talk includes report about latest developments on the topic about yttrium oxyhydride and possible applications in photocatalysis and energy efficient windows. In the last a few year, exciting results have been obtained on different types of solar cells such as Se-, Sb-S(Se), ZnOSe, $Cu_2ZnSnS(Se)_4$, and perovskite solar cells. The lecture reflects the latest developments.

Abstract of Plenary Talk – IV

Ways to tune metastable phases - a combined ab initio and experimental study

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A ‘metastable phase’ is a nonequilibrium configurational state of a system whose properties change reversibly at the time of experiment or observation. Metastability is ensured by the existence of an energy barrier associated with the path of transformation of the system into states with a lower potential energy. In other words, a metastable phase is a local minimum of the potential energy surface. Since the barrier separating metastable from stable states is never infinite in reality, at finite temperatures (and, including quantum fluctuations, even at a zero temperature), there is always a probability of transitioning into a more stable state in a certain time; i.e., there is always a characteristic `lifetime' of a metastable phase. Thus, the existence of a ‘metastable phase’ unavoidably introduces the factor of time (kinetics), absent in thermodynamics. Upon a quench, namely a sudden change of the external conditions, a system is initially in a nonequilibrium state. The relaxation processes to a new equilibrium state may be complex, especially if a phase transition boundary is crossed and more than one phase is locally stable. These metastable phases may exhibit physical and chemical properties very different from the equilibrium configuration, and thus be more suitable materials for certain applications. The tremendous increase of computational power over the last couple of decades, in combination with methodological improvements, opened the possibility of guiding the development of new materials and new phases using first principles calculations based on quantum mechanics. In this presentation, we are going to demonstrate a number of approaches to stabilize metastable phases and study their physical and chemical properties using state of the art density functional theory (DFT) calculations. These findings are complementary to the experimental observation (or to the lack of it) of metastable phases.

Photocatalytic Degradation of Methylene Blue Dye Using ZnO Thin Films-Effect of Area of Catalyst

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Abstract

Zinc oxide thin films were deposited on glass substrates using sol gel spin coating method. Zinc acetate dihydrate was used as a starting material. Isoproponol and monoethanolamine were used as the solvent and stabilizer respectively. The prepared solution was dropped on the cleaned glass substrates and the substrates were rotated at 2000 rpm for 20 s and the ZnO thin films were prepared by repeated coating. The prepared thin films were annealed at 450 ^{o}C. The annealed films were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), ultraviolet – visible spectrophotometer (UV-Vis), photoluminescence spectroscopy (PL). Photocatalytic activities of ZnO thin films annealed at 450 ^{o}C have been examined towards the photo degradation of methylene blue by varying catalyst area. A maximum efficiency of 90.4 % is reported using low watt (8W) UV source.

Keywords: ZnO thin films, photocatalytic activity, catalyst area

Greenly Synthesised Iron Nano Particles and Their Application for Degradation of Volatile Organic Compounds

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Abstract

Water pollution creates main issues due to the presence of organic pollutants such as benzene, Toluene, Ethylbenzene and xylene (BTEX), which has become an important global environmental demand. Currently, advanced oxidation shows a significant role in the degradation of BTEX in polluted water in the purification of waste water. However, most of the oxidation work use greenly synthesized iron nanoparticle (INP). We focus on a greenly synthesis of iron INP and degradation of BTEX in oil polluted water for the first time. INP is synthesized with green synthetic method using green tea as reducing and capping agent to keep particles in nanometer scale. The final INP and activated carbon composite are prepared by calcining at 500 ^{o}C for 1h. The synthesized nanoparticle is characterized by X-Ray diffraction and scanning electron microscope. The composite has been well formed with particle size ranges from 40 nm to 110 nm. The advanced oxidation activity of INP has been examined by the degradation of BTEX in an electrochemical cell. The reactivity of modified activated carbon was tested by the 100 ppb of BTEX standard solution in water. The oxidation of BTEX occurred in the presence of active oxygen and iron nanoparticles that imply the oxidation via the free radical pathway. Further, the oxidation of BTEX was fastest in the presence of 900 mA current through which iron nanoparticles cause vanishing of 90% of BTEX within 30 min. Oxidation of BTEX in water polluted by waste oil is vanishing of 90% of BTEX within 70 min. These observations suggest that the potential of INP can be used as water purification materials, and environmental therapy to remove or convert harmful organic substances.

Keywords: Iron nano particle, BTEX degradation, Oil degradation

Semi-Empirical Simulations of Interactions between Edge-Functionalized Graphene Oxides and Bisphenol A

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Abstract

This study reports for the first time an analysis of the interactions between edge-functionalized graphene oxide (GO) sheets and bisphenol A (BPA) examined by semi-empirical simulations. Bisphenol A (BPA), $(CH_3)_2C(C_6H_4OH)_2$, used in synthesis of a variety of polymers, is one of the chemicals produced in very high quantities worldwide, with more than 450 metric tons released annually into the environment. Due to its ability to mimic estrogen and it being an endocrine disruptor, it is a pollutant of serious concern. Graphene oxides have been studied extensively as electrochemical sensor materials for analytes, wherein the sensor performance (e.g., sensitivity) depends on the nature and amount of oxygen-containing functional groups present. This work considers a lattice containing 59 hexagonal cells ($C_{150}H_{34}$), with one edge modified by carbonyl/carboxyl groups, is used to examine interactions with BPA. Simulations are carried out at the semi-empirical PM6 level using MOPAC and the DH2 modification is employed to calculate interaction energies. It is seen that the hydrogen/oxygen atoms of the phenolic group(s) of BPA interact primarily with the oxygen atoms of the carbonyl/carboxyl group or the hydrogen atoms of the carboxyl groups/graphene edges. These interactions are predominantly polar and non-covalent in nature, e.g., hydrogen bonds, in addition to dispersion. The heat of formation of the GO-BPA complex decreases with increasing number of functional groups in GO and becomes exothermic. However, the strength of the GO-BPA interaction goes through a maximum at 4 carboxyl groups (for an edge with 7 carbon atoms). Beyond this, the carboxyl groups start interacting significantly amongst each other, weakening the GO-BPA interaction. Optimized structures, charges and the corresponding interaction energies are presented for eight different GO structures (2 containing carbonyl groups and 6 containing carboxyl groups).

Investigation on the Effect of Ultrasonication on the Morphology of BiVO4 Sonicated During and After Preparation by Chemical Co-Precipitation Method

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Abstract

Bismuth vanadate ($BiVO_4$) was synthesized by chemical co-precipitation and ultrasonic assisted co-precipitation method. The crystal structure of the samples was studied using X-Ray diffraction (XRD). The monoclinic scheelite structure was confirmed from the presence of (1 2 1) and (0 4 0) planes. The morphology and optical properties of the samples were analysed using scanning electron microscope (SEM) and UV–Vis diffused reflectance spectroscopy (DRS) respectively. Photocatalytic activity of the prepared BiVO4 was tested for the photo-degradation of Methylene Blue under visible light irradiation. The properties of as prepared BiVO4 is compared with the samples prepared using ultrasonic assisted co-precipitation method during and after preparation, and an optimal ultrasonic power output which leads to better photocatalytic activity is identified. The sample sonicated with 160 W during preparation yielded better catalytic efficiency which showed 93% degradation of Methylene blue. The improved catalytic activity could be attributed to its crystallinity, unique morphology and higher surface area compared to other samples.

Keywords: $BiVO_4$, chemical precipitation, photocatalysis

Response of Reinforced Concrete Panels Retrofitted with Elastomeric Polyurethane Coatings Under Blast Loads

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Abstract

Recent deterioration and damage to buildings and infrastructures caused by the extreme loading events have emphasized the necessity of adequate dynamic resistivity of those structures against such impulsive loadings. This innovation is on the use of palm oil-based polyurethane (PU) as a retrofitting material to enhance the structural capacity and resistance of reinforced concrete (RC) structural elements against impulsive effects. A numerical study was conducted using non-linear Finite Element (FE) code, LS-DYNA to study the dynamic resistance of bio-based PU coated RC slab elements subjected to blast load impact. FE models were developed based on an experimental investigation conducted by Tanapornraweekit et al. (2010). The material models were verified with the experimental outcomes of the varying strain-rate properties of materials which were investigated by the authors in the subsequent studies. Developed FE models were verified and validated using the experimental outcomes of the Tanapornraweekit's study. The contribution of coating thickness on the overall efficiency of the retrofitting scheme was assessed by four different coating thickness. The coating thicknesses were selected as the proportion to the total panel thickness, which are 2.5%, 5%, 10% and 20%. In addition, three concurrent studies on the coating thickness were undertaken, which are the influence of the coating thickness on impact face, rear face (with respect to blast) and, on both faces (with equal coating thickness). Findings indicated that the overall effectiveness of the proposed technique has shown great potential in terms of reduction in the panel deformations, support rotation and fragmentation effect in enhancing the blast resistance of RC elements.

Keywords: Bio-based polyurethane; Retrofitting; Reinforced concrete; Impulsive loading

Controlled Growth of Vertically Aligned ZnO Nanorod Array Via Polymer Assisted Hydrothermal Method

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Abstract

Hydrothermally synthesized vertically aligned Zinc Oxide (ZnO) Nano rod array are widely used in semiconductor device applications including LEDs, transducers, sensors and solar cells. It is an interesting material for third and fourth generation solar cells due to its thin and aligned morphology which increases the effective surface area and improve charge transport. The aspect ratio of the nanorods found to be a critical parameter for most of the device application particularly towards solar cell applications.

In this work, we report a simple solution process method to control the aspect ratio of the nanorods by a modified hydrothermal synthesis. ZnO nanorods were fabricated on a 100 nm ZnO thin film coated glass substrate. The growth solutions were prepared by mixing 100 ml of 50 mM Zinc acetate ($Zn(CH_3COO)_2 \cdot 2H_2O$) and 100 ml of 50 mM hexamethylenetetramine ($(CH_2)_6N_4$) (HMT). Polyethylenimine (PEI) with molecular weight of 600 was used as a controlling agent. Growth were carried out different times. Resulting Nano rods were characterized using Scanning electron microscopy (SEM), X-ray diffraction (XRD) and UV-vis spectroscopy (UV-vis). Resulting Nano rods exhibited vertical orientation and uniform distribution on the substrate with a hexagonal cross section. XRD confirmed that these nanorods grown with and without PEI show highly crystalline hexagonal wurtzite phase. We found that the aspect ratio of the nanorods increased when PEI is added to the growth solution. The average diameter and length of ZnO Nanorods were determined as 60 nm and 125 nm with and without PEI in to the growth solution. The length of the Nanorods was determined as ≈1 µm to ≈5 µm with and without PEI respectively. The variation of aspect ratio with and without PEI with growth time will be discussed in the presentation

Preparation, Synthesis and Characterization of Zeolite Faujasite for CO_2 Adsorption

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Abstract

Zeolites materials are mainly used as an adsorbent and also for the ion exchange and heterogeneous catalyst respectively. Though Zeolites are occurring in nature, some impurities were present inside it, therefore synthetic zeolite are getting more attention in recent decades. For synthesis, Sol-gel method is preferred because the crystal growth can be controlled by varying synthetic time and growth temperature. In this report, Zeolite Faujasite (FAU) X type was synthesised and their crystal structure were confirmed using X-Ray Diffraction (XRD), surface morphology was studied using Scanning Electron Microscope (SEM), functional group are identified by Fourier transform infrared spectroscopy (FTIR), the Si/Al ratio (1.5 to 3.0) determined by Energy-dispersive X-ray spectroscopy (EDS), From the N_2 adsorption/desorption isotherms the surface area and from Barrett-Joyner-Halenda (BJH) analysis its pore size distribution were studied.

Investigation of the Formation Mechanisms of Mesoporous Silica Structures by Local Dielectric Variations

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Abstract

Since their discovery mesoporous silica has been widely used in various fields like waste water purification, indoor air cleaning, catalysis, bio-catalysis, drug delivery, CO_2 capture, bioanalytical sample preparation. This is mainly due to their unique properties such as ordered pore structures, large pore areas and fairly high chemical inertness. Mesoporous silica can be synthesized in a wide range of morphologies such as spheres rods, discs, powders, etc. Unlike traditional porous silica, mesoporous silica exhibit exceptionally ordered pores.

