

EMERGING ENERGY TECHNOLOGIES SUMMIT AND EXHIBITION

Melbourne, Australia
5-7 December 2016

Book of Abstracts



PLENARY SESSIONS

Solution-Processed Organic Solar Cells: Current Progress and Challenges

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Organic solar cells potentially can offer low cost, large area, flexible, light-weight, clean, and quiet alternative energy sources for indoor and outdoor applications. In this talk, I will give an overview of the current progress and challenges in organic solar cells. Then, I will discuss recent progress at UCSB on the development of molecular donor materials for application in solution processed bulk heterojunction solar cells. Molecular donors offer potential advantages over conjugated polymer systems in terms of their ease of synthesis and purification; making them more affordable to produce on large scales. Additionally, small molecules do not suffer from molecular weight dependence and polydispersity, and thus large batch-to-batch variation as their polymer counterparts. Chemical structure and processing conditions can be used to tune the energy level, bandgap, solubility, molecular packing, film morphology, exciton diffusion, charge mobility, charge recombination, and therefore, the device performance. A series of compounds has been synthesized to establish structure-function-property relationships. A combination of techniques is employed to characterize material properties including steady-state and time-resolved spectroscopy, atomic force microscopy (AFM), photoconductive AFM, TEM, XRD, UPS, and GIWAXS. The results from these studies provide design guidelines for new generation of molecular-based materials for applications in organic solar cells.

Challenges for Large Scale Energy Storage and Transportation

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Energy Storage is critical for grid modernization and electrification of transportation infrastructure. For transportation, development of high energy and low cost battery technology with improved safety is a high priority. For grid scale energy storage, low cost and long cycle life are the key. This presentation will discuss challenges for high energy batteries, including challenges for the Battery500 Consortium, with an emphasis on progresses in the fundamental understanding of full battery reaction mechanisms and materials issues in next generation lithium battery systems. Currently lithium ion batteries are approaching its maximum energy density, but the cost is continuing to decrease. Replacing the current electrode materials with high capacity cathodes, silicon anode and lithium metal could significantly increase the energy density and reduce the cost, but requires breakthroughs in carefully controlling the electrochemical reactions in the whole battery system, particularly the interfacial reactions on both the cathode and anode sides. New electrolyte formulation and additives can significantly suppress the undesired reaction and increase the Coulombic efficiency and cycle life. This talk will also discuss many other technologies including redox flow, Na-ion and Li-S batteries.

Rechargeable batteries for renewable energy storage and conversion

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In this talk, I will report the development of advanced electrode materials for various high performance rechargeable batteries.

3D hyperbranched hollow carbon nanorod architectures were synthesised for high performance Li-S batteries. The nanorod composites delivered a high specific capacity of 1378 mAh/g with excellent cycle life.^[1] Multichambered micro/mesoporous nanocubes were also prepared as new polysulfide reservoirs for Li-S batteries with long cycle life.^[2]

Lithium-air battery is the most promising system as the power source for electric vehicles. The theoretical specific energy of the Li-O₂ battery is 3,505 Wh kg⁻¹, which is almost ten times higher than that of Li-ion batteries (387 Wh kg⁻¹). Porous graphene with different pore size architectures were synthesized as cathode catalysts for lithium-air batteries, which exhibited significantly higher discharge capacities than that of non-porous graphene. Moreover, the Ru nanocrystal decorated porous graphene exhibited an excellent catalytic activity with a high reversible capacity, low charge/discharge over-potential, and long cycle life.^[3]

Sodium-ion batteries are being considered as a promising system for stationary energy storage and conversion, owing to natural abundance of sodium. Several novel electrode materials were synthesized as either cathode materials or anode materials for lithium-ion batteries and sodium ion batteries.^[4-6]

Potassium-ion batteries are promising energy storage devices that offer a cost effective solution to store electrical energy on a large scale. An ongoing challenge has been to obtain satisfactory performances in each of the key areas of capacity, stability, cost, and safety. I will report a potassium iron (II) hexacyanoferrate nanocube cathode material that operates with an aqueous electrolyte to deliver exceptionally high capacities (up to 120 mA h g⁻¹). The cathode material exhibits excellent structural integrity, leading to fast kinetics and highly reversible properties (> 85 % capacity retention over 500 cycles at 21.4 C). All of the battery materials are safe, inexpensive, and provide superior high-rate, long cycle life electrochemical performance.^[7]

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Rethinking the challenges in supercapacitors: What makes graphene exceptional?

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On the basis of our recent research on graphene-based soft materials and their application in supercapacitors, this talk will present our personal perspectives on the following questions: (1) What really dictates the performance of a supercapacitor? (2) What are the intrinsic limitations of the traditional porous carbon materials for application in supercapacitors? (3) What makes graphene unique for use as electrodes in supercapacitors? (4) Future opportunities and challenges.

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Bioenergy and biofuels in the carbon-constrained future

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Biomass is among the cheapest renewable energy sources for power generation, especially base-load/dispatchable electricity. Biomass can also be used directly to produce drop-in liquid fuels and chemicals. Bioenergy and biofuels can be generated/produced with negative CO₂ emissions. Therefore, bioenergy and biofuels will play an important role in our energy supply mix in the carbon-constrained future.

This presentation will provide an overview of our recent research and development efforts on the thermochemical conversion of non-food lignocellulosic biomass. The presentation will be focused on the recent progress in the understanding of reactions taking place during the pyrolysis and gasification of biomass as well as those during the biorefinery of bio-oil. Our technology development efforts will also be summarised.

Emergency Target for Energy Storage

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One of the greatest challenges of the 21st Century is the maintenance of a sustainable development society under severe environmental constraints such as conserving resources and conserving energy. Therefore, it is imperative for Japan, with its lack of natural resources, to contribute to the global community by technology for energy storage and their effective use for a future society. As the energy storages in the renewable energy system, lithium ion battery (LIB) is one of the promising storage devices because of its high energy density and high power output. Diagnosis technology of LIBs is very important to use electric devices in safety as well as development of materials. Electrochemical impedance spectroscopy (EIS) is superior method for analysis of the battery health while in use. EIS has been utilized to characterize each factor of batteries, because it enables us to analyze dynamics of each elemental step sensitively and separately without destruction of the cell. In addition, un-destructive EIS is expected to utilize for premonitory diagnosis of batteries on board in electric vehicles. In our previous study, the equivalent circuit to express each elemental step in a commercial LIB by EIS has been carefully investigated. We proposed the designed equivalent circuit, and on the equivalent circuit, the impedance responses of LIB during capacity fading were analyzed with continuous charge-discharge cycling. EIS using conventional FRA – potentiostat systems is not easy to measure the impedance of the large-scale LIB because of its low internal resistance. Moreover, FRA – potentiostat system for conventional EIS measurement could not be mounted on the vehicle. Thus, impedance measurement system is needed without using FRA – potentiostat systems. In our study, application of square wave potential for input signals of EIS was investigated in simple electrochemical reaction to verify a new technique called “Square-potential/current electrochemical impedance spectroscopy (SP-EIS, SC-EIS)” which is a method for EIS without using the FRA systems. We applied SC-EIS to evaluate a state of a commercial LIB. Introduction of SC-EIS to diagnosis technology of laminated LIBs and the LIB module was discussed. [1]

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Progress towards hydrogen and ammonia from renewables

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Keywords: Hydrogen, Ammonia, Hydrogen carriers

One of the most efficient routes to hydrogen is by electrolysis of water, otherwise known as water splitting. While the technology of water electrolysis is well established, significant advances in efficiency are required to make the process competitive in economic terms. Such advances in efficiency require improvements in catalysts for both the hydrogen evolution reaction (the “HER”) and the oxygen evolution reaction (“OER”). The OER is particularly sluggish and thus much attention has been devoted to understanding and developing new catalysts and media[1] for this reaction in particular.

The energy source for this electrolysis process can be a variety of renewable electricity sources, including “excess” energy in power grids at times of excess supply over demand. Thus the process may offer a useful solution for the intermittency problem of power grids that include a large proportion of renewables. As an alternate to this “Grid connected” mode, recent work has demonstrated the levels of “Solar-to-Fuel Efficiency” (>22%) that can be achieved with careful tuning and “Direct connection” of the electrolysis cell to the photovoltaic cell [2]. There is also tremendous interest and effort devoted to direct solar reduction of water on photo-sensitized anodes or cathodes[3].

Where the source of the renewable energy is geographically distant from population centers (“Stranded Renewables”), the issue of hydrogen storage and transportation arises. One solution to this challenge that is being explored is the use of “renewable” hydrogen to generate liquid ammonia, a chemical that is relatively easily and safely transportable by both pipeline and marine tankers. At point of use the ammonia can be converted simply and efficiently into hydrogen (and nitrogen). For example, the capacity for the generation of both wind and solar power in the remote areas of northwest Australia is immense, and converted to ammonia could be easily transported in bulk tankers to Japan for conversion into hydrogen at a relatively local level. There is also growing interest in catalysts that could support the direct reduction of atmospheric nitrogen to ammonia[4, 5].

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CONCURRENT SESSIONS

Concurrent session 1: Photovoltaics

Dye-sensitized and perovskite solar cells

Udo Bach

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Polymeric interface materials and morphology control in polymer solar cells

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Polymer solar cells have gained considerable interest during the last decades. The most promising active layer material comprises so-called bulk-heterojunction blends of a donor polymer that is finely mixed with a fullerene acceptor. The photovoltaic performance has increased rapidly over the last years with high power conversion for lab-scale single-junction devices.

So far a number of different types of materials have been used as interface materials for work function modifications. We have synthesised and evaluated the stability of several such materials having different functional groups. The materials include modified fullerenes, polyfluorenes and the use of ethoxylated polyethylenimine (PEIE) and poly(4-vinyl pyridine) (P4VP). To evaluate the stability of the work function modification of ITO, UPS measurements have been performed on samples exposed to ambient conditions for up to four weeks. In devices we have seen a clear effect on the open circuit voltage and in some cases an improved thermal stability of the morphology as well. When using P4VP as the interphase layer on top of ZnO we have seen an increase in the power conversion efficiency from 5.1% to 6.5% for TQ1 devices.

In our search for environmentally friendly deposition methods we have concentrated our efforts on the preparation of water dispersion of nanoparticles. The most widely used preparation method involves the use of charged surfactants, for example sodium dodecyl sulfate (SDS). The morphology of the active layers is studied using different techniques including dynamic mechanical analysis (DMA) to for example determine a suitable annealing temperature for the coalescence of the nanoparticles. These methods present a promising way to deposit the active material in the solar cells from aqueous dispersions.

Getting around the current-voltage trade off in organic solar cells

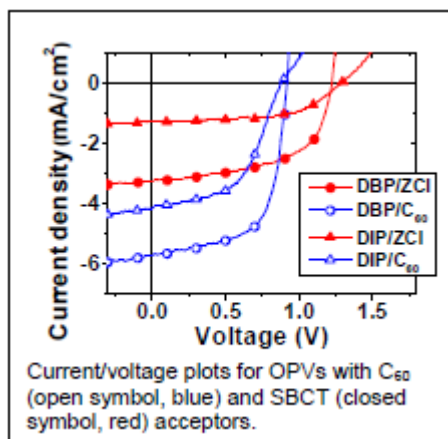
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A key limitation of OPVs are their low open circuit voltages (VOC), which are typically well below the energy of the light absorbed. I will discuss a new approach to achieve VOC values close to the theoretical limits, using materials that involve symmetry breaking charge transfer (SBCT). These materials are symmetric molecules that spontaneously form an intramolecular charge transfer complex, with nearly complete one electron transfer from one part of the molecule to another. This minimizes the energy offset needed at the donor/acceptor interface to drive charge transfer and charge separation. Incorporating the SBCT process into an OPV pushes the VOC close to the theoretical limits. We have characterized the SBCT process in a family of different materials, with high potential in OPVs. The kinetics of formation of the SBCT process have been characterized by ultrafast spectroscopic techniques. This intramolecular SBCT state readily forms a charge separated state at the D/A interface of the OPV.

We have explored these materials as both donors and acceptors in OPVs and found that they give good performance and high Voc. A proof of concept is seen when a zinc dipyrin, ZCl, is used to replace C60 as the acceptor layer in an organic solar cell. OPVs prepared with the zinc dipyrin give VOC values 400 mV higher than observed for analogous OPVs prepared with C60 (see Figure below), even though the two acceptors have the same LUMO energies. We will discuss our latest results with SBCT materials.