The interaction between inorganic precursor and organic template plays a major role in the mesoporous structure formations. Therefore, it is important to understand these interactions in detail to develop new porous materials as well as to modify existing materials. According to the conventional micelle chemistry, effective local surfactant parameter (p) is the mesophase deciding factor. Depending on the value of p different mesophases; $p < 1/3$ cubic –*pm3n*, $1/3 < p < 1/2$ hexagonal *p6m*, $1/2 < p < 2/3$ cubic *la3d* and $p = 1$ lamellar are formed.

Though there are several mechanisms proposed for these mesoporous material formations in scientific literature, none of the proposed mechanisms provides an exclusive and definite answers. So aim of this research is to shed some light on these unanswered questions on mesoporous silica formation mechanisms.

In this research silica based mesoporous material was prepared in the presence of Cetrialmethylammonium Bromide (CTAB) as a structure directing agent and Pyrene as the probe molecule. As probe material's emission spectrum is change due to its interaction with CTAB, the mechanisms in which micelle and silica formation were studied. Analysing spectroscopic data, Critical Micelle Concentration (CTC) and mechanism in which it interacts with Silica are present here.

Improved Method to Extract Kinetic Parameters from Thermograms

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Abstract

Thermogravimetric (TG) analysis and differential thermogravimetric analysis (DTG) are the most commonly used analytical techniques to find the kinetic triplet of solid state reactions. There are number of methods proposed in the literature for extracting kinetic parameters of solid state reactions from TG & DTG thermograms. MATLAB based computer simulation was used to investigate the dependence of DTG peak position on kinetic triplets. The numerical modelling shows that there is no significant variation in DTG peak position with the reaction model. Therefore, peak position is not a suitable parameter when determining reaction model. However, this enables a development of a common equation to link the activation energy and the pre-exponential factor. This relationship in turn be used to enhance the accuracy of kinetic parameters obtained.

Green Synthesis and Structural Characterization of Silver Nanoparticles Synthesized Using the Pod Extract of Clitoria Ternatea and Its Application towards Dye Degradation

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Abstract

Silver nanoparticles (SNPs) have multifaceted applications ranging from nanomedicine to nanoremediation. For the first time, silver nanoparticles were synthesized using the aqueous extract of *Clitoria ternatea* pods as reducing agent. The formation of SNPs was first confirmed by visual inspection and then by a characteristic peak at 418nm observed in UV-Vis spectrum. Spherical SNPs with few agglomerations were noticed in SEM image. EDS spectrum showed a strong signal for elemental silver at 3keV. The crystalline nature of the SNPs was confirmed from a sharp peak obtained in XRD at 38.58°. The involvement of biomolecules in the formation and capping processes was ascertained by specific bands such as (cm^{-1}) 3595, 1728, 2924, 1381, 1620 and 1049 in FTIR spectra. The average hydrodynamic size of the SNPs was 62.51 nm. A low PDI value of 0.264 was observed which validated the monodispersity of the SNPs. The stability of the SNPs was corroborated by the zeta potential value of – 24.6 mV. In addition, an important environmental application – degradation of methylene blue dye has been demonstrated in which SNPs acted as nanocatalysts. The first order kinetic constant for the degradation has been calculated as 0.1448 min^{-1}. This outcome may play an excellent role in the environmental remediation applications of the newly synthesized materials.

Green Synthesis of Silver Nanoparticles Using Thunbergia Grandiflora Flower Extract and Its Catalytic Action in Reduction of Congo Red Dye

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Abstract

Developing an eco-friendly approach for metallic nanocatalyst synthesis is important in nanoremediation research. The current study reports, a rapid, environmentally-friendly, and low cost production of silver nanoparticles from silver nitrate using the aqueous extract of *Thunbergia grandiflora* flowers and their use for the catalytic degradation of a hazardous Congo red dye. The UV-Visible spectral analysis confirmed the formation of silver nanoparticles by its characteristic surface plasmon resonance peak observed at 430 nm. SEM analysis resulted in the formation of spherical shaped nanoparticles. The EDX spectrum displayed the presence of elemental silver at 3.1 keV. The XRD analysis showed a sharp peak at 38.31° indicating the presence of (1 1 1) lattice plane. The FTIR analysis showed prominent peaks in the flower extract corresponding to the specific functional groups which involved synthesis and stabilization of nanoparticles. The DLS analysis revealed that the synthesized nanoparticles are less than 100 nm size. A negative zeta potential of – 24.5 mV implied the negative surface charges of the nanoparticles. The synthesized silver nanoparticles displayed excellent catalytic effectiveness in the reduction of carcinogenic azo dye (Congo red) which is a highly toxic environmental organic pollutant. The nanoparticles show excellent catalytic activities and follow pseudo-first-order kinetics. This finding may pave the way for the development of new nanocatalysts for remediation of organics.

Growth, Optical, Structural, FTIR and Dielectric studies on Pure and succinic acid doped ɤ-glycine single Crystals

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Abstract

Single crystals of pure and succinic acid doped ɤ-glycine were grown by slow evaporation technique. Many interesting results on several properties of pure and succinic acid doped ɤ-glycine single crystals have been reported. Succinic acid doped ɤ-glycine shows various morphology. The effect of doping on the growth, optical, dielectric and hardness properties has also been investigated. The presence of functional groups has been estimated by FTIR analysis. The lattice parameters of the grown crystals were studied by single crystal X-ray diffraction technique. Powder X-ray diffraction studies confirm the diffraction planes of the grown crystals. The UV-visible spectrum shows the cut-off wavelength at 220 nm. A study on the thermal properties has also been carried out. The photoconductivity study was carried out to know the conducting nature of the crystal. The NLO(Non-Linear Optical) property of the grown crystals was confirmed by SHG(Second Harmonic Generation) studies. The laser damage threshold was measured using Q-switched Nd:YAG laser (1064 nm). It was found that dopant concentration decreases the NLO property and proves to be a good material for photonic device fabrication.

Keywords: ɤ-glycine, succinic acid, Dielectric study, NLO Property

The Effect of Dissolved Gas on Synthesis of NiO/C Composite and Its Influence for Removal of Toxic Metal Ion from Wastewater

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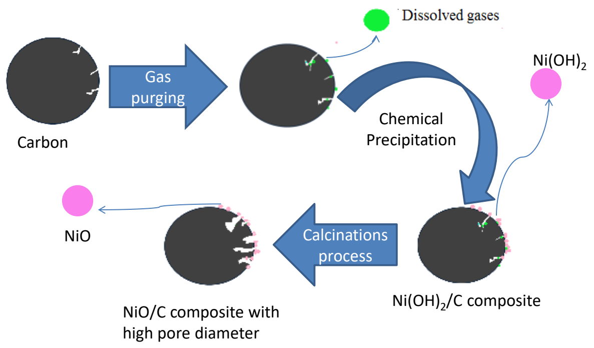
Abstract

The porous nickel oxide/carbon composite was successfully synthesized via a precipitation method in presence of dissolved gases medium. The porous NiO/Carbon composite was widely used in the supercapacitor, removal of toxic metal ion wastewater. In this study, carbon was prepared from Prosopisjuliflora wood by biochar process. Then NiO/Carbon was synthesized via two different precipitation method using Nickel nitrate, NaOH and dissolved air. This study explained the effect of dissolved gases on structural changes of metal oxide/carbon composite. The adsorption of dissolved air on carbon surface influenced the pore size variation on metal oxide composite. The mechanism of adsorption of dissolved gas on carbon surface in solvent explained. The apparent characters and physical chemistry performances of NiO/C composite were investigated by X-ray diffraction (XRD), BET adsorption, scanning electron microscopy (SEM) and Energy Dispersive X-Ray Analysis (EDX) mapping. The efficiency sorption parameters of both solid nano NiO/C composite, such as; pH study, contact time, the dosage of composite and competitive adsorption behaviours were studied. The surface area, pore volume, mean diameter were increased ~2 times presence of dissolved gases. The removal efficiency was also increased from 88% to 94% then Thermodynamic parameter values (ΔS1, ΔH1, ΔG1) indicated the dependency of temperature by the adsorption reaction process between adsorbent and adsorbate and their spontaneous and exothermic nature was also justified.

Graphical abstract:



Keywords: Biochar, NiO, NiO/C composite, dissolved gases, lead removal

Co-Synthesis of SnO_2-Core/ZnO-Shell and Zn_2SnO_4 Nanowires by Carbo-Thermal Reduction and Their Gas Sensing Properties

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Abstract

One-dimensional nanostructures made up of multiple metal oxides witnessed huge progress over the past years due to their applications in energy conversion and storage and environmental sensing. We report here a facile single step synthesis of SnO_2-core/ZnO-shell and Zn_2SnO_4 nanowires via a carbo-thermal reduction process and their gas sensing properties. Ball milled powders of ZnO and SnO_2 was used as precursors with activated carbon as the reducing agent. Growth was performed in a quartz tube placed inside a tube furnace at 900 °C. At the end of growth, we observed both SnO_2-core/ZnO-shell nanowires in the powder container and Zn_2SnO_4 nanowires on gold thin film coated alumina substrate. The growth mechanism for the SnO_2-core/ZnO-shell nanowires was found as vapor-solid (VS) and for Zn_2SnO_4 nanowires was vapor-liquid-solid (VLS). The fabricated nanostructures were examined using field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) to determine the structural properties. Gas sensors were also fabricated using the nanostructures and their sensing properties were studied against ethanol, methane, hydrogen and carbon monoxide. Sensors fabricated by SnO_2-core/ZnO-shell nanowires exhibited higher sensitivity for all the gases tested. In addition to that, SnO_2-core/ZnO-shell nanowires sensor exposed good selectivity to ethanol compared with Zn_2SnO_4 nanowire sensor.

Utilization of Ionic Liquids in Battery Technology and Medicine Science

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Abstract

Ionic liquids (ILs) have many excellent properties and have been utilized in many fields, including renewable energy, energy storage, CO2 capture, oil & gas process, medicine science, catalysis science, biotechnology, and nanoscience. Our laboratory focuses on utilization of ILs in battery technology and medicine science. In the conference, I will present the new important experimental results that we have obtained in our laboratory relevant to ILs for novel battery fabrication and new medicine science development.

First of all, we utilize ILs as electrolytes for novel battery fabrication. ILs electrolyte is a safe, low cost, high thermal stability, and high electrochemical performance electrolyte. The chemical structure of ILs electrolytes is investigated using Raman analysis. In addition, physical and thermal properties of ILs electrolytes, including density, viscosity, melting point and decomposition temperature, are investigated using density meter, viscosity meter, differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Moreover, the electrochemical properties, including the electrochemical windows, and ionic conductivity of ILs electrolytes are investigated using electrochemical instrument VMP and conductivity meter. It is found that some ILs obtained in our laboratory have excellent physical and electrochemical properties to utilize as electrolytes for novel battery fabrication. Nanomaterials, including carbon nanotube and nanoparticles are also characterized for battery electrode preparation. Finally, full cells are obtained in our laboratory. The electrochemical properties of full cells are investigated, including cyclic voltammetry curves, and specific charge-discharge capacity.

Due to excellent solubility, ILs can be designed to utilize in medicine science. In our laboratory, ILs based new anti-cancer drugs are synthesized for anti-cancer test. New disease diagnosis methodologies will also be developed using ILs.

Analysis of the Ability of Phase Change Material Coated Fabric to Maintain the Required Temperature Range

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Abstract

Phase change materials (PCM) help to regulate the microclimate temperature and body temperature by releasing or absorbing latent heat. This paper focuses on the use of PCM on traditional textiles as well as technical textiles and is the platform to analyse the behaviour and working principle of the phase change material on textiles even though it has been used in other industries. This research has been carried out to analyse ways of maintaining the microclimate temperature for a longer period of time by considering many parameters which influence the maximum performance of PCM. For the purpose of this research, the relative merits and demerits of organic and inorganic PCMs were considered, and organic PCMs were selected. Microcapsules were produced using a chemical method and encapsulated into the fabric using an in situ polymerisation method. Tests were carried out to ascertain the temperature range of phase change and the time to maintain the temperature. The research showed that the molecular weight of the PCM should be reduced to get the temperature close to the body temperature to keep the microclimate temperature at a constant level. The effects on thermal and aesthetic comfort of clothing were also explored as a part of the research.

Keywords: Phase change materials, Encapsulation, Pad-dry-cure method, Polyethylene glycol-1000

Experimental Investigation of Minimum Quantity Lubrication (MQL) of Coconut Oil Based Metal Working Fluid

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Abstract

Metal Working Fluid (MWF) is a liquid, which uses during machining for the purpose of heat removal, lubrication at tool chip interface, corrosion protection and wash away chips from the cutting zone. Due to unique properties like biodegradability, renewability and its adequate performance in wide range applications, vegetable oil based MWFs provide significant environmental benefits than the mineral oil based MWFs. Minimum Quantity Lubrication (MQL) is a technique of applying fine mist of MWF, instead a flood of it. This paper describes performance evaluation of novel coconut oil based MWF, during turning experiments executed with AISI 304 Austenitic Stainless Steel and Mild Steel as workpiece materials. The experimental set up was designed after evaluating several conceptual designs established through morphological analysis and finally the best design for the MQL system was fabricated. To corroborate the importance of novel vegetable oil based MWF, the machining performances in terms of surface roughness, tool tip temperature were evaluated and novel coconut oil based MWF could obtain better performances. Further flank wear and nose wear were investigated by observing SEM images. Turning of AISI 304, with presence of new MWF, has shown an improvement in tool flank wear compared with a standard mineral oil based MWF. Optimum decrease in tool tip temperature of 7.833 ^{o}C and best environmental conditions (negligible amount of mist) were identified, while machining of AISI 304, at 45 rpm of spindle speed, 5.231 m/min of linear cutting speed, 0.05 mm/rev of feed rate, 1mm of depth of cut, 2 bar pressure of compressed air and 0.186 ml/s flow rate of novel coconut oil based MWF.

Keywords: Minimum Quantity Lubrication, surface roughness, flank wear

Effect of Preparation of Pt-Sn Catalyst on Mixed-paraffin Dehydrogenation

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Abstract

Polypropylene and polybutadiene are high demand materials produced from propylene, 1, 3-butadiene. Currently, propylene and butadiene are produced either by dehydrogenation or by steam cracking of individual paraffins (propane and butane). But, paraffins are available as mixture from fluidized catalytic cracking and require separation before dehydrogenation. The products of dehydrogenation need to be separated again, due to their wide range. Feed separation, dehydrogenation and product separation result in high capital and operational cost. Hence, mixed-paraffin dehydrogenation is proposed. Platinum was reported to be a promising catalyst for paraffin (individual) dehydrogenation and suffers from coking. Promoters like tin were added to suppress coking. Further, the type of Pt-Sn alloy has a significant role on the extent of dehydrogenation, which is attributed to catalyst synthesis methodology, especially during reduction process. There are no studies in the literature on mixed-paraffin dehydrogenation. In this study, mixed-paraffin dehydrogenation was carried out using a Pt-Sn supported on Al_2O_3 catalyst. The catalyst was synthesized using impregnation method from platinum and tin precursors and was reduced by two different methods a) Liquid phase $NaBH_4$ and b) Hydrogen. The catalyst samples were characterized using SEM-EDX, XRD and XPS to confirm the formation of Pt-Sn alloy. The dehydrogenation was carried out in a packed bed reactor at 700 ^{o}C and 10 psi. The products were analysed using GC-FID detector. A conversion of 85 % and 38 % for propane and n-butane respectively with 225 % olefin selectivity was observed for catalyst reduced with $NaBH_4$. In comparison, the conversion for propane and butane for hydrogen reduced catalyst was observed to be 37 % and 62 % respectively with 407 % olefin selectivity. It was also observed that, the product profiles during mixed-paraffin dehydrogenation were different from individual paraffin dehydrogenation.

Design and Development of a Scuffing Load Capacity Tester for Comparision of a Novel Plant Based Lubricant with Standard Lubricants

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Abstract

Gear life is reduced due to the poor scuffing load capacity of gear oil and it caused to reduce the efficiency of power transmission. This paper describes a method to test the scuffing load capacity with Aluminium gears. In order to test the scuffing load, back to back test rig tester was designed and fabricated. Aluminium was chosen as the test gear material since it has a lighter weight and natural anti-corrosive material. The main parts of the scuffing load tester include, oil sump, shafts, motor, load application unit, test gears, temperature measurement unit, etc. The testing lubricant is poured into the oil sump and the load is applied to the testing gear and allowed to run 20 minutes. The steps continue with load increments until the scuffing appearance observed visually.

The developed tester was used to test the scuffing load capacity of a newly developed palm oil based lubricant which has a viscosity of 69.3 Cst at 40 ^{0}C. For comparison SAE30 engine oil also tested with the same developed machine. Apart from this weight loss of the testing gear and temperature variation of lubricants also measured. According to the test results, scuffing observed in Aluminium gear at 5th and 7th load stage for developed palm oil and SAE30 engine oil respectively. Where 5th and 7th stages represent the applied torques 17.5 Nm and 24.5 Nm respectively. Compared to the SAE30 engine oil, developed palm oil has lower scuffing load capacity. This variation of scuffing load capacity was caused high depreciation of the gear tooth and increased lubricant temperature in developed palm oil compared to SAE30 oil. However, as future works the scuffing load capacity of industrial oils (such as H68) are to be measured and compared. The developed tester is most suitable for comparing the different lubricant behaviours.

Keywords: Scuffing, Scuffing Load, Aluminium, Gear Lubricant

Degradation of dyes by TiO_2-loaded Graphene oxide (TiO_2-GO) materials under visible light illumination

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Abstract

Water pollution poses a threat to the sustainability of the Earth's ecosystem. In particular, the textile industry has been shown to discharge effluents containing compounds that are toxic to plant and animal life in aqueous environments. The dye materials in the effluent are broken down into various toxic substances, such as amines and cyanides under anaerobic condition. Therefore, removal of these toxic compounds is vital. In this regard, several studies are focusing on developing catalysts that can effectively remove these pollutants from the contaminated water. This study mainly focusses on degradation of a model dye, methyl orange (MO) by TiO_2 loaded Graphene oxide (GO) materials. $TiO_2$was loaded on the GO material using two different methods, such as mechanical-mixing and impregnation methods. 1, 2, 5, 10, and 20 % loadings of TiO_2 was made on the GO material, and the resultant materials were characterized by powder XRD method, which indicated the formation of amorphous TiO_2 over GO material. The synthesized materials were used to degrade a model dye, MO in the presence of visible light. Interestingly, 2 % TiO_2 loaded on GO using both mechanical-mixing and impregnation was found to be highly efficient in degrading methyl orange. In addition, a decrease in the rate of degradation was observed with increasing TiO_2 loading, whereas only adsorption of dye was attained with bare GO. The high degradation efficiency with the 2 % TiO_2 loaded GO material may be attributed to the good dispersion of the active TiO_2 nanoparticles on to GO.

Keywords: Titanium dioxide, Graphene oxide, Dye, Degradation, Visible light

Quantitative Studies of Cadmium Ion (Cd^{2+}) Adsorption on Oxidized Graphite Powder

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Abstract

The adsorption behaviour of cadmium ions (Cd(II)) on surfaces of oxidized graphite was investigated as a function of concentration of Cd(II) ions, contact time, and the amount of oxidized carbon used. Square wave anodic stripping voltammetry (SWASV) was used to measure the uptake of Cd(II) ions by oxidized graphite powder. Standard addition method was used to determine the amount of cadmium ion concentration. The adsorption of the metal ion specie on oxidized graphite was characterized by X-Ray Photo electron spectroscopy. Increase in atomic percentage of oxygen and decrease in atomic percentage of carbon after oxidation of graphite powder shows the successful oxidation of graphite with acid mixture of concentrated nitric and sulphuric acid. Adsorption capacity of bare graphite was found to be 37.37 %, where as that of oxidised graphite was 67.6 % when 10.0 ml of 100 µM cadmium ion solution was used with 100 mg of both sample. Also it was found that 300 mg of oxidized graphite powder adsorbed 92 % Cd^{2+} ions from 10 ml of 100 µM cadmium ion solution in 6 hours contact time. These results reveal that oxidized graphite has good adsorption capacity for adsorption of the cadmium ions.

Silver Nanowire Incorporated Wearable Thermogenic Smart Textiles Designed for Continuous Body Temperature Measurements

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Abstract

Conventional fabrics that have modified in to conductive fabrics by using conductive nanomaterials have novel applications in different fields. This kind of fabrics can be used as heat generators with the help of Joule heating mechanism, which is applicable in thermal therapies and to maintain the warmth in cold weather conditions in a wearable manner. The modified fabric can also be used as a wearable sensor for body temperature measurements using the variation of resistance with respect to the body temperature deviations. In this study polyol synthesized silver nanowires (Ag NWs) are incorporated to bare cotton fabrics by using simple drop casting method. The variation of sheet resistance of the fabrics with respect to the incorporated mass of Ag NWs was measured by using four probe technique while the bulk resistance variation with respect to the temperature was measured using ohm meter. Heat generation profiles of the fabrics were investigated by using FLIR T640 thermo graphic camera. Incorporation of 30 mg of Ag NWs in an area of 25 cm^2 of the cotton fabric gave electrically conductive fabrics which can be heated up to a maximum steady state temperature (at which heat generating rate is equal to the heat dissipation rate) of 45 ^oC, using a 9 V battery, with a resistance variation of 0.2 $\Omega\ ^oC^{-1}$. A simple microcontroller circuit was used to actuate the cotton as a heat generating wearable temperature sensor.

Acknowledgment: National Centre for Non-Destructive Testing (NCNDT) of Sri Lanka is gratefully acknowledged for providing laboratory facilities for IR imaging.

Optimization of Nano Zeolite-A Production Process by Contrasting Experimental Condition in Microwave - Assisted Synthesis Method as an Economically Viable Preference

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Abstract

Synthetic zeolites are used commercially more often than natural zeolites due to the purity of crystalline products and the uniformity of particle sizes. With the properties of synthetic zeolite, that can employ wide a variety of applications in comparatively natural occurrence. The synthesis of nano zeolites has received much attention in the past decade because those can have different of properties than their microscale counterparts. As usual, the reduction of particle size from the micro level to the nanometre scale can change several chemical and physical properties. However, due to the high cost of production and non-recyclable organic templates, this study aims to optimize the production process of nano zeolite-A, synthetic zeolite with the anionic surfactant of sodium dodecyl sulfate as a site directing agent under contrasting laboratory conditions. For that, microwave-assisted synthesis was performed under different conditions such as different time intervals, aging conditions as well as different temperatures. In order to achieve nano zeolite-A and after the purification, samples were subjected to characterization for structural determination. The Furrier transform infrared spectroscopy (FTIR), Scanned electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDX) and X-ray diffraction spectroscopy (XRD) were employed as a sample characterization. Results reveal that the process cycle one and two (Aging: 2 – 3 days at 40-50 °C, crystallization: 3 hours at 100 - 110 °C) was towards zeolite-A and third towards the formation of sodalite. While the cycle two conditions (Aging: 3 days at 40 °C and crystallization: 3 hours at 110 °C) was the most effective for nano zeolite-A production and XRD, SEM results of cycle two was emphasized the optimize production of nano Zeolite-A with 300-310nm size crystals. Furthermore, above results revealed that surfactant-based zeolite synthesis would be potentially important and viable option for nano zeolite-A synthesis.

Properties of Natural Intermediate Band in Cu_2CdGeS_4 for Intermediate Band Solar Cells: A First-Principle Insight

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Abstract

The development of intermediate band solar cells is an intermediate band in the band gap of the semiconductor, but it is generally produced artificially, which executes practical challenges on the synthesis side. Here, we found the natural intermediate band in the main band gap of Cu_2CdGeS_4 by first-principle calculations. Cu_2CdGeS_4 is I_2-II-IV-VI_4 group quaternary chalcogenide semiconductor, which had been proposed as promising light-absorber layer efficiency of Cu-based chalcogenide. For the first time, we found the isolated conduction band of Cu_2CdGeS_4 in the zincblende or wurtzite structure, which can be regarded as a natural intermediate band (partially filled) by employing a hybrid functional model. This evidence for the first time that absorption coefficient of both valance band to intermediate band and intermediate band to conduction band transition involving intermediate band are of significant by employing BSE method and corresponding to electronic transitions. The results imply that Cu_2CdGeS_4 being two-photon absorption in the visible light range. Additionally, the hole and electron effective masses of Cu_2CdGeS_4 are systematically studied using first-principle calculations. We show that Cu_2CdGeS_4 could make possible intermediate band solar cells of improved efficiency.