Concurrent session 2: Materials for energy storage

Controlling the Morphology of Materials for Li-based Batteries

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Li-ion batteries are commonly used in hand held, portable electronics, with significant research effort being focused on increasing their application in aerospace and electric vehicles. Associated with the need for highly efficient, larger batteries is the need for improved safety. Therefore, careful selection of anode and cathode materials is required. Our interests have focused on the morphology of the electrodes to enhance their electrochemical performance by incorporating porous structures. Porosity increases the electrolyte/electrode interface and thus enhances charge transport. To monitor the effect of pore size on the electrochromic properties we have used colloidal crystals as templates to vary the pore size within LiFePO₄ and fabricated mesoporous titania beads that varied in bead diameter and pore size.^{1,2} We have also studied porous metal oxide materials for hosting the sulphur in lithium sulphur batteries.³ This talk will focus on the fabrication of the porous structures, their morphological characterisation and their electrochemical properties.

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Considerations for industrial scale up of battery material manufacture

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The importance of considering scale up issues, even when we may only be involved with R&D at lab scale, is discussed. The more we anticipate scale up issues, the higher the probability of successful commercialization of our R&D and of dollars coming back to fund more research. Many issues with industrial scale up can be anticipated at lab scale, particularly during the selection of materials. Safety of the application is very important for consumer confidence, and it is an aspect that makes LiFePO₄ a good choice for large battery applications.

Small sizes of samples in lab scale synthesis are very forgiving with process choices. Increased sample sizes are required to reveal the true parameters that have to be controlled for high quality, reproducible powder manufacture. Examples of scale up issues will be given from previous experience on superconductor powder synthesis. Mention will be made of additional powder characteristics, which have impact on processing decisions, and where LiFePO₄ is no exception. Highlights of our pilot scale plant for LiFePO₄ manufacture will also be given.



Electrolytes for advanced metal batteries – Towards high performance, high energy density devices

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Recent progress of organic-inorganic hybrid perovskite solar cells

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Organic-inorganic hybrid perovskite materials have been of great interest due to their prominent properties such as high absorptivity via direct bandgap characteristics, long charge carriers' diffusion length due to the formation of shallow traps by ionic crystal structure, high open circuit voltage by large dielectric constant, and solution processability since Kojima *et al.* reported the liquid junction $\text{CH}_3\text{NH}_3\text{PbIX}_3$ (MAPbX_3 , $\text{X} = \text{Br}$ and I) perovskite-sensitized solar cells.[1] Currently the certified efficiency of lab scale perovskite solar cells reached over 22 % at 1 Sun condition. However, it has been known that the perovskite materials have some problems including poor stability such as humidity, thermal, and light soaking stability, poor reproducibility, and current density-voltage hysteresis. To find commercial applications in uses, further improvement of device efficiency, large scale coating technique, module design, encapsulation, and so on should be also studied more. From these aspects, I would like to introduce and discuss on our activities and research directions with you.

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Powering the future with printed solar films

Fiona Scholes

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Solar energy will clearly make an increasing contribution to global energy needs into the future. While traditional solar cells (based on silicon) are well known, printed solar films are an emerging technology with distinct features (cheap, flexible, lightweight) set to transform the future of solar energy. Since 2007, CSIRO has been working with university and industry partners to develop the capability to manufacture printed solar films in Australia. This talk will tell the story so far, including discussion of the key challenges and turning points, as well as a look towards the future.

Energy conversion and energy up-conversion in singlet fission sensitized organic heterojunctions

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Energy conversion and energy up-conversion forms a thrust area within the wider organic optoelectronic research. In photovoltaic operation of organic diodes, the external quantum efficiency (EQE) works as a figure of merit to efficient free charge generation. As such, the EQE depends on the product of the light absorption efficiency (number of excitations to incident photons), charge generation quantum yield (number of generated free charges to number of excitations) and charge extraction efficiency (number of extracted charges to generated charges). Generally, the upper limit of EQE is 100% as one incident photon gives rise to one electron-hole pair.

Organics semiconductors such as polyacenes among others have the unique ability of producing two electron-hole pairs per absorbed photon. This occurs due to the physical process of singlet fission where an excited singlet state breaks into two low energy triplets^[1]. In this paper, we will present our latest results on triplet exciton dynamics in pentacene and rubrene with strategies for energy conversion with EQEs >100%; spin branching ratio > 25% for light emission, and successful examples of energy up-conversion^[3, 4] in singlet fission sensitized organic heterojunctions.

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High efficiency perovskite on silicon tandem solar cells

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Concurrent session 4: Materials for energy generation and storage

New Battery Technology for Electrical Energy Storage

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Battery technology was initially developed for electric vehicles but is widely expected for electrical energy storage, which generate many new technical challenges for future battery technology. We have been working on various types of batteries for ten years, and achieved major improvement in the battery performance using nanotechnology and nanomaterials, including storage capacity, life time, and safety. This presentation will discuss safety issues of Li ion batteries, main challenges of high-energy density Li-S batteries and new electrode requirement for Na and K batteries. Further details can be found at <http://www.deakin.edu.au/about-deakin/people/ying-ian-chen>.

Clusters on Semiconductor Surfaces for Novel Catalysts

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Gold clusters with a size < 1.5 - 2 nm deposited on immobilized onto inert supports are known to be catalytic active with the size threshold often coinciding with the loss of metallic properties of Au nanoparticles. The size-threshold is established for both naked clusters prepared under UHV conditions [1] and chemically-synthesised [2] well-defined metal nanoparticles. Clusters can be deposited from the gas phase as size selected clusters [3] or from the liquid phase when using chemically synthesised nanoparticles [4] with the latter route offering the benefit of easy scale-up.

In the deposition process of chemically made clusters onto inert supports a few challenges need to be solved. First, it needs to be investigated whether or not removal of the ligands is required to make the chemically made clusters catalytic active. The presence of ligands might hinder gas molecules to access the catalytic active sites of the clusters. We have found that removal of the phosphorous ligands can be achieved with heating to around 200°C in vacuum [4]. Second, the agglomeration of the clusters needs to be avoided in order to keep the cluster size small. In particular heating for removal of the ligands could lead to agglomeration. We have deposited $\text{Au}(\text{PPh}_3)_y$ ($n = 8, 9$ and 101 , y depending on the cluster size) on titania and found that treatment of the titania prior to deposition influences the agglomeration in the ligand removal process. Treatments applied are amongst others basic and acidic treatment, calcination under H_2 and O_2 and UV/ozone treatment. Electron spectroscopy techniques (X-ray photoelectron spectroscopy (XPS)), scanning techniques (atomic force microscopy (AFM)) and microscopy ((scanning) transmission electron microscopy (STEM and TEM)) have been used to investigate the deposition process. Subsequent to deposition also the electronic and conformational structure has to be determined because these are the two properties which are believed to play the crucial role for catalysis. Metastable induced electron spectroscopy (MIES) has been used for determining the electronic structure of deposited clusters. Results of catalytic reactions will be shown.

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Computational Discovery and Design of 2D Materials with High Charge Carrier Mobility and Excellent Catalytic Properties for Energy Applications

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The discovery of graphene [1] has led to significant development of a new family of 2D materials including hexagonal boron nitride, silicene, phosphorene, borophene, metal dichalcogenides and metal oxides etc. Our recent research mainly focuses on (i) predicting new 2D Dirac materials with higher charge carrier mobility than graphene [2-3]; (ii) exploring 2D materials for hydrogen evolution reaction, solar cell and photocatalytic water splitting [4-5]; (iii) exploring functionalized 2D materials as efficient catalyst for converting carbon dioxide into alternative fuel cells [6]. In this presentation, I will share our most recent research progress in relation to the above topics.

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A Facile Fabrication of Doped Metal Oxide Electrocatalysts for Efficient Energy Conversion Application

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Electrocatalysts that convert electrical energy into chemical reaction energy, or vice versa, play an indispensable role in energy conversion technologies, such as dye-sensitized solar cells (DSCs), fuel cells and water splitting hydrogen production. Noble metal electrocatalysts, such as Platinum, Iridium, Ruthenium, demonstrate superior electrocatalytic activities towards key reactions but their high cost and scarcity place large hindrance to their future application. The search of high-performance, earth-abundant noble-metal-free electrocatalysts has therefore been a focused research topic in the energy conversion field.

Transition metal oxides represent one of the most abundant, stable groups of solid-state substance on earth but their electrocatalytic performances towards the key redox reactions are poor due to the lack of catalytically active sites. It has been demonstrated that introduction of exterior elements into pristine crystal structures (doping) can establish the active sites on metal oxide surface. Nevertheless, effective in situ doping for the electrocatalyst fabrication is still challenging. We herein demonstrate a facile vapour-phase hydrothermal (VPH) method to in situ dope the electrocatalytically inactivate metal oxides and convert them into electrocatalyst materials for energy conversion technologies, such as DSCs, and water splitting hydrogen production.

Robust Barrier Technology for Thin Film Photovoltaics

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The development of thin film barrier technology is critical to the packaging and reliability of thin film photovoltaics. Barrier films are used to limit moisture ingress into the photovoltaic cells and often require a water vapour transmission rate less than 10^{-4} g/m²/day for many applications. Several methods using vacuum deposition technologies such as atomic layer deposition and plasma enhanced chemical vapour deposition can be used to create ultrabARRIER films. However, assessing their durability must be done in terms of the impact of defects from the manufacturing process on their performance. Manufacturing defects and their growth over time can cause degradation of the barriers, leading to lower device lifetimes.

In this work, we use Ca corrosion testing to elucidate both the intrinsic and defect assisted WVTR permeation rates in vacuum deposited ultrabarriers. Through appropriate design of the barrier structure, we show that it is possible to reduce the impact of moisture ingress through localized defects. Next, we show the impact of the time-dependent propagation of defects in barrier films via channel crack growth under mechanical loading which can reduce device lifetime. Data shows that the concept of onset cracking strain that is often used to define the failure limits flexible barriers is insufficient. Data show that the time dependent crack propagation from defects in the barriers is a function of humidity, temperature, and applied strain (Figure 1). Thus barrier film reliability is strong function of environment and stresses experienced during application. Methods to ensure barriers are less susceptible to defect propagation will be discussed as well as demonstrations of integration with thin film photovoltaic devices.

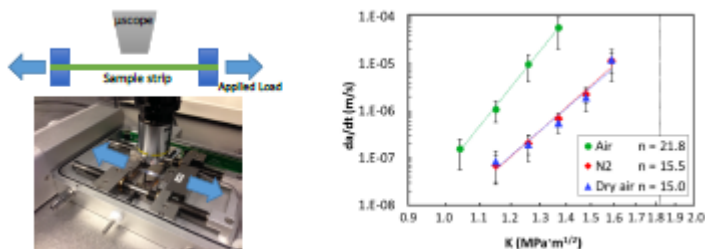


Figure 1. Mechanical test of a PECVD SiNx barrier on PET substrate and

the associated crack growth rates (da/dt) with applied loading

Third Generation Solar Cells - Challenges and Opportunities

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Development of cost-effective, stable semiconductor materials for efficient solar to electricity conversion efficiency devices is critical for deployment of low cost solar electricity. In the past two decades, different types of solar cells with variable device structure and light absorbing materials have been reported including dye/perovskite solar cells and $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) thin film solar cells. All these devices have demonstrated the potential to deliver cheap solar electricity by using earth- abundant materials and simple fabrication technology that is feasible for printing or roll-to-roll production. Nevertheless, all these new types of solar cells are still at the stage of intensive research and are yet ready for large scale production in practice. In my talk, I will share our recent research in the area of third generation solar cells including nanostructure dye/quantum dots-sensitized solar cells, perovskite solar cells and CZTS thin film solar cells. The challenges and opportunities of these devices will be discussed.

Interface Integrity in Organic Solar Cells

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Organic photovoltaics (OPVs) offer a number of advantages, such as fully solid state, compatible with high speed printing and production technologies, but they also a number of challenges related to efficiency and lifetime, many of which can be traced to instability in interfacial layers within the structure.

The ability to create, control and measure nanoscale structures is critical to the development of a range of new technologies. Understanding the properties of a wide range of systems that are generally thought to be “uniform”, “stable” and “consistent” are proving to be critical in the development of a number of options for new, low cost energy solutions which have the potential to change the way in which we harvest and collect energy. All of the approaches rely upon multi-layer structures with layers of the order of 10 - 200nm – a range that materials offer interesting chemical and electronic properties, but are also susceptible to subtle changes in chemistry that can drive significant performance differences.