Development of Nanofibrillated Cellulose (NFC) Reinforced Polypropylene Based Composite for Engineering Applications

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Abstract

Thermoplastics have very high demand over the world due to the low cost and reusability with better performances. Polypropylene has been used in thousands of applications including packaging, automotive, medical, and textile. The wide range of applications of Polypripylene is based on the advanced characteristics such as reusability, low toxicity, inexpensiveness, excellent chemical and water resistance, better process ability and high shelf life. Cellulose is a homo-polysaccharide and the most abundant biopolymer present on the earth. Nanofibrillated cellulose (NFC) consists of a bundle of long chains, flexible cellulose molecules with high aspect ratio. This can be used as a reinforcement nano material for various applications.

The objective of this research is to develop a NFC reinforced Polypropylene based composite for engineering applications. NFC have indicated a remarkable reinforcement effect on polymer composites due to the high specific area. However, the hydrophilic NFC is not compatible with hydrophobic polypropylene. Silane-based surface modification technique was used improve the compatibility of NFC and polypropylene. Polypropylene based composite was prepared by varing surface modified NFC up to 5% weight. Compression moulding technique was used to prepare the NFC and polypropylene based composite. The developed product was characterized by SEM, FTIR, XRD, TGA and DTA and mechanical property investigation techniques. 3.5% siylated surface modified NFC reinforced with polypropylene composite was given the optimum properties. Experimental results indicated that tensile strength, impact strength and hardness of the composites were higher than that of pure polypropylene samples. These results clearly showed the reinforcement effect of NFC with polypropylene materials. These composite materials can be used for various types of engineering applications due to significantly enhanced physical and mechanical properties.

Nano Silver Impregnated Polymer Coating for Food Packaging: Preparation, Applications, and Characterization

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Abstract

The ever growing demand for fresh food requires a packing that can extend the shelf life of food and capable of protecting it from contaminations that could leads to foodborne diseases. Silver nanoparticles exhibits very strong antimicrobial properties in variety of environmental conditions. Nowadays, there is a lot of attention in designing effective antibacterial material for food packing. Silver nanoparticles (AgNPs) based antimicrobial packaging is an innovative form of food packaging that extends the shelf-life of food and reduce the risk of pathogens. AgNPs are one of the most powerful inorganic antimicrobial agents known. The present research work describes the preparation of silver nanoparticles, their incorporation into cross-linked polyvinyl alcohol coating and the antibacterial activity of the coating. For every coating technology the adhesion is known to be critical. In general, factors that affect coating adhesion are mainly determined by the interfacial phenomena between the coating and the substrate. In this study, polymer substrates were activated by a controlled UV treatment. Contact angle measurements were used to measure the degree of activation. The work of adhesion was used as a measure of adhesion and was measured by employing peel off test. Optimum UV dose was determined by considering the degree of activation and work of adhesion. Thermogravimetric analysis was employed to study the thermal degradation of cross-linked nanosilver coating. Nanoparticles were characterized by Surface Plasmon Resonance (SPR) spectrums and Scanning Electron Micrographs (SEMs). The zone inhibition method was employed together with bacteria Escherichia coli to assess biocidal action. The developed product showed significant antimicrobial properties.

Structural and Optical Properties of Microwave Synthesized Silver Doped ZnS Encapsulated by NaCMC

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Abstract

The main aim of this work is to synthesize non-toxic, biocompatible inorganic luminescent nanoparticles (NPs) of zinc sulphide (ZnS) doped with Ag+ ions using chemical precipitation method. This communication reports synthesis of silver doped ZnS encapsulated by sodium carboxy methyl cellulose (NaCMC) and its characterization. The effect of efficient heating by microwaves were utilized to achieve faster reaction rates. The effect of dopant (silver) concentration on the photoluminescence behavior of the composite as a new approach for the preparation method was studied. Synthesis involves chemical co-precipitation method using zinc acetate and thioacetamide as ZnS precursors, silver nitrate as dopant salt, carboxy methyl cellulose as capping agent and water as solvent. The synthesized samples were characterized for their structural and optical properties. Substitutional doping of silver in to the ZnS lattice was indicated by the XRD studies. The nanocrystallite size increased with Ag concentration. The presence of silver dopants was indicated by EDS analysis. The band gap energies obtained from UV – Vis spectroscopy for all samples were higher than that of bulk value (3.68 eV) indicating quantum confinement effect. Photoluminescence measurements indicated maximum intensity at certain optimum concentration of added silver dopant. The difficulty in substitutional doping of Ag in to ZnS faced in earlier works has been overcome in our work due to microwave heating and this also influences the growth mechanism. As Ag is known for its antimicrobial properties, the Ag doped NaCMC capped ZnS samples are suitable for possible application as nanoscale fluorescent probes for potential biological and medical applications.

Method of Depositing Lithium Metal and Its Current Collector for Solid State Batteries

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Abstract

Lithium metal was deposited using specially designed compact thermal evaporation source and the deposition source can produce uniform lithium thin film on a four-inch wafer. Lithium deposition in solid-state electrolyte battery was performed with optimum metal weight using trial and error method. More than 3-micron thickness Lithium thin film was de-laminated after the Cu current collector deposition on to the lithium metal and the de-lamination could be stress induced de-lamination and poor interfacial adhesion with LiPON(Lithium phosphorus oxynitride) solid-state electrolyte. To avoid de-lamination of lithium from the LiPON solid-state electrolyte surface, we have optimized the lithium to copper thickness with different quantities of Cu and Li. We found that 1gm of Cu and 0.3gm of lithium was optimized as a suitable window for the right performance of the solid-state battery. Lithium stability with LiPON solid-state electrolyte was carried using cyclic voltammetry. The cyclability of lithium with the cathode and other anode materials were performed and it has shown stable performance for longer cycles. Time-dependent Lithium stability with LiPON interface and Copper as capping layer was evaluated and lithium metallic color was stable for 25 days or more for LCE 2 condition.

High Aspect Ratio Silicon Nanostructures Formed By Mace for Chemical and Biological Sensors

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Abstract

The use of high-aspect ratio silicon nanostructures as a sensor for detection of various analytes was investigated in the present study. Si nanostructure is a promising candidate due to ease of fabrication, large surface area, various accessible sizes and morphologies, controllable surface modification and its compatibility with conventional silicon processing technology. The optical or electrical properties of Si nanostructures are key sensing parameters that have been used in many chemical and biological sensing applications. Upgraded metallurgical grade wafers were used for the fabrication of nanostructures by metal assisted chemical etching (MACE). A detailed analysis of the optical properties is done by UV-Vis Diffused reflectance spectroscopy, Raman spectroscopy and photoluminance spectroscopy. Morphological properties, investigated by SEM, provides an insight into the physics of their formation. The adsorption of chemical or biological molecules into the pores modifies the electrical and optical properties, allowing convenient and sensitive measurement approach. The high aspect ratio of such nanoporous structures in chemical and bio sensing applications is addressed in the context of surface chemistry effects and nanostructures, measuring approaches and sensitivity and stability.

Keywords: Chemical sensors, Biosensors, Porous silicon, Optical, Electrical

Low Cost Quasi Solid State Electrochromic Devices Based On F-Doped Tin Oxide and TiO_2

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Abstract

In recent past, electrochromic devices (ECDs) have attracted much attention due to their potential applications as display devices with low power consumption and low cost. Expensive materials such as Tungsten oxide (WO_3) and CeO_2 have been extensively studied in ECDs as working and counter electrodes, respectively. In the present study, we investigated the possibility of replacing expensive WO_3 and CeO_2 with low cost, transparent, and nano-crystalline, titanium dioxide (TiO_2) as the electrochromic material and F-doped tin oxide (FTO) glass substrate as the counter electrode. A novel low cost electrochromic (EC) window device was fabricated by sandwiching a polymer electrolyte between mesoporous, nanocrystalline thin film of TiO_2 and FTO glass substrate. A quasi solid polymeric electrolyte composed of lithium chloride (LiCl), Ethylene Carbonate (EC), Propylene carbonate (PC) and Polyethylene Oxide (PEO) was employed as the electrolyte. ECDs with the configuration of FTO glass/TiO_2/EC:PC: LiCl:PEO electrolyte / FTO glass were fabricated and their electrochromic properties were examined. A considerable reversible colour change between dark blue and colourless states was observed, when 2.5 V was applied repeatedly to the device. The device changes its transmission between 63% (bleached state) and 0.98% (coloured state) at the wavelength of 600 nm at 3.7 V.

Design and Manufacturing of Electrocoagulation Based Domestic Water Purification System

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Abstract

Water is one of the basic needs for every living being. However, the amount of drinkable water available on the earth surface is considerably low due to human activities and other natural disasters like flooding. With increasing population, demands for the drinking water also increases and need to apply various techniques to purify water in rivers and reservoirs to fulfil the drinking water demand. Therefore, it is essential to find the ways to remove heavy metals, microorganisms, sediments, organic compounds and fluoride in water obtain from rivers and reservoirs. Various techniques have been used to purify water taken from rivers and reservoirs before use as domestic purposes. In this work, domestic scale water purification system was designed and studied on the effect of different parameters in purification process. Heavy metal like arsenic was removed by electrocoagulation technique with aluminium electrodes. This process was carried out by changing the reaction time and the settling time with supply voltage of 12 V (DC). Current density was kept as 0.55 mA/cm^2. The highest arsenic removal was obtained at the reaction time of 5 minutes and settling time of 24 hours. Suspended particles were filtered by a cloth mesh of 149 micron. Fluoride was removed by using a bed type filtration device with different absorbents materials. In this defluoridation process, kaolinite which was used as absorbent material, showed 77.47 % of fluoride absorption. According to the results, the parameters tested herein for the water sample was found to be in good proximity with the World Health Organization requirements for drinking water.

Extraction and Characterization of Nanocellulose from Agricultural Waste

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Abstract

Polymers are class of substances composed of very large molecules. Most of the polymers are usually made from petroleum-based by-products. However, petroleum-based polymer production has created economic and environmental sustainability issues. To satisfy the increasing demand for polymers, innovative technologies are required to produce polymers from sustainable materials. Rice is the main agricultural crop in Sri Lanka today. It is cultivated in most parts of the country and rice straw is the main agricultural waste product. Rice straw is a harvesting residue that is traditionally burned and contributes heavily to air pollution today. Rice straw is a lignocellulosic biomass comprising of lignin, cellulose and hemicellulose materials. Nanocellulose is a naval nanomaterial derived from cellulose that acts a major role in the nanotechnology related researches and applications.

The objective of this research was to extract the nanocellulose from Sri Lankan rice straw. First, chemically purified cellulose was extracted from rice straw using de-waxing, delignification, hemicellulose and silica removal processes. Nanocellulose synthesis was performed from extracted cellulose by subjecting acid hydrolysis, quenching, centrifugation, dialysis, sonication and freeze drying process. Extracted product was characterized by Fourier Transform Infrared Spectroscopic techniques (FTIR), Scanning Electron Microscopic techniques (SEM), Differential Thermal Analysis (DTA) and Thermo Gravimetric Analysis (TGA) techniques. SEM images indicated that extracted cellulose fibres and nanocellulose having diameter less than 10 µm and 50 nm respectively. Experimental results verified that extracted cellulose and nanocellulose had very high chemical purity. TGA results indicated that extracted nanocellulose thermally stabilized up to 300 ^{0}C. This extracted product can be used as a naval and sustainable raw material for various applications.