A range of unique techniques have been used to investigate the materials that make up the layers and interfaces in these devices, including:

- a) X-ray photo-, UV photo-and metastable induced electron spectroscopy (XPS, UPS and MIES). The combination of these techniques allows for analysing the electronic structure at the interface and discriminating between the outer layer and the region close to the surface;
- b) neutral impact collision ion scattering spectroscopy (NICISS) for analysing the elemental composition across interfaces to a depth of about 10nm;
- c) electron microscopy.

This presentation will discuss the chemical and electronic properties of a number of interface layers within organic photovoltaic devices, with a particular emphasis on understanding the relationship between processing conditions and properties and the structures that are actually forming.

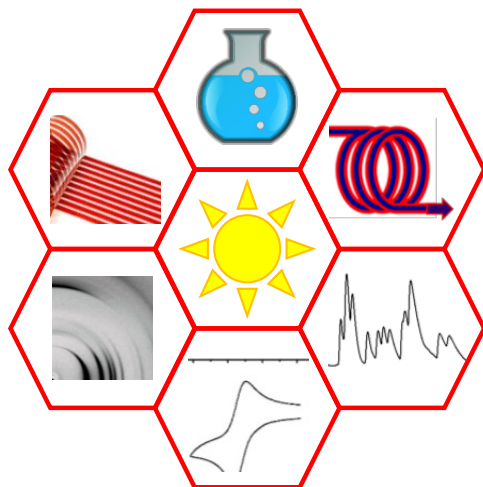
High Performance Organic Solar Cell Materials – Design, Synthesis and Scale-up

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State-of-the-art thin film organic solar cell devices have breached the 10% power conversion efficiency barrier in recent years. Progress in this research area can be attributed to development of new materials, new device architectures and overall understanding of device operation. Our experience reflects the multidisciplinary nature of this area where materials development facilitated device improvements and vice versa. This resulted in reports of a polymeric material^[1] as well as a molecular material^[2] with high solar cell performance from our group.

In this report, we will share our experience of designing and making these high performance materials with a view towards their use in fully printed large area solar cells.^[3] Examples will be presented to show the influence of synthesis methods and molecular structural modifications. We will also briefly discuss our research into scaling up the synthesis of materials using continuous flow methods.



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Concurrent session 6: Solar thermal

Solar thermal energy: From power generation to kerosene synthesis

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High-flux solar irradiation obtained with optical concentrators is an excellent source of clean process heat for high-temperature physical and chemical processing. Solar thermal power, the area that has traditionally driven developments in concentrating solar technologies, experiences renewed research interests, primarily in the context of large-scale dispatchable power generation. The area of solar thermochemistry aims at direct thermochemical production of chemical fuels and commodity materials. Cheap and efficient solar production of synthesis gas, the precursor to synthetic drop-in hydrocarbon fuels such as petrol, diesel and kerosene, is an intriguing approach to transform today's fossil-based to tomorrow's renewable-based transportation sector. In the most ambitious scenario, synthesis gas is obtained from sunlight, water and captured carbon dioxide. This presentation gives an overview of recent developments in high-temperature solar thermal and thermochemical processing, from basic research to applications.

Emerging Technologies in Concentrating Solar Thermal for the New Economy

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Concentrating solar thermal (CST) energy technology has potential to play a major role in transforming the energy-intensive processes that underpin Australia's mineral and resource exports to generate low-carbon products for the new economy. Emerging technologies include high-temperature CST reactors to directly calcine alumina and lime with high flux radiation, through to the production of renewable fuels, such as syngas, or oxidants that can be used directly in existing production processes. The production of syngas with CST from biomass sources also offers the potential to achieve carbon-negative emissions and can alternatively be transformed to a liquid transportation fuel, with its high energy density and storability, either for local use or for export. The complementary drivers for these various types of technologies will be discussed, together with options with which to maintain continuous operation from a variable resource.

Solar Thermal Power and Key Material Technology

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Key words: Concentrated solar power, Solar selective absorbing coating, Thermal stability

Solar thermal energy is one of clean and renewable energies with great potential usages. Solar spectral selective absorbing coatings are the fundamental component of a solar photo-thermal conversion absorber which is required to have a high absorptivity in the wavelength 300-2500 nm and a low thermal emissivity in the wavelength 2.5-50 μm . The situation and development of solar thermal power is reviewed. A solar absorptivity above 0.95 and a normal emissivity below 0.06 have been obtained in our new designed coatings, such as $\text{Al}_2\text{O}_3/\text{AlNi-Al}_2\text{O}_3/\text{AlNi-Al}_2\text{O}_3/\text{Mo}$, $\text{SiO}_2/\text{NbMoON}/\text{NbMoN}/\text{Al}$ and $\text{SiO}_2/\text{ZrSiON}/\text{ZrSiN}/\text{Mo}$ multilayer coatings. The thermal stability above 500°C was evaluated for the potential applications in parabolic trough concentrated solar power (CSP).

The correlation between uniaxial negative thermal expansion and negative linear compressibility in $\text{Ag}_3[\text{Co}(\text{CN})_6]$

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Density functional theory (DFT) calculations are used to investigate the correlation between the uniaxial negative thermal expansion (NTE) and negative linear compressibility (NLC) behaviors in $\text{Ag}_3[\text{Co}(\text{CN})_6]$. First, we reproduce the uniaxial-NTE and NLC behaviors under temperature- and pressure-field. And then the temperature dependence of elasticity is studied. The abnormal nature of elastic constants C_{33} and $C_{11}+C_{12}$ as the function of temperature is predicted. The hardening of phonon modes (below 564 cm^{-1}) with increasing temperature can be as an indicative for abnormal physical properties of $\text{Ag}_3[\text{Co}(\text{CN})_6]$. Through analyzing the vibration mode with the strongest phonon hardening, the deformation of wine-rack motif in anisotropic framework can be identified as the mechanism that leads to the coexistence of uniaxial-NTE and NLC in $\text{Ag}_3[\text{Co}(\text{CN})_6]$. The response of phonon group velocity along c -axis is intense and quicker than that of a -axis on heating and on compression, facilitating c -axis itself to be the carrier of abnormal uniaxial-NTE and NLC properties.

Concurrent session 7: Energy storage

Renewables, electric vehicles and energy storage

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The key to a low carbon future is the elimination of almost all of our current hydrocarbon energy sources. In the USA the two largest sources of CO₂ are transportation and electricity generation. Considerable research into the replacement of coal plants using renewables and the development of electric vehicles are underway and significant progress is being made. Recent analysis at NREL has identified that only limited CO₂ reductions can be achieved from BEV and PHEVs utilizing a high carbon electrical grid. However, as the deployment of renewable generation increases, issues with grid integration and curtailment are becoming more apparent. The intersection between these problems is energy storage. In this presentation

I will discuss the requirements for energy storage in both vehicles and grid and detail the NREL approaches to both systems and materials development.

Automotive energy storage is currently dominated by lithium ion technology, and major improvements in materials for both the cathode and anode are underway. At NREL we are focusing on the development of high-energy high-voltage cathodes and the fundamental chemistry of lithium-silicon electrodes and the formation and evolution of the solid electrolyte interface on Li-Si alloys. The challenges of high nickel high voltage cathodes and silicon anodes will be discussed.

Energy storage on the grid is much less developed, than vehicle applications, and many more options are open for the future. Again lithium ion is dominating the current deployments, but other applications such as mechanical storage, flow batteries, and beyond lithium ion concepts are all potentially on the road map. While the technical challenges for grid storage are different from those of vehicles they are not less challenging and cost is going to dominate technology deployment. I will discuss the major technical challenges of some of these technologies and the approach NREL is taking to enable future grid storage for renewables.

Renewable organic batteries

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Keywords: green batteries, aqueous batteries, organic electrode materials, p-type reaction

Accelerated progress and innovation in the development of new and potentially “greener” electrochemical storage devices, is imperative. In this regard, the past decade has seen significant progress with respect to redox-active organic compounds, attracting much interest from the energy storage community. This is evidenced by the rapid increase in the number of studies and recent reviews on the topic although this approach is still in its infancy [1]. Based on the tailoring of naturally abundant chemical elements (C, H, N, O, S, in particular), organic chemistry also provides great opportunities for discovering innovative electrode materials, which could be prepared (i) from renewable resources (biomass) and (ii) via eco-efficient processes (green chemistry principles, making the concept of “greener and sustainable” Li-ion batteries possible [2]. Additionally, two types of electrochemical mechanisms can be used in practice: n-type structures involving a charge transfer between the negatively charged state and the neutral state of the organic backbone (with cation release/uptake), and p-type structures involving a charge transfer between the neutral state and the positively charged state of the organic backbone (with anion uptake/release) [3-5].

We launched recently several new projects dealing with greener organic non-aqueous and aqueous batteries. In this communication, we report on new materials and their uncommon reaction mechanism, for both technologies.

The first part of the lecture deals with the elaboration of a novel non-polymeric crystallized organic positive electrode material belonging to low-weight aromatic amines, for the non-aqueous application. We show this new material is able to reversibly host anions even without a carbon additive, which is very unusual behavior for an organic electrode material.

The anion insertion process relies on the electrochemical activity of neutral secondary amino groups incorporated into a robust terephthalate backbone. XRD, TEM and EELS studies reveal the attainment of a lamellar morphology conducive to the oxidative insertion of anions (including the bulky TFSI⁻). In a dual-ion cell configuration using lithium as the negative electrode, this organic structure can react reversibly at high operating potential (~3.2 V vs Li⁺/Li) with good cycling performance.

For stationary applications such as storage of renewable energy sources, low cost is a must. We decided to focus on sodium aqueous organic batteries as a new promising technology, barely studied yet, for which negative electrodes are missing. In the second part of the lecture, we address this issue and we show our on-going results on several n-type diimide materials, delivering a cycled capacity ~100 mAh/g at low voltage in neutral aqueous electrolyte.

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Mechanically-assisted Electrochemical Production of Graphene Oxide for Energy Storage Application

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Graphene oxide (GO) is promising for a variety of applications due to its excellent dispersibility and processability. However, current chemical oxidation routes have several drawbacks, including the use of explosive oxidizing agents, residual metal ions contaminations and the creation of irreparable hole defects on GO sheet. The electrochemical exfoliation and oxidation of graphite is a potentially greener approach without the need for extensive purification steps. Most reported electrochemical methods employ a single preformed bulk graphite as electrode, which limits their scalability, reproducibility and degree of oxidation. Herein, we reported a novel mechanically-assisted electrochemical method to produce graphene oxide directly from graphite flakes. The electrochemically-derived graphene oxide (EGO) shows a good degree of oxidation but with less physical defects than chemically-derived graphene oxide (CGO). EGO has good dispersibility in water and various solvents and, in particular, displays better long-term stability in ethanol when compared with CGO. Notably, unlike conventional CGO, EGO can undergo facile thermal reduction at 200 °C in air to produce conductive reduced EGO, which is highly desirable for heat/chemical sensitive applications. In this talk, the application of EGO as supercapacitor electrodes will be discussed.

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Three dimensional computational fluid dynamic analysis of producer gas fuelled solid oxide fuel cell operation

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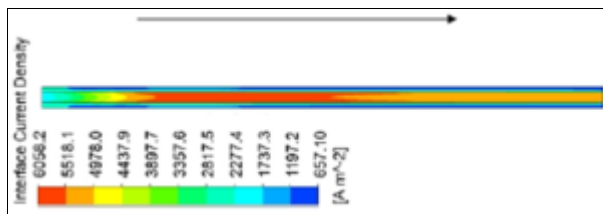
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The performance of a single channel fuel cell fuelled with producer gas is reported in the current article. Producer gas, generated from thermo-chemical conversion of biomass is a green chemical energy source with near zero carbon foot print and is currently being explored in internal combustion engines for power generation. With significantly higher conversion efficiencies as compared to engines (close to double) fueling of fuel cells with producer gas potentially represents the environmentally most benign power generation solution and is numerically investigated for performance in the current article.

A single channel solid oxide fuel cell is modeled using the ANSYS-FLUENT package adopting the unresolved electrolyte model (hence the electrolyte is not modelled). The model is validated based on hydrogen fuelled operation (from literature) with the model indicating average current density of 4013 A/m^2 (refer figure) against literature data of 5000 A/m^2 , the difference attributed to stack being considered in the literature.