Enhancing the Synthesizing Efficiency of Graphene from the Expanded Version of Vein Graphite

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Abstract

Sri Lankan vein graphite comprises extraordinary purity, exceeding 99+% and occurs substantially as veins in colossal, underground sedimentary rocks. This carbon rich resource comes up with a unique potentiality to produce high quality graphene nevertheless, a number of obstacles are recognized to hamper the large scale production. Underground mining process at the boundary of the vein consistently brings about graphite lumps, consist of stone pieces hence, a substantial aggregate of graphite has been disposed off while hammering. In this study, it was intended to explore promising approaches to recover these graphite lumps and subsequently, to synthesize graphene from recovered graphite more efficiently. Lumps of graphite consist pieces of stones were treated with a dispersion of conc.H_2SO_4 and conc.HNO_3 in the way that 1:8 volume ratio in room temperature thus, the leaching of dispersion in to graphite layers facilitates the stripping off and obtains delaminated graphite together with stone pieces. Subsequently, the delaminated graphite was filtered and after several washing steps the sample is heated at 600^0C to acquire expanded graphite; the precursor for scalable synthesis of graphene. Hummers method with a few modifications enables a feasible production route concurrently, the expanded graphite enables the obvious penetration of the intercalating agent (conc. H_2SO_4) together with amenable oxidation. The spontaneous expansion of graphite influences in the way that, achieving the milestone of the study by acquiring yield of graphene about two times more than manipulating ball milled graphite as the precursor. The results give an insight into large scale, cost effective and industrially viable synthesis of graphene thus, pave the way towards massive production of enormously important graphene applications.

Polarization-Controlled Interface Charges for Generation of Open-Circuit Voltage Higher Than the Band Gap Towards "Polarization Photovoltaics" Solar Cell

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Abstract

Recently, solar cells have gained significant interest due to renewed attention to sustainability. The energy harvesting effectiveness of a solar cell centres are critically influenced by surface and interface properties inherent in the manufacturing of these devices. Conversion efficiencies over 40% have been achieved using conventional III–V semiconductor compounds as photovoltaic materials. The fundamental bandgap of the group III-nitride alloy system covers over a wider spectral region (from 0.64 to 6.2 eV) with tunable bandgap and strong absorption coefficient. However, bottleneck limiting the performance of such device arises from the potential barrier at the heterointerface due to the electron affinity difference. Another important factor is the existence of significant interface charges induced by spontaneous and piezoelectric polarizations due to non-centrosymmetric crystal structure. In turn, results in surface band bending depending on the interaction with surrounding atmosphere. Heterojunction (HJ) between n-ZnO and p-Si has a potential to perform as efficient and inexpensive solar cell. However, the relation between the polarization bound charges and the electronic properties of the HJ interfaces is not yet well understood. Calculated work function, φZnO (or barrier height) for ZnO varied from 5.02 to 0.33 eV as a function of Zn/O molar ratios. Surprisingly, a non-centrosymmetric crystal structure can develop a giant photovoltage. Specifically, the electron processes: photo-excitation, scattering, and relaxation occur with different probabilities. Considering, a hetero-structure with cubic and non-centrosymmetric material, each non-centrosymmetric layer can act as a photovoltaic, so that the overall open-circuit voltage across the multi-junction is large, potentially much larger than the bandgap. Fundamental issues considering wurtzite-GaN/cubic GaN and wurtzite-ZnO/cubic-CdO hetero-structures will be discussed towards next-generation solar cells.

Effect of Surface Morphology of Hydrothermally Synthesized Nickel Ferrite Magnetic Nanoparticles on Photocatalytic Water Remediation

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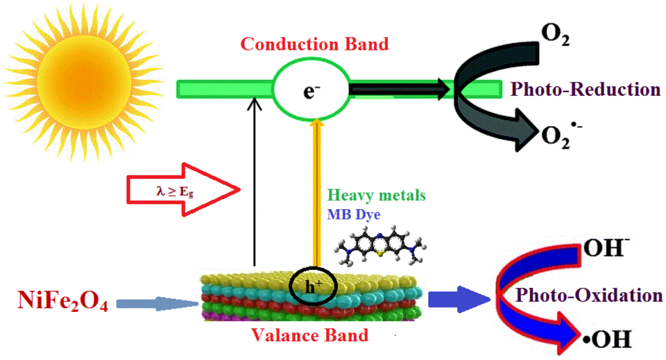
Abstract

Many research studies have been reported in the last decade on the significant utility of nanoferrites in waste water treatment. AB_2O_4 spinel, and spinel-like nanoferrites (with A=Divalent and B=Trivalent transition metal cations) are of great interest for applications in various fields due to their unique physics and chemistry and our ability to control the spectrum of properties by various processing techniques. The great advantage of nanoferrites in waste water treatment is their physical seperability (phase separation) using an external magnetic field which facilitates reuse. In this study, $NiFe_2O_4$ nano-ferrites have been synthesized by a hydrothermal treatment method. The material was characterized by x-ray diffraction, field emission scanning electron microscope and vibrating sample magnetometer studies. Two different morphologies, spherical and octahedral have been found in the synthesized samples with varying surfactant concentrations. These ferrites are photo-catalytically active even in the visible range of the solar spectrum. The effect of different morphologies on the photo-catalysis has been studied. The saturation magnetization and coercivity are also important parameters in addition to the optical band gap of nanoferrites for their usage in waste water remediation. The different structures, protocols and characterization parameters are analysed and compared to extract discernible patterns.

Graphical Abstract:



Keywords: Surface morphology, Nickel ferrite, Water remediation, Band gap, Magnetic Nanoparticles

Symposium on

Bioenergy, Wind Energy, Hydrogen Energy and Storage, and Environmental Applications

Hydrogen Fuel from Water

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Hydrogen gas is considered as the zero-emission fuel because, when hydrogen is combusted with oxygen in air, it produces water vapour as the only product. Hydrogen can be used in electrochemical devices such as H_2/O_2 fuel cells, or in internal combustion engines to power devices or motor vehicles. Hydrogen is the fuel with highest energy density, i.e., energy per unit mass. Hydrogen compressed at 700 bar has chemical energy density of 142 MJ/kg. However, hydrogen as H_2 gas does not exist naturally in our planet though H and He dominates over 98% of elemental abundance of the Universe thus making all other elements only 2%. Hydrogen is naturally available in our planet mainly as water and hydrocarbons. As such, hydrogen gas has to be obtained from these widely available hydrogen resources. In the petroleum industry, cracking of large hydrocarbons produces hydrogen gas though almost all is used onsite and for the production of urea in the Haber process and in the production of methanol. Decomposition of water to H_2 and O_2 is a thermodynamically uphill process which requires energy to carry out. The cheapest and cleanest way to provide this energy is from solar energy. Fujishima and Honda have first demonstrated water photo-splitting using illuminated TiO_2 electrodes in 1972. Solar spectrum incident on the Earth surface contains only 5% of UV radiation that is required for electronic transition in TiO_2 semiconductor and hence 95% of the incident radiation is wasted. This review investigates the up-to-date developments in water photo-splitting starting from this famous experiment of Fujishima and Honda and explores strategies to produce hydrogen from water in efficient manner for practical application of hydrogen gas in fuel cell devices and in motor vehicles.

Abstract of Plenary talk – I

Supercapacitors for Energy Storage

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Present world has a soaring demand for energy due to the full use of various appliances deeply integrated into day today activities. Upon detrimental environmental impact and cost of fossil fuels, a significant attention has been paid on energy generation from renewables. This has automatically highlighted the importance of energy storage devices because of the dependence of renewables on location and time. Supercapacitors have emerged as a class of competitive energy storage devices that bridge the gap between the batteries and conventional capacitors in terms of power and energy. They are being currently employed in a diverse range of applications covering memory backs ups in CD players, cameras etc., hybrid and electric vehicles, aircrafts and smart grids. Supercapacitors are designed utilizing high surface area electrodes separated by a thin electrolyte with the prime objective of receiving higher capacitance than conventional capacitors. They are capable of retaining characteristic high power density and also reaching high energy density. Basic taxonomy of Supercapacitors is three fold namely electrochemcial double layer capacitors, redox capacitors and hybrid capacitors according to the variation of electrode materials. The first and second types are using carbon based electrodes and conducting polymer, transition metal oxide materials based electrodes respectively. Hybrid supercapacitors have blended electrodes used in the first and the second category. Some of the key attributes of supercapacitors are higher power density, shorter charging time and longer life time. According to the current pursue for green energy concepts and low cost, there has been an exceptional progress on supercapacitors in terms of materials and design variations. But, still the energy density is acting as a crucial factor restricting the popularity in global level. With the present state of R&D dedicated on Supercapacitors, it can predict that more refined and well matured supercapacitors will emerge in the near future facilitating all clean, sustainable and efficient scenarios.

Abstract of Keynote speech – II

Bioenergy: Is It Sustainable

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Current wastewater treatment technologies have energy- and cost-related limitations and therefore wastewater recovery is difficult to achieve and sustain. Anaerobic membrane bioreactors and microbial fuel cells (MFCs) have been researched and are now recognized as an innovative technology that offer sustainable solutions for distributed power systems and energy positive wastewater treatment overcoming environmental problems. This presentation discusses the viability of biofuels and the concepts and different designs of anaerobic membrane bioreactors and Microbial fuel cell. Several case studies on anaerobic membrane bioreactors are also discussed with energy production.

Keywords: Microbial fuel cell (MFC), biofuel, anaerobic membrane bioreactor, wastewater treatment

Abstract of Plenary Talk – II

Biomass Energy in Sri Lanka: Retrospective and Prospective Analysis

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Access to energy is a pre-requisite to achieve broader development goals. Biomass is a significant source of primary energy in Sri Lanka. The dominance of biomass in the primary energy mix has declined from 69% in 1989 to 38% in 2016 although the overall consumption is on the increase. While households consumed 85% from the total of biomass in 1989, it has dropped to less than 62% in 2016. Heavy use of wood-burning stoves contributes to indoor air pollution, while WHO estimates the number of deaths attributable to indoor air quality in Sri Lanka in 2004 to be 4,300. Government's attention is to promote biomass for industries for their thermal energy use. Power generation from grid connected biomass is insignificant with 5 projects on ground with 16MW capacity by 2017, and another 9 projects of 39MW in pipeline. Fuelwood depots are established to facilitate supply chain. SLS released national standards for improved cook stoves and sustainably produced fuelwood while product standards for fuelwood is being formulated. Efforts are made on human capacity development, introduce technologies, identification and removal of barriers, resource assessments, and study movement of biomass, while studies have been commissioned on incentive and financing schemes. National energy policy and its revision captures biomass, but inadequately. Initiatives for national renewable energy policy having some attention to biomass did not materialize. *Gliricidia* was declared the fourth National Plantation Crop in Sri Lanka by cabinet of ministers in 2005, and a programmes to plat of 1,000 million trees 'The *Gliricidia* Initiative' in 2016 were launched, but with no more progress. Sustainably produced biomass being a source of renewable energy has a significant potential to meet Sri Lanka's energy demands in the future it being a country situated closer to equator with plenty of sunshine, fertile soil and considerable rainfall.

Facile Solvothermal Synthesis of 3D Biocooh Architectures for High-Performance Photo-Supercapacitor and Water Splitting Applications

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Abstract

In this present work, we synthesized a three dimensional (3D) BiOCOOH micro flowers by a solvothermal approach and applied to photosupercapacitor application for the first time. When it is used as electrode material for photosupercapacitor, the BiOCOOH material shows long cycling stability (5000 cycles) during the continuous charge-discharge process. This improvement in the cycle life of the BiOCOOH material is ascribed to its highly stable three dimensional structures. The as-prepared BiOCOOH exhibits a maximum specific capacitance value of 140 Fg^{-1} and outstanding cycle life with maximum specific capacitance retention of about 78% after 5000 cycles. This rational synthesis provided an effective strategy to enhance the photosupercapacitor performance towards commercial application. With the good electrical conductivity, and outstanding specific surface area, the as-prepared BiOCOOH electrode presents great potential for high performance applications. The 3 wt% Pt modification of the BiOCOOH generates 441 µmol g^{-1} h^{-1} of H_2, upon 5 h illumination.

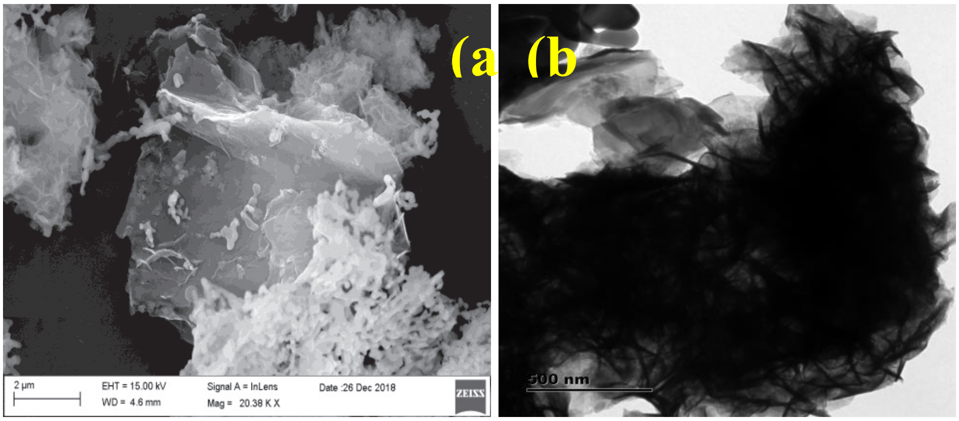

Fig.1 SEM and TEM images of BiOCOOH composites

Synthesis of Visible Light Active $CuFe_2O_4$/g-C_3N_4 Photocatalyst for Water Splitting

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Abstract

A facile g-C_3N_4 supported $CuFe_2O_4$ composite photocatalyst has been prepared by a simplistic one-pot calcination approach using urea and a $CuFe_2O_4$ gel as precursors. The compounds obtained were analysed with Raman Spectroscopy, X-Ray Diffraction (XRD), X-Ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy(SEM) and Energy Dispersive Spectroscopy (EDS) in order to obtain their morphological and structural properties. Optical behaviour was studied by UV–vis Spectroscopy. In this composite, $CuFe_2O_4$ was finely dispersed in g-C_3N_4 matrix, resulting in much improved efficiency of $CuFe_2O_4$/g-C_3N_4 heterojunction in photocatalytic H_2 production by water splitting under visible light. The peak 104 μmol h^{-1} was obtained at optimized loading amount of 3% $CuFe_2O_4$ in the composites, which was about 4 times of that on the pure g-C_3N_4 obtained from urea. This remarkable improvement can be attributed to the enhanced visible light absorbance, improved surface area and charge carrier separation and transfer ability.

A Novel Energy Storage Model to Improve National Electricity Load Profile of Sri Lanka

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Abstract

It is proposed to introduce a low-cost battery storage system which will get charged during off-peak hours & use this stored energy during peak demand time. This will be a low-cost option to level off the daily electricity demand cycle, by flattening the peak and filling the valley. It is revealed that two peaks in the daily load profile which had been caused due to the usage of the domestic sector and the significant high peak is observed in the evening from 6.30 pm to 10.30 pm. The concept of storing energy gathered from the main grid during the off-peak hours and reusing it during the peak hours is introduced. To develop the model three types of the household were selected based on the monthly consumption of 90 units, 150 units, and 180 units. Analysis of the household load profile of an average middle-class house utilizing 180 kWh, 150 kWh and 90 kWh per month shows that during peak hours, it will utilize around 3 kWh, 2 kWh and 1 kWh per day respectively. This can be stored in a low-cost battery by charging it during off-peak hours (say from 11.00 pm to 5.00 am) and can be utilized during peak demand time of 6.30 to 10.30 pm. As a storage device, a novel household battery technology will be introduced with 160 Ah (~2kWh) and 250 Ah (~3kWh) capacities. The model house that has been considered uses 3 kWh per day during the peak demand time, therefore proposed, 3 kWh storage battery to be installed with charging and inverter circuits. This house will not draw electricity from the national grid during peak hours. This energy saving option, even though it will not generate electrical energy by way of installation of a solar panel or any other renewable option, this will be a low-cost option to the household while saving a massive cost to the nation. This will also maximize the capacity utilization of all existing generation plants.

Experimental Investigation of High Alcohol-Low Viscous Renewable Fuel in DI Diesel Engine

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Abstract

An experimental investigation of orange oil methyl ester with ethanol (E) and diethyl ether (DEE) is presented in this work. The biodiesel preparation was carried out with the clear knowledge on performance and emission characteristics of stationary single cylinder agriculture purpose direct injection diesel engine subjected to the hybrid combination of orange oil methyl ester (OME) and oxygenated additives. Prepared orange oil methyl ester was analysed using GC-MS. On engine analysis, it was observed that there was an increment in BTE with a decrement in BSEC with oxygenated fuel blends than neat diesel. Also, increase in CO emission was observed for all oxygenated fuels with a decrease in HC and NOx emissions at all loads except for DEE blended fuels. Reduction in smoke emission observed for all oxygenated fuels. It was found that addition of oxygenated additives to biodiesel improved performance and reduced emission.

Keywords: Orange oil methyl ester, oxygenated additives, performance and emission

Performance of New Aminothiazole Schiff Base Sensor for Cation Detection

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Abstract

The 2-hydroxybenzaldehyde-2-aminothiazole ligand was synthesized from benzaldehyde and 2-aminothiazole by direct condensation method using methanol as solvent. The formation of 2-hydroxybenzaldehyde-2- aminot hiazole compound was confirmed by FTIR, ^{13}C NMR, ^{1}H NMR and mass spectrometry. The band at 1658.78 cm^{-1} confirms the presence of C=N group. The total number of carbon atoms was confirmed by ^{13}C NMR. The chemical shifts (100 MHz, DMSO:d$_6$, ppm) were noticed at (C$_1$-130.14), (C$_2$-122.72), (C$_3$-128.32), (C$_4$-117.70), (C$_5$-154.62), (C$_6$-128.53), (C$_7$-140.48), (C$_8$-139.36), (C$_9$-128.96) and (C$_{10}$-129.07). The total number of hydrogen atoms was confirmed by ^{1}H NMR .The chemical shifts of ^{1}H NMR (400 MHz, DMSO: d$_6$, ppm) were noticed at (1H-6.857), (2H-6.945), (3H-6.964), (4H-6.983), (5H-6.993), (6H-7.013), (7H-7.126), (8H-7.157) and (OH-9.237). The molecular mass of the compound was confirmed by mass spectrometry and found to be m/z=204.23 and the molecular formula of the compound was $C_{10}H_8N_2SO$. The synthesized compound was investigated for chemosensor application. The synthesized ligand was complexed with various metal ions like Na^+, K^+, Ba^{2+}, Ca^{2+}, Mg^{2+}, Ag^+, Cu^{2+}, Co^{2+}, Cd^{2+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Hg^{2+}, Ni^{2+}, Mn^{2+}, Zr^{2+}, Zn^{2+}, Pb^{2+}, Al^{3+} and Ce^{2+} and extent of complexation of the metals with the ligand was analysed using absorption and emission spectroscopy. The 2-hydroxybenzaldehyde-2-aminothiazole was analysed for high selectivity & sensitivity towards a particular metal ion. The compound was further studied for its performance on antibacterial, and antifungal activities.

Development and Characterization of Bio-Mix Fuel produced from the Mixture of Waste Chicken Fat, Used Cooking Oil and Its Impact on CI Engine Application

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Abstract

In India, food industries are growing fast day by day. The wastage coming out from these industries like meat waste and used cooking oil are nearly 4.9 million tons/year. Due to the lag of waste management, these wastes have been dumped in landfills which increase environmental pollution and health problem for human as well as animals. To solve this problem, an attention has been made to develop a renewable catalyst from egg shell which is a poultry waste product for the production of biodiesel. Fourier transform-infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) were used to characterize the synthesized catalyst. For biodiesel production, chicken fat and waste cooking oil were used. The chicken fat was extracted from the waste poultry meat and used cooking oil was taken from the college canteen. These chicken fat and waste cooking oil were mixed together to form a raw bio-mix oil. This raw bio-mix oil was converted to bio-mix methyl ester through the transesterification reaction. The reaction parameters like methanol/oil ratio, catalyst and reaction time were investigated. Two samples of bio-mix biodiesel (BMB-I and BMB-II) were prepared, BMB-I from the developed catalyst and BMB-II from the base catalyst (KOH). Furthermore, fuel properties were investigated and found to be within the standard values. Engine study shows that both bio-mix biodiesel samples (BMB-I, BMB-II) have higher brake specific fuel consumption (BSFC) and lower brake thermal efficiency (BTE) as compared to diesel fuel. Exhaust emissions like NOx, CO, CO_2, HC and smoke were found to be lower for BME-I as compared to BMB-II and diesel fuel respectively. Thus the catalyst developed in this study was found to be cost effective and low toxic for biodiesel production.

Wastewater Treatment and Energy Harvesting Employing Microbial Fuel Cells (MFC)

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Abstract

Wastewater is recognized as making a major contribution to environmental pollution. Current wastewater treatment technologies have energy- and cost-related limitations and therefore wastewater recovery is difficult to achieve and sustain. Microbial fuel cells (MFCs) have been researched and are now recognized as an innovative technology that offers sustainable solutions for distributed power systems and energy positive wastewater treatment overcoming environmental problems. This is particularly the case in isolated areas that are supplied with biosensors, bio hydrogen production, as well as *in-situ* power sources for bioremediation and wastewater treatment. This study explores the use of a single-chamber air-cathode microbial fuel cell (SCMFC) having a 0.5 mg/cm^2 platinum catalyst cathode treating simulated domestic wastewater. Two similar air-cathode SCMFCs were operated for simultaneous electricity production and wastewater treatment. Operation with a hydraulic residence time (HRT) of 24 h and feed COD concentration of 0.5 g COD/L-day produced the highest current density of 294.4 mA/m^2 and 108.31 mW/m^2 power density. Overall, the COD removal at each HRT was high, between 71 – 85%. It is envisaged that there is scope to develop a novel, cost-effective SCMFC design for achieving simultaneous electricity generation and wastewater treatment.

Keywords: Microbial fuel cell (MFC), air cathode, wastewater treatment, power density

Electrochemical Double Layer Capacitor based on Commercial Graphite and Gel Polymer Electrolyte

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Abstract

Today, technology has made our life styles luxurious and as a result, many appliances such as mobile phones, laptops and computers are in full use. They all need un-interrupted power that has created a high demand for energy storage devices. This has given a substantial attention on supercapacitors, which are known to be lying between batteries and conventional capacitors in terms of power and energy. Electrochemical double layer capacitor (EDLC) is one type of supercapacitor that uses carbon based electrodes. In the present study, an EDLC was fabricated with a gel polymer electrolyte (GPE) and commercial graphite electrodes. Its performance was evaluated using cyclic voltammetry techniques and electrochemical impedance spectroscopy. The potential window within which the cycling is done and the scan rate are affecting the single electrode specific capacitance. No redox reactions could be observed in cyclic voltammogrammes (CVs) implying the non-faradaic nature of capacitance. The characteristic rectangular shape of CVs for ideal EDLCs was also present in each case. EDLC has the ability to withstand continuous cycling process. Even though there were some ups and downs of specific capacitance, they were reversible maintaining more or less constant value. This in turn shows the self-healing property of GPEs. The average single electrode specific capacitance was about 1.8 Fg^{-1}. In the Nyquist plot, resistive and capacitive properties were present at high and low frequency regions. The spike corresponding to the capacitive features was tilted due to the problems in electrode surface.

A Natural Rubber based Electrolyte to be used in Electrochemical Double Layer Capacitors with Sri Lankan Graphite

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Abstract

In the modern technology based world, it has become a great challenge to seek solutions for fulfilling the enormous demand for energy efficiently and effectively. Renewable energy sources have been identified as viable candidates for this purpose due to their safety and low cost. Automatically this has highlighted the importance of energy storage devices. Batteries and capacitors have been used as energy storage devices but, the present demand exceeds their supply. Supercapacitors have emerged as a new link to bridge the gap between batteries and capacitors. In the present study, an electrochemical double layer capacitor (EDLC) which is a type of supercapacitor was fabricated and its performance was evaluated. The novelty of the investigation is use of Sri Lankan natural rubber (NR) and natural graphite (NG) as the electrolyte and electrode respectively. Electrolyte was prepared using solvent casting method. Graphite was used with polyvinylidene fluoride as the binder. Cyclic voltammetry and electrochemical impedance spectroscopy were the characterization techniques used in the study. Single electrode specific capacity increased with widening the potential window of cycling. But, some additional reactions were observed with wider potential windows. When increasing the scan rate, single electrode specific capacity showed a decreasing trend. At the scan rate of 2 mV/s, it was about 740 mF/g whereas at the scan rate of 100 mV/s, the value was 85 mF/g. EDLC withstood continuous cycling with low capacity degradation. An initial specific capacity of 300 mF/g reduced to 122 mF/g with continuous cycling for 500 cycles. Charge storage mechanism is taken place electrostatically only. Capacitive properties became dominant at low frequency regions. This EDLC showcases the suitability of using NR and NG for energy applications while adding value to the raw materials.