Fuelling the single cell with producer gas at air to fuel ratio of 50:1 provides an average current density of 223 A/m^2 with CO utilization factor of 23% and H_2 utilization of 9%. The lower current density is attributed to the higher activation over-potential, 0.26 V, (energy lost due to slowness of electrical reactions) due to the presence of CO. Extended analysis indicates the possibility of partially overcoming this effect by steam wherein the activation over-potential is reduced to 0.15 V. The potential for carbon deposition on anode, due to the presence of CO, has also been assessed and is found to be directly proportional to the CO fraction.



A Novel Hybrid Compressed-Gas/Pumped-Hydro Ground-Level Integrated Diverse Energy Storage System

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Due to the increasing generation capacity of intermittent renewable electricity sources and an electrical grid ill-equipped to handle the mismatch between electricity generation and use, the need for advanced energy storage technologies will continue to grow ^{1,2}. The novel Ground-Level

Integrated Diverse Energy Storage (GLIDES) system was recently introduced and extensively studied analytically ³. A first proof-of-concept prototype in the base system configuration has been demonstrated at Oak Ridge National Laboratory. Previous analytical studies and prototype performance have shown that GLIDES can achieve round trip efficiency in the 66-82% range, and energy density in the 2.46-3.59 MJ/m³ range.

Efforts to drastically increase system energy density are underway, including the use of condensable gases as primary working fluid. A proof-of-concept bench-top prototype utilizing R134a as primary working fluid has been built and initial performance evaluated. These results are presented here.

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Concurrent session 8: Bioenergy

Feedstock Options for Renewable Jet Fuel Production in New Zealand

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New Zealand has an unusual makeup of electricity supply wherein 80% is generated from renewable resources. However, as a nation New Zealand still imports 75% of its fossil fuel based liquid petroleum products.[1] To lower fossil fuel sourced carbon dioxide emissions, it makes sense to transfer more of New Zealand's transportation to electrically powered modes of transport. For airline travel, electrically powered modes of long haul flight appear to be infeasible, and will continue to depend on high energy density liquid fuels. In this paper we explore the possibility of generating aviation fuel from several different renewably based feedstocks in New Zealand. Specifically, three feedstocks will be explored in detail: tallow from beef and lamb; woody biomass from commercial forestry; and purpose grown canola oil. For tallow feedstock, a process based upon Honeywell UOP's patented process [2] was investigated in which the tallow is hydrogenated, deoxygenated and isomerized to create a mix of fuels which were further refined and separated into their various fractions. For the woody biomass feedstock, a gasifier was used to create synthesis gas which was then passed through a Fischer-Tropsch reactor to produce a mix of hydrocarbons. For the third feedstock, purpose-grown canola oil was reacted with methanol in a fatty acid transesterification reaction, and the methyl-esters were upgraded to aviation fuel in a downstream process. A detailed description of the three processes will be given comparing and contrasting the technical benefits and drawbacks of each. Furthermore, the process economics will be explored including projections of both capital and operating costs and the influence of governmental policy and consumer based purchasing decisions

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From concept to pilot-scale demonstration: Thermochemical biomass conversion research at the National Renewable Energy Laboratory

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The National Renewable Energy Laboratory (NREL) is developing gasification and pyrolysis processes for the cost effective thermochemical conversion of biomass to biofuels and biofuel intermediaries. NRELs thermochemical research abilities range from computational modeling to catalyst development through pilot scale demonstrations. Overarching research to support the thermochemical efforts include developing novel pyrolysis oil characterization methods and technoeconomic analyses.

The Thermochemical Process Development Unit (TCPDU) is a 0.5 ton/day pilot plant, used to scale-up and test a variety of technologies including feedstocks, catalysts, and engineering designs. This state-of-the-art thermochemical conversion pilot plant consists of several complementary unit operations that can be configured to accommodate the testing and development of various reactors, filters, catalysts, and other unit operations.

It is capable of being configured for multiple thermochemical biomass conversion pathways including gasification with syngas reforming, fast pyrolysis, and ex-situ catalytic fast pyrolysis.

This research and development pilot-plant is highly instrumented to obtain process measurements, such as temperature, pressure, and flowrates, throughout the entire system. Online analytical equipment, including gas chromatographs, nondispersive infrared detectors, and molecular beam mass spectrometer provide real-time analysis of process stream compositions.

Bioenergy Systems for Sustainable Energy Access

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The lack of access to modern energy carriers and services is the most serious global challenge of the current times. About 3 billion people in the developing countries fall in this bracket and India faces the highest challenge of eradicating energy poverty. Transition to modern energy carriers and services such as electricity and cleaner cooking fuels is not simple. Issues in accessibility, reliability, quality, affordability, availability, and cultural & past preferences can make such transitions difficult. To bring transformations, the need is for implementation of some radical and out of the box solutions. The proposal is to develop an innovative Package of

Solutions which is a blend of local renewable resources, modern technologies, enabling policies, efficient local institutions and inclusive business models. The aim is to combine technologies that produce affordable clean energy, create access to preferred energy services, and at the same time promote productive, income generating enterprises.

In this paper, we discuss implementation of such an approach, which involves adoption of (i) modern bioenergy technologies as effective solution for providing affordable, reliable and adequate access to both electrical and cooking energy, (ii) establishing inclusive and participatory local institutions to build, own, operate and manage the energy services enterprises, and (iii) enable establishment of productive energy use enterprises and livelihood opportunities through modern energy, and several by-products. Next, this approach is subjected through three-pronged evaluation for its effectiveness by assessing (i) implications for energy resources, energy needs and environment, (ii) financial feasibility analysis, and (iii) long-term sustainability of outputs and outcomes. This demonstration attempts to establish, demonstrate and sustain bioenergy led development pathway while simultaneously creating improved lifestyles, value added products, micro-enterprises, markets and grass-root institutions to sustain this path at village scale. Locally available bio-resources will be transformed into clean and modern energy carriers such as electricity and biogas to meet the entire set of energy services required for sustainable human development.

Method for Hot Real-Time Analysis of Pyrolysis Vapors at Pilot Scale

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Biomass Pyrolysis has been an increasing topic of research, in particular as a replacement for crude oil. This process utilizes moderate temperatures to thermally deconstruct the biomass which is then condensed into a mixture of liquid oxygenates to be used as fuel precursors. Pyrolysis oils contain more than 400 compounds, up to 60% of which do not re-volatilize for subsequent chemical analysis. Vapor chemical composition is also complicated as additional condensation reactions occur during the condensation and collection of the product. Due to the complexity of the pyrolysis oil, and a desire to catalytically upgrade the vapor composition before condensation, online real-time analytical techniques such as Molecular Beam Mass Spectrometry (MBMS) are of great use. However, in order to properly sample hot pyrolysis vapors, many challenges must be overcome.

Sampling must occur within a narrow range of temperatures to reduce product composition changes from overheating or partial condensation or plugging of lines from condensed products at cooler temperatures. Residence times must be kept at a minimum to reduce further reaction chemistries during sampling. Pyrolysis vapors also form aerosols that are carried far downstream and can pass through filters resulting in build-up in downstream locations. The co-produced bio-char and ash from the pyrolysis process can lead to plugging of the sample lines, and must be filtered out at temperature, even with the use of cyclonic separators.

A practical approach for considerations and sampling system design, as well as lessons learned are integrated into the hot analytical sampling system of the National Renewable Energy Laboratory's (NREL) Thermochemical Process Development Unit (TCPDU) to provide industrially relevant demonstrations of thermochemical transformations of biomass feedstocks at the pilot scale.

Bioinspired catalysts- mimicking the active site of enzymes

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Enzymes as nature's catalysts exhibit remarkable control over biological reactions and their use in industrial applications is widespread^{1,2}. In particular, the application of the lipase and protease enzyme families in the production of biodiesel has been well established³. The utility of enzymes as industrial catalysts however, is reduced by their low stability, limited operating range and high cost. Despite the complex structure of enzymes, they employ a relatively small functional area- the active site- to mediate their important reactions (Figure 1)^{4,5}. In this presentation I will outline our efforts towards a bioinspired hydrolytic catalyst by mimicking the structure and function of a proteolytic enzyme active site. Our artificial active site (AAS) incorporates the key functional groups present in the enzyme's functional core, and exhibits a significant hydrolytic effect in our selected catalysis assays. Furthermore, the AAS moiety has been used to functionalise a hydrophobic polymer backbone to deliver greater control over the AAS secondary structure and self-assembly in solution. These materials exhibit a wider operating range and increased stability over the natural enzyme, which may provide a novel, efficient and cost- effective route to biodiesel production.

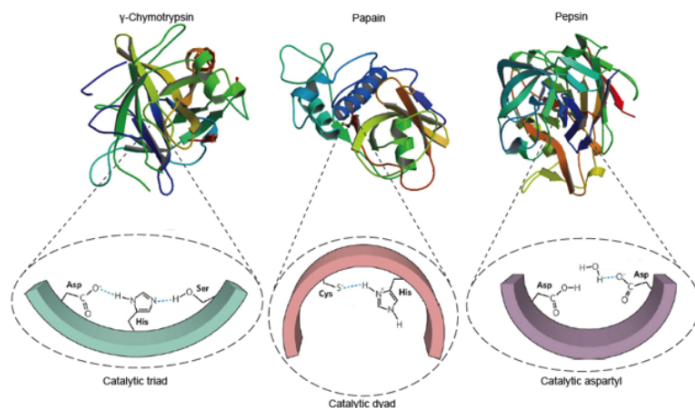


Figure 1: The amino acid residues present in the active site of some proteolytic enzymes. The interplay of these functional groups is chiefly responsible for the catalysis observed by the parent enzyme⁶.

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Making bioenergy sustainable by creating value added by-products – transforming biomethanation outputs

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Bioenergy technologies have always suffered a non-level playing field and usually carry a significant burden of generation costs therefore alternative methods to overcome or offset this imbalance are often required to make bioenergy sustainable. CST has attempted to offset this by converting surplus gas, digested residue (DR) and digester liquid (DL) from biogas plants into value added products (VAP) such that they are not merely sustainable energy options but become economically and socially attractive to its potential rural users. This paper discusses the current status of research and future potential for conversion of biogas digested residue (DR) to edible mushrooms, natural fibers, etc. through secondary processes. About 5 species of mushroom fungi (*Pleurotes*, *Hypsizygus*) have been successfully raised on biogas digested residue and results are encouraging. Also about seven biomass (banana sheath, rachis, leaves; pineapple, Areca, hemp, agave, etc.) feed stocks have been anaerobically digested to biogas, natural fibers and compost. Based on the level of conversions achieved the mass, nutrient and energy balance are discussed to indicate resource, nutrient and economic sustainability that becomes possible through such interventions. Biogas plants operated with single or mixed biomass feedstocks as indicated above could therefore become key-stone technologies that not merely produce a source of sustainable energy but could also be linked to several value added byproducts and local value addition extending the horizons of sustainability for bioenergy.

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Crossing energy borders: from nano-processing using plasmas to nano-plasmas

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Selected examples in this presentation include: 1) Plasma-nano-catalysis [1]; 2) Sustainable, green-chemistry based nanotechnology; and 3) Nano-plasmas generated by intense radiation [2]. In each area, plasma-specific effects and phenomena will be the main points for discussion. For example, in area 1) I will provide some examples of synergistic actions of low-temperature plasmas and nanometer-sized (mostly) inorganic catalysts that lead to value-added products. In area 2), I will introduce the sustainable life-cycles of natural-resource-derived plasma-made nanomaterials. In area 3), I will pose a fundamental question if it is feasible to reduce the size of plasmas, the fourth state of matter, to the nanoscale and will discuss the physical limitations. Some of the interesting effects that arise due to the nanoscale plasma-surface interactions and the interesting properties of the nanostructures [3,4] in relevant cases are discussed. These interactions can be enabled by low-pressure and atmospheric-pressure plasma discharges. One featured example [5] is focused on sub-micrometer graphene microwell structures which are used to improve liquid penetration into tiny gaps. The plasma enables nanoscale texturing of the graphene microwells. This leads to water purification by capturing nanoparticles and to improvement of the performance of supercapacitor electrodes.

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Supercapacitors on silicon and perspectives for integrated energy storage

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It is expected that by 2020 several billions of interconnected “things” will aid the daily life and operations of about 4 billion of interconnected people and businesses. This whole system will require to be powered uninterruptedly in permanence, leading to the necessity of delocalized power sources, seamlessly integrated in the single nodes. Power sources are one of the most challenging units in term of miniaturization, because of the need for large energy storage volumes and the use of materials and electrolytes not always compatible with integration on a semiconductor platform.