Synthesis of $MnNiO_3/Mn_3O_4$ Nanocomposites for Water Electrolysis Process

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Abstract

Hydrothermal method was optimized to produce highly efficient, novel $MnNiO_3/Mn_3O_4$ nanocomposites for water electrolysis process. The predominant peak observed at 36.6^o corresponds to the X-ray crystal plane orientation of (1-10) and confirmed Rhombohedral phase $MnNiO_3$ and other well resolved peaks attributed to the $MnNiO_3/Mn_3O_4$ nanocomposites. Vibrational properties and metal oxygen vibration present in Fourier transform infrared profile around ~570-620 cm^{-1}. The oxygen vacancies and electron trapping mechanism were revealed from photoluminescence spectra. The combined morphology of nanorods and distinguished nanopetals was achieved for highly active $MnNiO_3$ nanocatalyst. The band structure and modification was thoroughly studied by UV visible diffuse reflection spectroscopy and the observed band gap was 2.8 eV for $MnNiO_3/Mn_3O_4$ nanocomposites. Cyclic voltammogram and linear sweep voltammogram studies investigated the redox behaviour and water oxidation nature of the novel $MnNiO_3/Mn_3O_4$ nanocomposites. The excellent conductivity and ionic mobility were confirmed by electrochemical impedance spectroscopy. Long-time durability of 24 h stability test was carried out and reported for the optimized electrocatalyst. Hence, the present study completely dealt with the preparation of novel combination of $MnNiO_3/Mn_3O_4$ nanocomposites using controlled synthesis technique and the exploration of optimized candidate for efficient water electrolysis process.

Keywords: Novel $MnNiO_3/Mn_3O_4$, Nanorods-distinguished nanopetals, Water electrolysis process.

Assessment of Impacts on Tropical Marine Environment for Off-Shore Clean Energy Development

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Abstract

Off-shore floating solar photovoltaic and wind power installations are two potential future clean energy technology options, being considered by energy developers. Whereas technical feasibility of these options is well demonstrated in many parts of the world, the associated socioeconomic and environmental impacts remain to be investigated. Indeed, associated impacts must be evaluated on project-by-project basis, as these are site-specific and depend on size of the project. Quantitative methods of environmental impact assessment are important because these generate useful inputs for decision makers. The inputs desirably should be accurate, authentic and reliable. In the present work, we demonstrate method for determining ambient noise characteristics of the under-water sound-scape in tropical marine coastal waters, in quantitative terms. The results presented are based on in-situ measurement of noise spectral density underwater, during the period from the year 2012 to 2016. The ambient noise at an underwater site, 30 m deep in tropical littoral shallow waters, has been measured in winter and summer every year during the said period. The site is located near Grande Island (Latitude 15°18'N, Longitude 73° 41'E) 18 km off-the-western-coast of Goa, India. The site is known to be ecologically sensitive zone, which is close to commercial and military air-port, sea-port, fishing areas and popular tourists' island. The results show that during the period of observation, the average power spectral density of underwater ambient noise at the site varies over a range from 82 dB to 116 dB, at 10 Hz frequency. Corresponding variation of average power spectral density of under-water ambient noise is 56 dB to 88 dB at 100 kHz frequency. This indicates that there are wide variations in ambient noise power at frequency spectrum from 10 Hz to 100 kHz. Also, it is observed that the underwater ambient noise power is higher at low frequency in the range from 10 Hz to 1000 Hz and is lower at frequencies in the range from 10 kHz to 100 kHz. The quantitative results presented here are useful reference for measuring environmental impacts due to future on-shore and off-shore developmental activities.

Electrochemical and Safety Performance of Lithium Rich (Li-Mn-O) based Cathode Materials for Li-Ion Batteries

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Abstract

The lithium ion (Li-ion) batteries are rechargeable batteries and reliable to store electrical energy in electronic devices such as Mobile Phones and Hybrid Electric Vehicles (HEV). Among other cathode materials, Li-Mn-O based materials are most attractive for their safe, durable and high energy density. In this paper, nanostructured Li-Mn-O based cathode materials were synthesized by sol-gel method using acetate materials as precursors with chelating agent in a stoichiometric ratio. From the TGA/DTA measurements of the sample, weight loss intervals were identified to study the decomposition temperature and mass loss. The XRD analysis of the sample indicates that the synthesized material was crystalline in nature and found to be in monoclinic phase. From the FESEM images, layered stack like morphology was observed and the elemental composition of the materials were studied using EDAX. The cathode materials were coated on aluminium foil and the half-cells (2032) were coined. The fabricated cells were studied using Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), and Charge-Discharge curve and its cycle life behaviour was investigated.

Keywords: Li-ion battery, monoclinic phase, layered stack morphology, cyclic voltammetry, Electrochemical Impedance Spectroscopy, cycle life behaviour

Influence of Prevailing Air Quality on Physiological Attributes of certain Plant Species in Industrial Area

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Abstract

In this research a systematic attempt was made to screen and investigate twenty-two species of plants grown around the SIDCO industrial area, Coimbatore for their ability to improve the design of the urban industrial area. The relative water content, total chlorophyll content, ascorbic acid content and leaf extract pH of plants were analysed and the air pollution tolerance index of the plant species were computed. On the basis of high air pollution tolerance index, the plants were screened for their tolerance to air pollution. The identified tolerant species of plants, such as *Annona squamosa* and *Magnolia champaca*, with high air pollution tolerance index value from selected area were recommended for air pollution management during plantation programme to minimize pollution and to create a healthy environment.

Keywords: Plants, air pollution tolerance index, total chlorophyll, ascorbic acid, plantation programme

A Review of the Current DFT Simulations and Experimental Work done on Solar Powered Water Splitting

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Abstract

Over the last years, there has been a steadily increasing focus on clean, renewable energy sources as a way to hinder the irreversible climate change we are facing and to meet the continuously growing energy demand. The direct harvesting of solar light and its conversion into electrical energy in photovoltaic cells or into chemical energy by photoelectrochemical reactions are the most relevant technologies to address this challenge. Conventionally, both technologies rely on the collection of light in semiconductor materials with appropriate bandgaps, matching the solar spectrum and thus providing a high-energy conversion efficiency. In this presentation, we describe the most recent theoretical simulations and experimental work within this field, with the intention of providing a clear overview of the current state of solar driven hydrogen production and of the main issues to be addressed before the technology can become competitive. We will discuss various photocatalysts, including metal oxides, nitrides, sulphides, lanthanides, nanocomposites and doped materials, providing an evaluation of their strengths and shortcomings. The interesting case of TiO_2 is presented in a separate section, in which we address the well-known issues related to its too wide band gap, the quick electron-hole recombination time and the large overpotential for hydrogen evolution reaction. We propose a number of solutions, including a variety of dopants, surface modification, amorphization of the crystal structure, heterojunction catalysts and noble metal deposition. The tremendous increase of computational power over the last couple of decades, in combination with methodological improvements, has made it possible to guide the development of new materials using principles and calculations based on quantum mechanics. Model simulations can work as a great tool for screening a large database of materials, thus identifying new promising materials. Future work should focus on improving the current technology by enhancing visible light absorption, physical and chemical stability, lifetime as well as charge transfer.

Palladium Nanoparticles - Poly(3,4-Ethylenedioxythiophene)-Carbon Nanotube Composite as Oxygen Reduction Catalyst for Direct Methanol Fuel Cells

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Abstract

Palladium, multi walled carbon nanotube (CNT) and poly(3,4-ethylenedioxythiophene) (PEDOT) composite, (Pd/CNT/PEDOT), is prepared as an electrocatalyst towards Oxygen Reduction Reaction (ORR). This composite is characterized using X-Ray diffraction, Fourier Transform Infrared, X-ray Photoelectron spectroscopy, X-Ray Fluorescence and Scanning Electron Microscopy to understand its properties and morphological characteristics. AC impedance analysis and the electrochemical analysis are also carried out to study its catalytic properties. Pd/CNT/PEDOT, which has 10% palladium content out of total mass, shows competitive performance in catalytic activity in both acidic and basic media and is better than that of commercially available Pt/C (20% Pt loading). Durability and methanol tolerance are extremely high for this catalyst. Therefore, this material can be used as the cathode material in Direct Methanol Fuel Cell applications.

Pretreatment of Rice Husk using Hot Water Washing for Ash Removal

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Abstract

Biomass from agricultural waste is renewable source of energy to use in boilers and furnaces. Rice husk which is abundant in Sri Lanka is a potential source of biomass, but ash content containing alkali and alkali earth metals and silicates create operational and corrosion problems. This study investigates the effect of temperature (40, 50, 65, and 75 ^{0}C) and particle size (1.0-1.4, 1.4-2.8, and 2.8-5.6 mm) of rice husk by 2 hours of water washing. Conductivity of leachate was measured at regular intervals to identify the leaching behaviour of ash with time. The removal of ash was compared against unwashed sample. Compositions of K_2O, Fe_2O_3, CaO, MgO, SiO_2, Al_2O_3, TiO_2 and P_2O_5 of ash were determined after combusting the treated and untreated rice husk to understand the leaching behaviour of ash constituents and to calculate the fouling indices. A linear positive relationship was obtained between percentage removal of ash *vs* temperature for all particle sizes. The effect of particle size is more significant compared to temperature; as particle size reduces, more ash is removed even at lower temperatures. Maximum of 25.2 %(w/w) of ash was removed by washing 1.0-1.4 mm particle size at 75 ^{0}C. Up to 90 % of K, 70 % of P and over 40 % of Fe, Al and Ti had been removed; however, the source of water has an effect on some constituents (increase in Ca and Mg). Overall improvement in fouling index can be achieved by increasing temperature and/or reducing particle size.

Keywords: Rice husk, ash removal, hot water washing

Investigatıon of Self Discharge Mechanism of Local Activated Carbon based Supercapacitor

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Abstract

Activated carbon is a popular material used in the fabrication of supercapacitors due to its high specific surface area. Sri Lanka is one of the main produces of activated carbon. Due to availability of high quality activated carbon, this is an area of potential interest to Sri Lanka. Activated carbon based ionic electrolyte supercapacitor was fabricated and its electrical properties were investigated to identify the drawbacks in these supercapacitors. Supercapacitors fabricated with local activated carbon and aqueous sodium sulphate (Na_2SO_4) electrolytes were used in this study. Self-discharge is inevitable in this type of supercapacitors. It was believed that the discharge is mainly due to electrical conduction through ionic electrolyte. However, this study proposes that in addition to the above mechanism, there is another dominant mechanism which governs the early stage self-discharge.

Catalytic and Magnetic Properties of Yellow and Red Iron Oxide for Water Splitting

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Abstract

The commercial red iron oxide (Fe_2O_3) and hydrated yellow iron oxide ($Fe_2O_3.xH_2O$) powders were characterised for catalytic and magnetic properties for water electrolysis. The structural and morphological properties were determined by X-ray diffraction, Scanning Electron Microscopy and Transmission Electron Microscopy. The mixed phase of *alpha* and *gama* iron particles is found in the yellow iron oxide. The X-ray fluorescence and EDAX revealed the elemental composition of the iron oxide samples. The optical characterisations were performed by Photo Luminescence (PL), UV-absorbance and reflectance by Diffuse Reflectance Spectroscopy. The temperature dependant magnetic properties were studied by Variable Sample Magnetometry (VSM), which revealed only red iron oxide exhibits ferromagnetic properties. Electrocatalytic properties of red and yellow iron oxide were characterized by various techniques such as CV, Linear Sweep Voltametry (LSV) and impedance spectroscopy. Thermo gravimetric analysis revealed 7 % weight loss for yellow iron oxide. The as-received iron oxide samples were annealed at 600 °C and similar characterizations were performed. The electrocatalytic behaviour in terms of polarization in iron oxide will be presented in detail.