We have recently demonstrated a nickel assisted thin film approach to obtain graphene from a SiC surface on silicon wafers. The SiC layer acts as both the template and the source of carbon [1]. The obtained material system can be used as electrode for supercapacitors. We have assessed such approach with different electrolytes, including a solid -state “gel” medium with a 2 V operation window [2]. We will show that this platform offers a broad range of avenues for further improvement, leading to energy densities that are compatible with Li-ion thin film technologies, while also offering key advantages as high reliability, safe operation, and high power densities. This method also eliminates the use of conductive additives and binders. Additionally, the electrodes can be easily patterned at the wafer-level to produce on-chip interdigitated structures.

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The development of an all-climate sodium ion battery

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Large capacity, high power density and low cost energy storage is critical for the electrification of the transportation and energy infrastructures. Recently, many types of rechargeable battery technologies such as aqueous lead-acid batteries based on conversion reactions and organic lithium ion batteries (LIBs) based on intercalation have been developed. However, they both suffer from severe power loss and slow charging at low temperatures. Meanwhile, severe voltage drop at low temperatures could be also detrimental to some electric applications (such as electric vehicles) and cause safety hazards. In this work, we have achieved all-climate high-rate performance of sodium ion batteries by utilizing electrode materials with Na Super Ionic Conductor (NASICON) crystalline structure. A designed NASICON structured carbon-coated $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ (NVP@C) nanocomposite exhibits an excellent performance at high rates in a wide temperature range (i.e., from 20 to 55 °C). Even at a low temperature of 20°C, the NVP@C cathode can still maintain a discharge capacity of 91.3 mA h g⁻¹ or 85.2% of the room performance at 10C, and secure an average output voltage of 2.86 V (vs. Na⁺/Na). These excellent wide temperature accomplishments can be ascribed to fast three-dimensional Na⁺ hopping transportation mechanism in the NASICON structure. The finding in this work offers a promising strategy to address the long-standing inherent wide-temperature issues of rechargeable batteries and extends the potential application of sodium ion batteries.

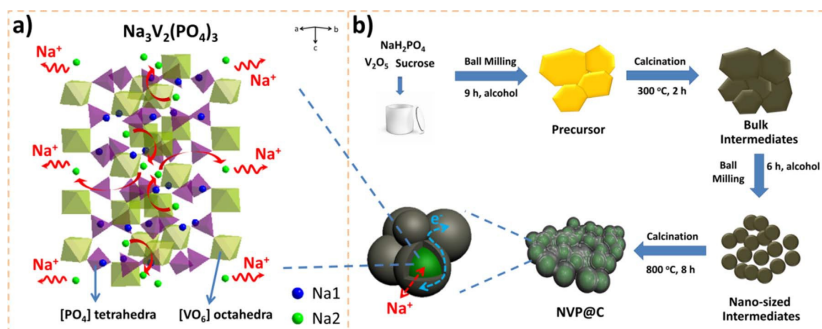


Fig. 1, The Na⁺ hopping transportation mechanism for the all-climate battery (a) and synthesis of the NVP@C nanocomposite (b).

Focused Ion Beam Reduced Graphene Oxide Micro-Supercapacitors with Unprecedented Energy and Power Densities

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Miniaturization of energy storage devices with high energy and power densities can reduce the footprint of micro-devices being used in our daily life. Micro-supercapacitors with planar geometries offer several advantages, such as, the ability to control and reduce the distances ions travel between two electrodes, easy integration to micro devices as the separator and the electrodes are in the same plane, and offer the potential of being extended into 3D without compromising the inter-electrode separation distances. In this study, we have used focused ion beam technology (which is capable of producing reduced graphene oxide patterns and complex shapes in insulating films of graphene oxide with a possible spatial resolution down to ~20 nm in a mask-less and direct write approach) to directly write miniaturized planar electrodes of reduced graphene oxide on films of graphene oxide (GO). We have optimised the ion-beam irradiation and have investigated the influence of ion beam irradiation on the resultant microstructure and the electrochemical properties of the resultant reduced graphene oxide films. Subsequently, using the optimized ion-beam irradiation, interdigitated electrode designs (40 μm long and 3.5 μm wide fingers with ultra-small inter-electrode spacing of 1 μm) have been generated, which have demonstrated a large capacitance (102 mF/cm^2), ultra-small time response (0.03 ms), low equivalent series resistance (0.35 $\text{m}\Omega/\text{cm}^2$), and have retained 95 % of the specific capacitance after 1000 cycles at an ultrahigh current density of 45 mA/cm^2 . These performance metrics show unprecedented improvements on several aspects of supercapacitor performance over existing reports due to the miniaturized electrode dimensions and minimal damage to the graphene sheets. We believe our results can provide opportunities for large-scale fabrication of arrayed, planar, high performance micro-supercapacitors with a small environmental footprint.

Heterogeneous catalysis with MOFs for CO₂ conversion to fuels

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Metal organic frameworks, a relatively new class of porous periodic structures are being investigated as heterogeneous catalysts for the conversion of CO₂ to fuel products. Under typical reaction conditions (usually >300°C and >2 MPa) it has been found that certain MOFs are transformed into metallic nanoparticles (2-10 nm) that are highly active hydrogenation catalysts. By way of example, the MOF MIL-140C, containing 10 % bipyridyl linkers with coordinated Ru(CO)₂Cl₂, was successfully tested as a precursor for a catalyst for CO₂ reduction to methane. The catalyst was found to be stable for up to six days of continuous operation, converting more than 95 % of the hydrogen offered, yielding almost stoichiometric conversion at an overall space velocity of 195,000 ml hr⁻¹ g_{catalyst}⁻¹. This is far superior to a commercially available catalyst employed as a benchmark. Transmission electron microscopy (TEM) studies show that the Ru is highly dispersed in a nanocrystalline matrix of Zr oxides while X-ray photoelectron spectroscopy (XPS) studies indicate that it is in a reduced (Ru⁰) form. These features probably account for the very high activity that is observed.

Australian opportunities for small wind turbines

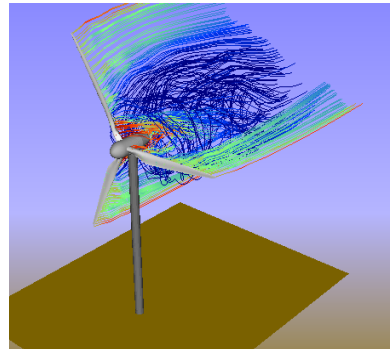
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The wind energy market has witnessed enormous growth in the past. The world's cumulative installed capacity reached 432,883 megawatts (MW) in 2015, from 23,900 MW in 2001 [1], at a Compound Annual Growth Rate of 23%. While most of the attention in wind engineering has been focused on large wind turbines producing energy in the MW range, small wind turbines have been increasing their market share significantly within the last years. While small wind turbines produce less energy than their larger counterparts, they have the advantage that they can be installed almost anywhere on existing structures and can produce the energy right where it is needed, e.g. within urban areas or in remote locations.



This provides an opportunity for Australia, as it provides a method to produce electricity in remote and off-grid communities and allows to diversify from solar power. However, due to the low Reynolds-numbers observed on small wind turbines, the aerodynamic performance suffers and requires optimization. To this end, I will present research directions to improve the usability of small wind turbines and in particular with respect to Vertical Axis Wind Turbines.

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Pellet shaped polyethyleneimine type sorbents for CO₂ post combustion capture

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The post combustion capture (PCC) of CO₂ is considered essential to help mitigate the negative effects of the current global warming trend [1]. Adsorption based technologies are of interest to provide simpler and more energy efficient process designs than incumbent absorption based technologies [2]. Supported polyethyleneimine (PEI) type adsorbents are of particular interest to provide high CO₂ selectivity and capacity, and water tolerance, however, their shaping into pellet forms was found to be complicated by product stickiness and/or extrusion [3]. Recently, we demonstrated novel shaping technology which overcomes these problems; pellets, rather than powders, being preferred for industrial applications [3].

A series of pellet shaped mesocellular siliceous foam (MCF) supported PEI composite powders were thus prepared in accord with the invention; a large volume of one sorbent being shaped via an automated single punch tablet press, demonstrating scalability. The shaped products were subjected to CO₂ partial pressure swing adsorption processing under various conditions, and so, found to exhibit up to ~5 wt % and ~14 wt% CO₂ working capacity for vacuum swing adsorption (VSA) and thermal swing adsorption (TSA) type processing respectively (105 °C), with H₂ ads (CO₂) of ~100 kJ mol⁻¹ (105 – 115 °C). Additionally, the working capacity of the bulk pellet product was found to be maintained after up to 60 hours exposure to a highly wetted simulated flue gas. The sorbents were thus found prospective for CO₂ PCC.

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Predicting key features of a substation without monitoring

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Understanding domestic electricity behaviour has never been more important, hence Distribution Network Operators (DNOs) are installing monitoring devices at the low voltage (LV) substation level. However, monitoring devices need to be allocated with consideration. This paper seeks to quantify the relationship between key information from a substation electricity profile, and type of properties it supplies. Often the number of properties is the most significant predictor for key substation features. Additionally, the proportion of properties which are small-to-medium enterprises (SMEs) affects nearly all key features considered: from the overall load mean and variance, to the annual trend, to peak behaviour.

Do you want to maximise Intellectual Property protection of your Nanotechnology research? Then don't do this...!

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The path that takes a promising laboratory result to commercial success begins with a careful consideration, planning and generally hard work in the laboratory. Protection of Intellectual Property (IP) rights relating to the research can be a key step along the path to commercial success. However, the timing of research and IP protection are often unsynchronised, and mistakes made at the onset of promising research can compromise the ability to capitalise on that finding in the long run.

Scientific Research and IP protection can travel at different speeds, which can make securing IP protection particularly challenging. For example, while it may be advantageous to pre-empt research by competitors with an immediate communication of a relevant result, a premature disclosure of potentially patentable subject matter may preclude its protection in a patent.

This presentation will highlight common oversights by researchers that can limit the scope of IP protection available to an otherwise solid IP position text.

Examples of such oversights include premature or accidental self-disclosures of potentially patentable subject matter, which may occur in circumstances other than publications and conference papers. This presentation will outline an exemplary range of such circumstances as experienced throughout years in assisting researchers seeking IP protection for their research.

On a positive note, premature disclosure or research results may not necessarily be fatal to the ability of seeking IP protection. In that regard, it is important to be aware of legal mechanisms that are available in a number of countries (including Australia) that would limit and contain the loss of IP rights that may derive from a self-disclosure, either intentional or accidental.

The presentation will be of a practical nature and should assist researchers in devising an effective strategy for the management of early discoveries both in terms of disclosing their research and securing effective IP rights.

Scalable Flame Synthesis of Ultra-Transparent and Robust Nano-Layers for Water Oxidation Catalysis

Anotoni Tricoli

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Direct chemical storage of solar energy is an attractive concept for off-the-grid renewable power generation. Currently the poor transparency of the thick low-cost catalyst layers required for water oxidation hinders the large-scale fabrication of efficient photo-electrochemical cells for artificial photosynthesis and hydrogen production. Flame synthesis of tailored nanoparticles and direct aerosol deposition is a scalable technology for the production of ultra-porous layers of photo-catalysts and optoelectronic devices¹. Nevertheless the fragility² of this gas-phase self-assembly has limited their application in liquid environments with most studies requiring the in-situ high temperature annealing of the depositing particle to obtain sufficient mechanical stability. This results in a drastic drop of the layer porosity and hinders the fabrication of optimal architecture for electrochemical systems.

Here, we report the engineering of robust high performance photo-electrodes with tunable porosity and composition.^{3,4} We discuss the critical parameters controlling the self-assembly of these nanoparticle layers and present a flexible approach for their mechanical and chemical stabilization. We apply this concept to the fabrication of photo- and electrochemical cells for water splitting demonstrating very high turn-over frequencies, controllable light absorption and efficient electron collection. We envision that this scalable synthesis approach can be readily implemented for the commercial production of low-cost devices for chemical energy storage and renewable fuel production.

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Solution Processing of Metal Oxide Nanostructures for Plasmonics and Optoelectronics

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Solution processing is an accessible and versatile approach for the synthesis of structurally and chemically controlled nanomaterials. However, the quality benchmarks are mostly set by expensive vacuum depositions. The ability to control the purity, surface chemistry, and microstructure of solution-processed materials will enable to move away from vacuum-based processes, reducing the cost and improving the scalability of material synthesis and device fabrication. This will facilitate the commercialisation of cheaper technologies conducive to highly efficient, large area devices for a variety of energy-related applications, such as solar cells.

In this talk a few strategies to develop metal oxide nanostructures will be presented, along with their applications within optoelectronic devices. First, the scalable synthesis of highly doped plasmonic ZnO nanocrystals will be described, focusing on doping strategies and on the fabrication of infrared plasmonic absorbers and transparent electrodes. Then the aqueous bath deposition of both intrinsic (semiconductive) and doped (conductive) ZnO thin films will be discussed, highlighting the possibility to deposit highly crystalline materials on large area substrates at low temperatures, and with excellent control on their morphological, structural and optoelectronic properties. The high quality of these thin coatings will be demonstrated by using them to replace vacuum-processed buffer layers and electrodes within high efficiency solar cells and light emitting devices.

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Quantitative Femtosecond Charge Transfer Dynamics at Organic/Electrode Interfaces Studied by Core-Hole Clock Spectroscopy

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Organic semiconductors have important applications in organic photovoltaics and other novel hybrid energy-related devices. In organic solar cells, the transport of photo-excited charge carriers across the interfaces between organic molecules and electrodes plays an important role in determining the device performance. Charge transfer dynamics at these interfaces usually occurs at several femtoseconds timescale which presents tremendous challenges to conventional pump-probe based time-resolved techniques. In this talk, I will introduce our recent work in the application of synchrotron-based core-hole clock (CHC) spectroscopy on the quantitative characterisation of charge transfer dynamics in several model organic/electrode systems with relevance to the operation and performance of organic solar cells and molecular devices. 1, 2 The CHC technique allows us to quantify the interfacial charge transfer times with element and site/orbital specificity. Combined with other soft x-ray spectroscopies, it enables us to identify a few critical factors affecting the charge transfer dynamics at organic/electrode interfaces, thus allowing us to rationally engineer the organic/electrode interfaces at molecular scale for enhancing device performances.

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Copper Antimony Sulfide: Nanomaterials, Thin Films, and Solar Cells

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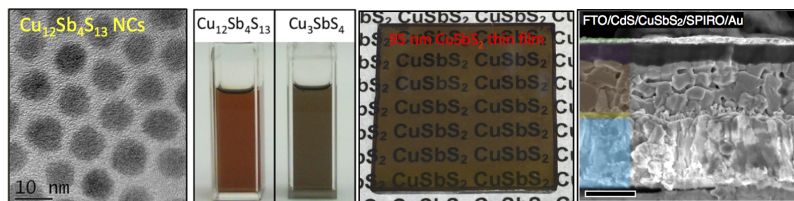
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Solution processing is a low-cost, effective means to produce thin films for photovoltaic (PV) devices.^[1] In an effort to find new materials with properties appropriate for PV devices, the exploration of (nano) materials has recently expanded to include antimony-based semiconductors.



This talk provides an overview of recent work on copper antimony sulfide (CAS) nanocrystals (NCs) and thin films. CAS is a p-type semiconductor with a direct bulk band gap that varies between ~1–1.8 eV depending on the crystal structure. Beginning from the first reported synthesis of a CAS nanomaterial,^[2] the synthetic conditions required to produce CAS NCs and

CAS thin films of various phases is presented alongside comprehensive characterization data.^[3,4] Preliminary data on PV devices is also presented with an outlook on how to improve device performance.^[4]

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Concurrent session 12: Smart grids

Grid independent customers: Challenges and opportunities of PV and storage

Nando Ochoa

University of Manchester (UK) and University of Melbourne (Australia)

Techno-economic modelling the integration of renewables into the grid

Ariel Liebman

Monash University (Australia)

Direct Current Micro Grid Bus Voltage Regulation for Photovoltaic and Wind Integrated Systems

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The rise in energy demand in the grid distribution network and grid isolated areas, the renewable energy sets with micro grid setup trendy to meet the challenge. The electricity generation from renewable sets specifically from photovoltaic cells and wind turbine is of stochastic nature. Since, the demand regulation of voltage output in order to meet the standard load requirements. Therefore an integration of these renewable sets in a direct current micro grid (DCMG) setup has been proposed. This is considered due to practicability and economic viability to transform voltage output in DC and maintain the DC bus voltage at 12V. The simulation of two sources have been considered and maintained at a level of 12V under various conditions. The appropriate dc load has been deployed for DCMG system performance measurements. The results show that the dc voltage level has been maintained satisfactorily at the dc-bus for both loads and sources. Thus, the proposed model is significant for integrating multiple renewable energy sets for dc supply under isolated dc micro grid setup.

Acknowledgement

The authors are grateful to USPCAS – E Peshawar for project grant (USPCAS-E ARG-Dec15-042) to carry out the research. They would also like to acknowledge Mehran UET Jamshoro & UET Peshawar for joint carrying of the project.

Concurrent session 13: Photovoltaics

Nanocarbons in novel solar cells

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One of the most important issues facing society is the ability to supply the world's energy requirements via both environmentally responsible and sustainable means. Renewable energy, and in particular solar energy, has the potential to address current issues in energy production but costs, both in terms of the energy required for production and final price to the consumer, as well flexibility in terms of system deployment are problems that will need to be addressed. This talk will focus on work using carbon nanomaterials to make new architectures for solar cells. Methods to pattern or control the morphology of the nanomaterials will be discussed and the impact on solar cell performance examined. Future directions leading to carbon only solar cells will also be explored.

Interface Engineering of Solution-Processed optoelectronic materials & devices

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Nanophotonics solar cells

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The concept of using photonics nanostructures to manage light in solar cells has offered an unprecedented potential for dramatically increased solar energy conversion efficiency that breaks the previously predicated efficiency limit. To facilitate the transformation of the nanophotonics solar cell concept to a viable high efficiency technology solution for the solar industry, it is essential to address key fundamental as well as practical challenges including the detrimental absorption of metallic nanostructures, narrow band absorption enhancement in the active layer, high cost and scarcity of noble metals and expensive and complicated photonics nanomaterial fabrication and integration methods. In this paper, we present our strategies to use innovative photonic methods to tackle these challenges.

Semiconductor nanocrystals and their application to photovoltaic devices

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Semiconductor nanocrystal is one of the most attractive nanomaterials for solar energy conversion devices. With their relatively large extinction coefficients and a wide light absorption range over visible wavelengths, the nanocrystals can be effective light absorbers. However, despite these attractive properties, when they are employed in solar cells, their function, particularly exciton states, charge separation and recombination dynamics has not been well understood. For example, the excited electron and hole can readily be trapped by the surface states, losing initial excited energy, however their relations to the solar cell function is not clear. In this presentation, we will discuss underlying key parameters controlling interfacial charge separation and recombination dynamics [1,2], and relationship of the nanostructures with the interfacial electron transfer reactions [3].

Several types of narrow band gap nanocrystals with a narrow size distribution are synthesized to control the potential energy levels of the conduction and valence bands. We analysed influence of nanocrystal surface states on the interfacial charge transfer dynamics [3], and their interfacial structure is modified to control the dynamics.

This work was financially supported by the JST PRESTO program (Photoenergy Conversion Systems and Materials for the Next Generation Solar Cells) and by JSPS KAKENHI Grant Number JP16K05885, Japan. The author also acknowledges Australian Research Council (ARC) LIEF grant (LE140100104) and the Office for University-Industry Collaboration, Osaka University, for the financial supports.

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Molecular engineering approach for designing nonfullerene acceptors

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Ionic liquid-based redox electrolytes for thermal energy harvesting

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Thermoelectrochemical cells are increasingly promising devices for harvesting waste heat, particularly at temperatures <200°C such as from power plants or geothermal sources. This technology offers the promise of continuous and cheap operation, with low maintenance and no carbon emissions. Thermoelectrochemical cells utilise two electrodes, held at different temperatures, separated by an electrolyte containing a redox couple. The temperature dependence of the electrochemical redox potential results in a potential difference across the device. The magnitude of this temperature dependence is given by the Seebeck coefficient, S_e .

Until recently, research into thermoelectrochemical cells had primarily focused on aqueous media with the ferri/ferrocyanide redox couple.¹ However, the good thermal and electrochemical stability, non-volatility and non-flammability of many ionic liquids (ILs) makes them promising alternative electrolytes for these devices. Potential advantages include increased thermoelectrochemical device efficiencies, longer lifetimes and the ability to utilise waste heat in the 100 – 200°C temperature range.

Here we discuss our research into the influence of the IL on the temperature-dependant thermodynamics of Co^(II/III) redox couples. We also discuss how different solvent/IL mixtures can yield significant improvements in thermoelectrochemical cell power output.²

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Enhancement of Seebeck Coefficient of Thermo-electrochemical Cell by Supramolecular Chemistry

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Energy harvesting from natural source is one of the important agenda in today's world. We focused on thermo-electrochemical cells (TEC) that can generate electric power by the difference of electrochemical potential between hot and cold electrodes. We report the novel method to improve the Seebeck coefficient of the TEC by using host-guest chemistry. We added α -cyclodextrin (α -CD) into iodide / triiodide TEC system (Fig. 1). α -CD captures the I_3^- at low temperature and releases it at elevated temperature. The capture and release of I_3^- evokes the difference of concentration of the triiodide ion between both electrodes, which makes difference of voltage according to Nernst equation. We succeeded in enhancing Seebeck coefficient of I^-/I_3^- TEC from 0.8 to 1.4 mV K⁻¹ by the addition of α -CD.¹

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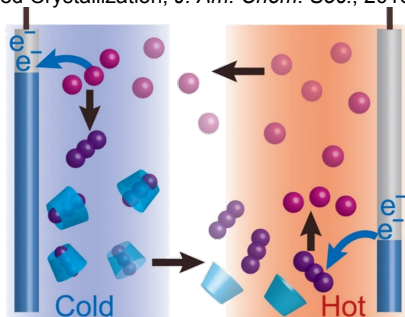


Figure 1 Scheme of Host-guest thermos electrochemical cell

White-Light Light-Emitting-Diodes using Carbon Nanodots

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Current progress in white-light light-emitting diodes (LEDs) technology, which is a green innovation of this 21st century, relies on the mixture of blue-LEDs emission with green and red lights that are down-converted within the 'phosphors' (rare-earth materials) coating under blue excitation to generate white-light illumination. However, the need of costly 'phosphors' defeats the purpose of energy saving and reduction of carbon emission. The restriction of dirty mining and refining contributes to the high production cost and inevitable environmental damage. Hence, it is necessary to replace 'phosphors' with eco-friendly and abundant element like carbon.

Recently, researchers had discovered that graphite of nanometer sizes (i.e., carbon nanodots) coated with organic passivation exhibits unexpected behavior – intense visible light emission under either optical or electrical excitation at room temperature. This luminescence behavior of nanostructured carbons can in fact replace 'phosphor'. In this presentation, we would like explain how to i) optimize the optical and physical characteristics of nanostructured carbons, ii) to use different approaches to obtain intensive light emission from the nanostructured carbons and iii) to realize remote carbon-nanodots white-light LEDs. The impact of our effort will not only generate new knowledge in using nanostructured carbon as light-emitting devices, it will also contribute to the development of low-cost and environmentally friendly solid-state lightings.

Is the Imidazolium Cation a Unique Promoter for Electrocatalytic Reduction of Carbon Dioxide?

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There has been considerable recent interest in the use of the imidazolium cation as a promoter in the heterogeneous and homogeneous electrocatalysis of CO₂ reduction. However, despite its widespread use for this purpose, the mechanism by which imidazolium operates is not yet fully established. The present work reveals that enhanced catalytic activity is achieved by addition of many cations other than imidazolium. Under cyclic voltammetric conditions at a Ag electrode in acetonitrile solutions (0.1 M *n*-Bu₄NPF₆), 2.0 mM concentrations of imidazolium, pyrrolidinium, ammonium, phosphonium and (trimethylamine)-(dimethylethylamine)-dihydroborate cations can all enhance the kinetics of catalytic CO₂ reduction with imidazolium and pyrrolidinium being the most active. Analysis of the voltammetric data suggests that imidazolium cations achieve their impact by directly acting as co-catalysts with Ag whereas the other cations affect the reaction rate by modifying the electrochemical double layer. The results also confirm that the active form of the co-catalyst is the reduced imidazolium radical which forms a complex with CO₂ before being further reduced to CO or other products at Ag and not an imidazolium carboxylate formed between an imidazolium carbene and CO₂. In fact, imidazolium is deactivated during CO₂ reduction by the latter reaction. Addition of water inhibits this deactivation pathway allowing the imidazolium cation to act as in a long term for CO₂ reduction. In contrast, the pyrrolidinium cation, where enhanced catalysis is attributed to an electrochemical double layer effect, retains its catalytic activity for very long periods of time regardless of the presence or absence of water.