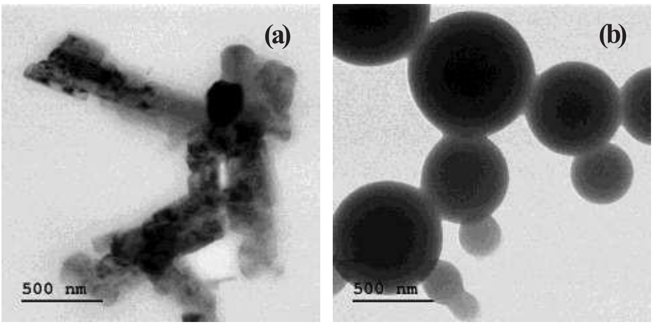

Figure: TEM image of (a) Yellow iron oxide and (b) Red iron oxide

Design of Small Horizontal Axis Wind Turbine for Low Wind Speed Rural Applications

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Abstract

In this study, a 2 kW small scale horizontal axis wind turbine with a rotor radius of 1.8 m and a Tip Speed Ratio (λ) of 6 was designed to work at low wind speed for rural applications. Aerodynamic analysis was performed on 10 airfoils, *viz* Aquila, BW-3, E387, FX63-137, NACA0012, NASA LS-0413, RG-15, S1223, SD7080 and SG6043 using QBlade software. These airfoils were used to analyze lift coefficient (C_L) and lift to drag ratio (C_L/C_D), with different angles of attack (α) and compared with one another. From the analyzed results, SD7080 airfoil was found to be the best due to its wide and maximum lift to drag ratio of 46.30 for the angle of attack (α) of 5^o and comparatively high power production at low wind speed operation. It showed a high soft stall behaviour in the α range of $4\text{-}9^o$. The blades were specifically designed for various airfoils by applying Blade Element Momentum Theory (BEMT). The power coefficient (Cp) of the selected airfoils varied according to the values of tip speed ratio (λ). From the results, it was detected that the SD7080 airfoil blade has an optimum power coefficient of Cp = 0.34, at λ = 6 for Reynolds number (Re) = 81712. SD7080 airfoil blade was analysed for different Re values of 30642, 40856, 51070, 61284, 71498 and 81712 in comparison with tip speed ratio and power coefficient. A considerably high power coefficient of 0.29 was produced when Re as low as 40856 at λ = 6. Therefore, from the numerical simulation, it was found that SD7080 was the most suitable airfoil to start producing considerably high power under low wind speed applications.

Keywords: Small horizontal axis wind turbine, BEMT, numerical simulation, QBlade software.

Synthesis and Characterization of Silver deposited Iridium doped Titanium Dioxide Nanocomposites and their Applications in Photon Upconversion

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Abstract

Photon Up Conversion (PUC) is a physical optical phenomenon in which several low energy photons are added to get one high energy photon. This can be used to convert infrared (IR) photons into visible or ultraviolet photons. PUC stands out to be a very convenient way to harvest over 55 % of infrared radiation incident on the Earth surface for its utilization in solar energy conversion devices, such as Dye Sensitized Solar Cells (DSSCs) and water photosplitting. This research is concerned with the up conversion of infrared radiation, by developing suitable materials capable of doing so, for utilization in DSSCs and photosplitting of water to produce hydrogen gas. In this research, TiO_2 nanoparticles were doped with Iridium (III) cations to introduce the electronic energy levels within the band gap of TiO_2 using our own sol-gel/hydrothermal method to produce the specific nanostructures. Finally, silver islands were deposited on the above nanoparticles to enhance the absorbance of the material by localized plasmon resonance. This Ag-Ir(IV)-TiO_2 nanocomposite materials were characterized by XRD, UV-Visible spectroscopy, SEM, EDAX, XRF, I-V and FTIR techniques. The applications of photo water splitting and DSSCs were discussed by introducing the synthesized material.

Keywords: Water splitting, DSSC, photon up conversion, Iridium, silver, localized plasmon resonance

Cobalt Disulfide embedded TiO_2 Nanocomposites for Hydrogen Production under UV Irradiation

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Abstract

Hydrogen gas is greener and reliable energy source, which can contribute to fill the gap between the energy demand and energy supply. Several photocatalyst materials, such as TiO_2, ZnO, CdS, WS_2, mixed oxides, perovskites, dye and metal doped oxide materials have been used as phototcatalysts for energy production, such as water splitting applications and environmental remediation. Development of efficient non-toxic photocatalyst has opened a new avenue for several other applications, such as in lithium ion batteries, solar cells, etc. The production of hydrogen through water splitting is a green route for converting solar energy directly in to clean fuel. Recently, the transition metal chalcogenides have intensively been focused on hydrogen production due to their stronger edge and the quantum confinement effect. This work mainly focuses on synthesis of cobalt disulfide (CoS_2) embedded TiO_2 nanocomposites using hydrothermal approach; and, the hydrogen production efficiencies of pure CoS_2, pure TiO_2, and different wt% of CoS_2 in TiO_2 were compared under UV irradiation. Nanocrystalline TiO_2 having 10 wt% CoS_2 exhibits higher hydrogen production of 2.5492 mmol/$g_{catalyst}$ in comparison with the pure CoS_2 or TiO_2 used in this study. The bare CoS_2 material was found to be inactive due to its very low bandgap energy of 2.5 eV; however, the enhanced activity of the CoS_2 loaded nanocomposite may be due to the heterojunction frame work that causes the effective electron-hole pair separation. In summary, the metal dichalcogenide, CoS_2, acts as an effective co-catalyst, whereas titania serves as active site by effectively separating the photogenerated electron-hole pair. This study lays down a new approach to develop transition metal dichalcogenide materials with significant bandgaps that can effectively harness solar energy for hydrogen production.

Keywords: Transition metal chalcogenides, titania, hydrothermal, hydrogen, water splitting

Coordinated Control of STATCOM with Distribution Network Devices for Wind Farm Integration

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Abstract

The global warming and greenhouse effect have increased potential for renewable energy technologies. The wind power generation is proven as a prominent renewable energy source for producing electricity. The most wind potential is available in remote areas, where the distribution networks are constrained by the power quality and reliability issues. Usually the distribution network consists of several devices such as De-Energized Tap Changer (DETC) and On-Load Tap Changer (OLTC). Further, the STATCOM is also used to solve power quality and reliability problems. This study investigates a practical situation of a small and remote distribution network, connected with wind farm and STATCOM, using PSCAD simulation. A worst case analysis is studied using critical wind data. A coordinated control technique is proposed to operate DETC, OLTC and STATCOM to reduce voltage variations. Here, the STATCOM detailed model using IGBT switches and small scale distribution network were modelled. The DETC and OLTC control and STATCOM, converter control, AC terminal voltage drop control and DC link voltage regulatory control were designed to operate accordingly to solve the voltage variations. The above DETC and OLTC controls were based on to operate the distribution system at the middle set point of the stable limits. The STATCOM control used park transformation for locking phase angle for synchronization. Accordingly, STATCOM system control, its internal voltage was developed. The STATCOM converter control used the sine-triangular PWM to generate the gate pulses. This is to eliminate the voltage violations during the steady state as well as the transient operations. The proposed coordinated control technique with the DETC, OLTC and STATCOM has proven better performance of the small distribution network. This allows to increase the wind farm integration to the remotely operated distribution grid.

Structural and Photoelectrochemical Characterization of Heterostructured Ag_2MoO_4-SnS_2 coated Carbon Sheet Photocapacitor

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Abstract

Photocapacitors that can harvest solar energy and store it in the form of electrical energy, are expected to solve the problem of unstable power output of solar cells under fluctuating sunlight. In the present study, a novel heterostructured Ag_2MoO_4-SnS_2 photocapacitive device was developed. In this device, SnS_2 nanoparticles act as capacitive platform *via* redox pseudocapacitance, whereas Ag_2MoO_4 molecules act as the active core of the device. The crystalline structure and the surface morphology of Ag_2MoO_4-SnS_2 coated carbon sheet was examined by powder X-ray Diffraction method (XRD) and Scanning Electron Microscopy (SEM) respectively. The XRD pattern indicates that Ag_2MoO_4 coated on carbon sheet is in β phase with respect to Ag_2MoO_4. The SEM analysis reveals Ag_2MoO_4 coated carbon sheet as hexagonal nanorods, and Ag_2MoO_4- SnS_2 coated carbon sheet as spherical nanoparticles. The device, when subjected to visible light illumination, showed a specific capacitance of 780 mF/cm^2 with an open circuit potential of 0.8 V *vs* Ag/AgCl electrode. The high capacitance obtained with this novel device may be attributed to the large specific area and high conductivity of the Ag_2MoO_4- SnS_2 coated carbon sheet. This research study has open up a new avenue for an effective heterostructured photocapacitor.

Keywords: Photocapacitor, photoelectrochemical characterization, specific capacitance, silver molybdate, carbon sheet

Sustainable Biomass Energy for Rural Bangladesh

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Abstract

Bangladesh is a densely populated country with limited natural resources, and suffering from severe energy crisis since the past few decades. Due to the limitation in fossil fuel reserve, the only way to minimize the supply-demand gaps in the energy sector is switching towards the alternative renewable energy sources. Kazi Shahid Foundation (KSF) has been working in partnership with rural villagers for over 15 years. In order to make rural people’s lives healthier and more productive, KSF has developed an innovative “Biogas Program”. The continuous burning of biomass fuels leads to long term health issues, predominantly among women. The amount of wood consumed, also contributes to an increase of greenhouse gas (GHG) emissions and partly responsible for deforestation. Bangladesh has a long standing tradition of utilizing dung exclusively as the feedstock for biogas plants whereas India has focused mainly on food waste. Attempting first in Bangladesh, KSF is utilizing the “no cash” microfinance repayment system, where KSF will be reimbursed the cost of the biogas plant through the effluent slurry, as well as, excess cow dung or milk. This bio slurry and dung are used for organic tea plantation at the Kazi & Kazi tea estate (Teatulia organic tea) in Panchagarh district and as well, for organic farming of fruits and vegetables to supply all over the country’s chain of super shops. In order to make biogas a viable alternative to the current biomass fuels used in cooking, this multi-purpose approach was developed through careful research into the latest technologies, fiberglass bio-digesters that is now available in Bangladesh. Fiberglass bio-digesters are portable, easy to install, need less space, and the use of water (as charging material) is half compared to the conventional brick-layered biogas plants.

Keywords: Biogas, fiberglass,

Low Temperature Deposition of Lithium Cobalt Oxide for Stable Performance as the Cathode of Solid-State Thin Film Batteries

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Abstract

There has been a considerable amount of work on the deposition of lithium cobalt oxide thin films on the metalized silicon substrate using room temperature deposition and post-deposition annealing at 700 °C. High-temperature annealing leads to tensile stress-induced cracking in the lithium cobalt oxide thin film. After film cracking, a considerable amount of tensile stress gets stored in the cathode material, that leads to further degradation during the charge-discharge process. The other issue with high-temperature annealing is, lithium desorption that leads to the reduction in the lithium content in the cathode materials. To address this issue, we have developed a deposition process at a lower temperature of 500°C. The substrate used in the process was aluminium and the reason for choosing aluminium was its widely used current collector property in lithium-ion battery fabrication process. The deposited films at 500°C showed predominantly (104) orientation, which is a favourable texture for high diffusivity of lithium. SEM micrographs showed columnar growth and different textures for the films which were deposited with different thicknesses. The Raman spectra showed single phase lithium cobalt oxide and high crystalline nature. To avoid temperature induced effects, magnetron efficiency was also monitored during 500°C substrate temperature. The ideal target to substrate distance was optimized as 6 cm and the sputtering magnetron efficiency was unchanged. The electrochemical performance was evaluated using chronopotentiometry technique and the capacity of the deposited lithium cobalt oxide film was 120 $\mu Ah/cm^2$. The performance of the cathode was stable even up to 80 cycles.

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