A scale factor model for the design of spiral coil-type horizontal ground heat exchangers

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Owing to the higher heat transfer performance, the spiral coil-type horizontal ground heat exchangers (HGHEs) have been increasingly used in a ground source heat pump (GSHP) system. Many researchers have conducted field tests and simulations in order to investigate the heat transfer mechanism and established design methods for the spiral coil-type ground heat exchanger. However, there is a limitation to widely utilize the proposed methods as a universal design method for HGHEs because of its complexity. Therefore, a scale factor model, which could be used to design the coil-type exchanger based on the design length of line-type heat exchanger, was presented in this study. With the consideration of various design factors, the ratio of mean thermal transfer energy between the line-type and spiral coil-type heat exchangers was investigated numerically.

The three dimensional finite element model was developed using COMSOL multiphysics. The effect of shape of heat exchanger, ground thermal properties, and weather conditions was also investigated. Based on the numerical results, the artificial neuronal network (ANN) was employed for the model development. The scale factor model was then validated using the numerical and field experimental results. The proposed scale factor may provide a fast and efficient way for the design of spiral coil-type HGHEs design.

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POSTER SESSION

Application technology of TEC (Tidal Energy Converter) in low velocity environmental regions

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Various types of renewable energy have been introduced with great international efforts to reduce carbon emission. The importance of renewable energy development has been increased with great concern for global climate changes. Ocean energies have a high potential to substitute fossil fuel considering the large amount in the earth. Tidal energy is considered as a reliable, sustainable and predictable energy source. Even tidal barrage is also predictable energy, many projects in the world have been delayed or cancelled due to significant environmental impacts. Tidal current power is now regarded as one of the best ocean energies with the minimum environment impact. As the energy is proportional to cube of current speed, a duct implementation can increase the inflow velocity resulting in higher power production. This approach can extend the application to tidal energy in relatively low current regions. The effect of duct is dependent on various parameter including its configurations of inlet and outlet, inner and outer diameters, overall length, etc. Also to reduce the cost, the mooring system can be applied to secure the TEC (Tidal Energy Converter) at the location. As the floating concept for TEC can improve the economic feasibility, it is very important to understand the dynamic behavior for various flow attack conditions. In this research study, the optimized duct has been designed for a floating TEC and the extensive CFD analyses based on the hydrodynamic coefficients in frequency domain using impulse response function (IRF) method, Orcaflex software and Matlab together with the physical model test in a circulating water channel (CWC) are introduced. Also the actual field application of a duct TEC installed at a low current region is introduced in the paper.

Acknowledgement

The work was supported by the project titled "Manpower training program for ocean energy" funded by the Ministry of Oceans and Fisheries, Korea (KIMST) and also the project titled "Development of active-controlled tidal stream generation technology" funded by the Ministry of Oceans and Fisheries, Korea (20110171)

Optimising the Performance of Thermoelectrochemical Cells

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Thermoelectrochemical cells are a promising energy conversion technology for utilizing waste heat. Low grade waste heat (<200°C), such as that generated by industrial processes, represents a large source of potential energy. Thermoelectrochemical cells can convert this thermal energy to electrical energy via the formation of a temperature gradient across a cell containing two electrodes in an electrolyte containing a redox couple. The temperature gradient between the two electrodes creates a potential difference due to the temperature dependence of the redox potential. This causes the reduction and oxidation of the redox couple, generating a continuous power output.

The performance of thermoelectrochemical cells is determined by different properties of the system, including the redox couple, the supporting electrolyte and the electrode material. Recently, research focus has shifted from aqueous electrolytes ¹ to non-aqueous electrolytes, particularly ionic liquids (ILs). ILs offer many advantages over aqueous electrolytes, namely, good electrochemical stability, low volatility, non-flammability and higher operating temperatures ².

In this work, the optimization of thermoelectrochemical cell properties for high performance is investigated. This includes examining the effects of different redox couples and electrolyte compositions on the performance of these devices.

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Energy, Culture & Institutional Networks: Residential Solar Energy and Islandic Energy Regimes

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Small-islands are unique geographies that by their very nature have traditionally had finite resource portfolios, and cultural identities attached to these resources and the lack thereof. Therefore the local availability of economically valuable though also limited resources like fossil fuels is a major determinant of their sustainable energy transition evolution.

The research focuses on the island of Trinidad in the Caribbean referencing the neighbouring Barbados, as well as Oahu in the Pacific-Oahu and Barbados having no substantive fossil fuels unlike Trinidad. The three islands are in turn at three different points along their residential solar energy transitions.

The research subsequently compared residential electricity actor-networks, innovation-mainstream dichotomies, and residential energy cultures (norms, material culture, and practises) to tease out the lessons-learned and knowledge-transfer opportunities existing within such insular regimes.

Oahu and Barbados' import bills have consequently incentivized residential solar but Trinidad has instead nurtured a path-dependent institutional orientation that has yet to adopt it. This comes with a concurrent cultural evolution centred on convenience and energy-complacency- historically reinforced by subsidized electricity tariffs.

Energy, and electricity were thought to be separate semantic domains with the former defined by notions related to 'oil and gas' and the latter, lifestyle-salient energy services. However, energy is synonymous with electricity in the residential energy culture and is energy service-oriented through norms tied to cultural perceptions and even misconceptions surrounding peak demand, appliance ownership, and electricity billing.

So as a regime that has had no prior interaction with distributed residential solar energy, its introduction would need to be increasingly practical, transparent and affordable at both the institutional and cultural levels.

Nitrogen-doped Activated Carbon derived from biomass for High Performance Lithium-ion Supercapacitor

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Developing advanced energy storage device has become an urgent demand in various fields, such as electrical vehicle, portable electronics and power grid [1]. Among different energy storage device, Lithium-ion battery (LIB) and supercapacitor (SC) have attracted tremendous attention. LIB can deliver high energy density while exhibit a low power density [2]. In contrast, SC can provide higher power density with a relatively poor energy output. In order to bridge the gap between these two devices, a novel energy storage apparatus called lithium-ion capacitor (LIC) is proposed. LIC, which combine capacitor-type electrode (activated carbon) and lithium ion battery-type electrode (graphite, silicon and transition metal oxide), can provide high energy while maintain the power density [3].

In this work, nitrogen-doped activated carbon with high surface area was achieved from biomass by a facile activation and carbonization process. A LIC was assembled utilizing the AC as cathode and Si/C composite as anode. This device shows high energy density, high power density and good cycling stability.

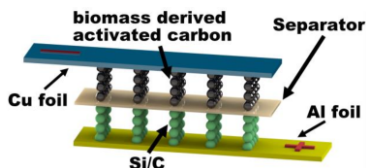


Fig.1 Schematic illustration of the LIC.

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New Cobalt-based Redox Active Ionic Electrolytes for Thermal Energy Harvesting.

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Thermoelectrochemical cells are devices capable of converting heat directly into electricity. The conversion of energy is based on the Seebeck effect: when a temperature gradient is applied across two identical electrodes in contact with a redox active electrolyte, a potential difference is created. The Seebeck coefficient S_e of a redox couple is related to the entropy change of the redox reaction, and is given by: ¹

$$S_e = \frac{\Delta V}{\Delta T} = \frac{\Delta S_{rc}}{nF}$$

In recent reports ionic liquids have been investigated as electrolytes, to overcome the high temperature limitations and volatility problem associated with aqueous systems. Previous work in our group has demonstrated high Seebeck coefficients in ionic liquids using a cobalt bipyridyl redox couple. ² We report here the use of new cobalt (pyridine-pyrazole) redox complexes in ionic liquid electrolytes for thermal energy harvesting applications. In this work we look into the fundamental effects of redox couple structure on the Seebeck coefficient as well as device performance. The effects of redox couple concentration on performance are discussed. In addition, we demonstrate a stable and continuous device energy output over time.

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Effect of feedstock, temperature and residence time on pilot-scale pyrolysis products

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The Thermochemical Process Development Unit (TCPDU) at NREL is a thermochemical pilot-scale process currently focusing on conversion of cellulosic biomass to liquid fuels. This paper explores the impact of changing feedstock, temperature and residence time on pyrolysis production, in particular quantifying the effects on chemical composition and physical characteristics of the resultant oil and char. Four feedstocks –oak, clean pine, and two, low-cost blends with varying ratios of clean pine, construction and demolition waste, forest residues, and switchgrass – were pyrolyzed at two reaction temperatures (500°C and 480°C) and two residence times (~3.5 seconds and ~2.9 seconds). Multiple tests were performed to characterize the oil and char products, complementing the online analysis of the hot pyrolysis vapors and light gases. The results show greater differences in the pyrolysis oil between feedstocks than between operating conditions using the same feedstock.

Hybrid organic-inorganic perovskite solar cells: Investigations in varying the metal-oxide and polymer additives

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Perovskite based solar cells have gained significant worldwide interest due to their remarkable efficiencies demonstrated within a short period of time. Investigations in this field are still at an early stage with much exploration and optimisation efforts required. In this study we investigate hybrid lead halide perovskite solar cells fabricated with poly (3-hexylthiophene) (P3HT) polymer as the hole transport material. This study investigates variations to the concentrations of additives tert-butylpyridine (tbp) and lithium bis (trifluoromethanesulfonyl) imide (Li-TFSI) in the P3HT film. We also investigate varying the TiO₂ metal-oxide nanoparticles in the nanoporous film. We compare the standard nanoparticle paste used in many studies (DSL-18NRT) in comparison with a novel TiO₂ paste (DSL 30-NRD) with larger nanoparticle size (30 nm). Performance variations in the perovskite devices with different metal-oxide layer thicknesses are also investigated in order to optimise the perovskite device with polymer hole transport layer.

Will the Integration of Renewables enable Sustainable Transition of Indian Electricity System?

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Electricity systems worldwide are transitioning from conventional carbon intensive firm power generating systems to intermittent and variable renewable energy dominated low carbon systems. Although the dimensions of the transition vary from one electricity system to another, there is concurrence in terms of need for and the subsequent issues related to renewable energy integration and the enabling operational regimes. In this research, an attempt is made to verify whether these transitions lead to a sustainable electricity system as measured through three dimensions – economic, social and environmental. This is performed by adopting an integrated framework which connects the indicator based multi-hierarchical and multidimensional macro model of electricity system sustainability assessment with the bottom up optimization model of electricity system generation expansion planning and generation scheduling, and implementing it in the context of Indian electricity system. We explore multiple scenarios for a planning horizon of 18 years till 2032, and characterize Indian electricity system on select indicators under three dimensions of sustainability for each year. We aggregate this annual characterization of Indian electricity system to compute National Electricity System Sustainability Index (NESSI). NESSI value for base year is 0.377 (2013) and within the select scenarios, NESSI value in the terminal year (2032) varies from 0.481 to 0.504. We observe that although renewable energy is not selected in the cost optimal expansion plan, its compulsory deployment results in better NESSI value. This is due to the positive impact of renewable energy integration on environmental sustainability, which more than offsets the negative impact renewable energy integration has on other NESSI dimensions. We throw some light on how the important questions concerning generation technology pathways for electricity system sustainability transition are queried and the underlying choices this process involves.

Concentrated Li-doped plastic crystal and polymer nanofibre based composite electrolytes: Ion transport and Li battery studies

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Safer electrolytes for better energy devices such lithium batteries and dye-sensitized solar cells are in urgent need. Organic ionic plastic crystals (OIPCs) are a class of solid-state electrolyte material with good thermal stability, non-flammability, non-volatility and good electrochemical stability. These materials deform easily under stress and can also allow fast transport of ions such as Li^+ through the rotational and translational motions of the matrix ions. Doping with lithium salts can increase the conductivity¹, and makes them increasingly promising for future energy storage applications².

However, waxy or powdery OIPCs cannot form a flexible membrane. Using electrospun polymer fibres as a matrix is a viable way of developing all-solid-state, free-standing and flexible electrolytes. We have recently reported that the plastic crystal N-ethyl-N-methylpyrrolidinium tetrafluoroborate ($[\text{C}_2\text{mpyr}][\text{BF}_4]$), doped with lithium tetrafluoroborate (LiBF_4) and combined with electrospun PVdF fibers can successfully support stable lithium cell cycling, with a capacity over 140 mAh g^{-1} . The conductivity was also enhanced with incorporation of the PVdF³. To further the development of such composite electrolytes, it's important to investigate the influence of polymer nanofibre on the thermal, structural, morphological, and electrochemical properties of OIPCs. Further, understanding the influence of composite composition on electrolyte parameters such as Li transference number, battery cycling performance and stability is key.

In this study, 1:1 (mole) LiFSI doped $[\text{C}_2\text{mpyr}][\text{FSI}]$ and PVdF electrospun nanofibers were successfully developed as composite electrolyte membranes (Fig 1.). The effects of PVdF incorporation in the Li-doped plastic crystal were investigated by differential scanning calorimetry, impedance spectroscopy, SEM, and nuclear magnetic resonance. The optimized ratio was determined to be 8wt%PVdF-92wt% ($[\text{C}_2\text{mpyr}][\text{FSI}]$ -50mol%LiFSI). Use of a thicker electrolyte membrane supported lithium symmetric cell cycling at a current density of 0.13 mA/cm^2 at 50°C and ambient temperature.



Fig 1. Flexible composite electrolyte

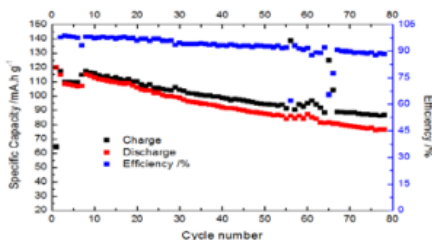


Fig.2 Cycle at room temperature

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Meeting the energy needs of the village using biomass - concept to implementation

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The project 'Rural hybrid energy enterprise system' (RHEES) adopts both a targeted R&D and technology demonstration through participatory enterprise models. The concept involves meeting all rural energy needs and energy services required for modern-day and emerging life-styles to be met predominantly from bioenergy technologies wherein we firstly prove on ground their optimally combined operation to demonstrate resource and end-use sustainability. This concept is meant to transcend most of the conventional rural energy program conceptualization and implementation by evolving bioenergy technology and bioenergy service packages and rural enterprise institutions that create, institutionally aggregate and market various value added products from these bioenergy technologies such that in addition to energy and energy services, there are various saleable outputs that greatly enhance the economic viability capabilities that were difficult to achieve in the past. This paper presents three novel components not hitherto included in typical renewable energy projects namely biogas from herbaceous biomass feedstocks for family use, multiple forms of value-added byproducts emerging from biogas and gasification units that make bioenergy economically viable. Finally many participatorily derived micro-enterprises for bioenergy and value added products that make them socially sustainable are described and assessed.

Chanakya HN (2015). Towards a biogas centric bioenergy system for rural Asia. *MGIRED Journal* 2015. 1, 67-79. ISSN 2393 9605

Pyrolysis of mallee wood residue after washing with bio-oil

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Pretreatment of biomass prior to pyrolysis is an important way to modify the structure and property of biomass, which could change the yield and quality of bio-oil from the pyrolysis of the treated biomass. This study aims to investigate the effects of biomass pretreat on the yield and composition of bio-oil. Mallee wood biomass was washed with different fractions of pyrolysis bio-oil of the same biomass. The pre-treated biomass was then pyrolysed in a fluidized bed reactor. The washing procedure was effective in reducing the inorganic contents of the biomass. The washing has resulted in significant changes in the yields of pyrolysis products as well as the composition of bio-oil. While the yield of some bio-oil components decreased, those of other components decreased.

Keywords: bio-oil, pyrolysis, pre-treatment, composition, mallee biomass

Phase behaviour and electrochemical performance of phosphonium plastic crystals mixed with sodium salt

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Organic ionic plastic crystals are highly promising solid state conductors for battery applications which have attracted much attention recently. Their unique properties include various solid-solid phase transitions before melting which cause a disordered phase after each transition. Combined with negligible volatility, electrochemical and thermal stability these properties have prompted researchers to investigate different kinds of OIPCs, especially for Li device applications. Due to some advantages of Na batteries versus Li devices, (including potential cost and safety) this work focuses on a study of the physicochemical and electrochemical behaviour of the phosphonium cation organic ionic plastic crystal (OIPC) triisobutyl(methyl)phosphonium bis(fluorosulfonyl)imide (P₁₁₄₄₄FSI) (figure 1) and NaFSI mixtures. We determine their phase behaviour and try to attain a fundamental understanding of the structure and dynamics in these systems, and finally investigate their application as Na battery electrolytes.

The phase behaviour of these novel materials has been determined over the whole composition range using Differential Scanning Calorimetry (DSC). In order to acquire information about the morphology and topography of the materials, Electron Microscopy (SEM) was used. The ionic conductivity measurements have also been conducted on the pure OIPC and several compositions for the mixtures, using electrochemical impedance spectroscopy (EIS). Na symmetric cells were constructed to study the ability of the electrolyte to cycle Na metal with good efficiency.

The partial phase diagram for the P111i4 NTf2/NaNTf2 binary systems is determined and shows complicated phase behaviour with depression of the melting point upon NaFSI addition, suppression of crystallisation in the middle of the phase diagram, and finally a higher melting point at compositions beyond 60mol% NaFSI. This work indicates that solid state sodium batteries can be developed using a solid state Na ion conductor based on OIPCs.

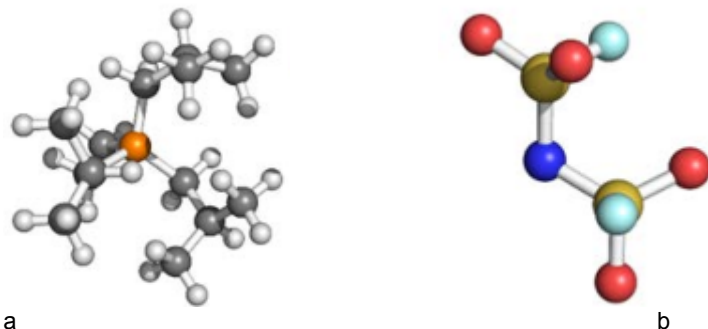


Figure1. Structure of (a) $[P_{1444}]^+$ and (b) $[FSI]^-$

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Roll-to-Roll Printed Silver Nanowire Semitransparent Electrodes for Fully Ambient Solution-Processed Organic Solar Cells

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A combination of silver nanowires (AgNWs) and zinc oxide (ZnO) is demonstrated as a cost-effective replacement of ITO for OSCs [1]. AgNWs/ZnO are deposited on flexible substrates using fast roll-to-roll (R2R) printing in ambient conditions. OSCs are further fabricated on this electrode on a laboratory roll-coater using all additive printing and coating methods under ambient conditions. These processing conditions are directly transferrable to large-scale R2R processing upon availability of materials. Additionally, AgNWs/ZnO is compared with a previously reported large-scale printed ITO alternative known as Flextrode which comprises polyethylene terephthalate (PET)|silver grid|poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS)|ZnO. The results indicate AgNWs/ZnO is a significant improvement over Flextrode. It has >80% uniform integrated optical transmission which takes both the diffusive and the direct components of transmission into account. The corresponding sheet resistance was 10-20 $\Omega \square^{-1}$. These attributes lead to higher power conversion efficiency in OSCs on AgNWs/ZnO than on Flextrode. The effect of higher transmission is especially pronounced in tandem cells which shows up-to 80% improvement in efficiency than Flextrode.

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Towards Higher Energy Density Redox Flow Battery: Imidazolium Ionic Liquid for Zn Electrochemistry under Flow Environment

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Currently, Redox flow batteries (RFBs), such as all vanadium and Zn-Br, are limited to stationary energy storage applications due to low practical energy density resulted by poor solubility of active materials, dendrite formation and corrosive nature of acidic solvents. This has initiated the search for novel electrolytes to overcome these limitations. Ionic liquids (ILs) constitute a promising type of electrolyte composed entirely of ions, and are liquid below 100°C; and depending on the composition they can offer many advantages such as chemical and electrochemical stability, ionic conductivity, safety due to negligible vapor pressures and non-flammability.¹ Previously, our group has successfully demonstrated reversible Zn deposition and dissolution at low onset potential (0.23 V) with 1-ethyl-3-methylimidazolium dicyanamide, [C2mim][dca], resulting high current densities (32/61 mA/cm² - red/ox) under static conditions.² The presence of 3 wt% H₂O in the IL mixture was found to be crucial for obtaining a uniform, dendrite free morphology.² Our research will present the first demonstration of Zn electrochemistry in IL under real flow conditions. The higher [Zn²⁺] was found to be favourable under flow due to lower onset potential for Zn deposition/dissolution (0.18 V), high discharge peak current densities (100mA/cm²), higher cycling efficiency (45 ± 3%) and uniform morphologies. Further results on the effects of salt concentration and flow rate on Zn cycling performance and deposition morphology will be discussed.

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Air bubble frequency distribution in the cavity zone

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As a clean and safe energy, hydroelectric power, together with thermal power and nuclear power, constitute three central pillars of the power in today's world. In design for large-discharge chutes of the dam, it is necessary to prevent the risk of cavitation erosion. Therefore, spillways and flood-discharging tunnels are usually equipped with chute aerator, which is quite widespread as it has been proved to be a successful countermeasure in the Grand Goulee Dam since 1960. Chute aerators separate the flow from the chute bottom, and air can enter into the flow through the lower surface in the cavity zone due to high turbulence eddies close to the air-water interface. In this paper, the chute in the downstream of an aerator was partitioned into four zones: the cavity zone, the impact zone, the disjointed zone and the far zone. A series of experiments were carried out on the air concentration distribution. In the cavity zone, the air bubble frequency distribution was similar to the air concentration distribution. The air bubble frequency increased from the bottom and then decreased near the unaerated black water region. The position of the maximum air bubble frequency f_{\max} moved downwards. In the cavity zone, the position of the maximum air bubble frequency was generally in the region of high air concentration, where bubbles were the main type of air-water structure because of the water drops. At the air-water cross section, the relationship between the air bubble frequency and the air concentration was self-similar; the position of the maximum air bubble frequency caused by the air-water discontinuity gradually approached $C=0.50$ with the development of aeration. Meanwhile, the dimensionless air bubble frequency in the cavity zone followed a parabolic function of $f/f_{\max}=4C(1-C)$, where C was the air concentration.

Keywords: chute; air bubble; air concentration; frequency

Fabric heat-gain assessments of building walls with alternative options of PCM and insulation

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Heat gain assessment of a building is a prime factor estimating the overall building electrical power consumption. There are various factors which affect the heat gain profile of a building. Present study attempts to assess some of the strategies which are utilized as building load abatement factors pertaining to thermal comfort and electrical power consumption. The study brings forward the efficacies of various options ranging from ordinary brick wall to Phase Change Materials (PCM) integrated wall constructions having the ability to store large amount of heat at constant temperature. A parametric analysis comparing four different types of ASHRAE compliant PCMs integrated walls has been carried out to compare them with standard thermally insulated walls. Effects of climatic variation pertaining to various climatic zones have also been studied to approach the best possible design.

Efficacy of CFD in estimating thermal behaviour of a naturally ventilated house

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“Analysis led design” helps us to understand the system behavior without the actual system construction. With rapid urbanization and stringent energy conservation building codes, it is essential that a detailed understanding of the building physics be made before the actual building constructions. Therefore computational analysis becomes a very useful tool to predict such system behaviors where massive urbanizations are envisaged. Present study is attempted to describe the efficacies of CFD as an “Analysis led design” tool, where a computationally modelled house is analyzed to estimate the energy consumption patterns, thereby providing opportunities in rectifying any anomalies pertaining to it, prior to the actual construction. The house considered in the present study, numerically analyses the effects of natural ventilation through the established PMV model [1] specifically describing the thermal comfort and indoor air quality.

A genetic algorithm approach for modelling low voltage network demands

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Distribution network operators (DNOs) are increasingly concerned about the impact of a low carbon future on the low voltage (LV) network. Smart meters can potentially provide better analysis of LV networks through power flow modelling. However, such data may not be readily available for DNOs. If not, it may need to be purchased for all customers, which could be expensive. In this poster we outline some simple methods for modelling a large number of unmonitored residential customers at the LV level. We do this by buddying these customers with a limited number of monitored customers who have smart meter data. Hence the presented methods require a significantly smaller amount of data to model all LV end points with half hourly resolution data. Using real LV network modelling we show that our methods perform significantly better than a comparative benchmark for modelling half hourly energy demand, and gives a fuller picture of the peak demand behaviour compared to standard planning measures currently used by DNOs.

Proton Conducting Membranes for Energy Applications

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Proton conducting membranes are one of the most crucial components in several electrochemical applications such as fuel cell, flow battery and CO₂ reduction etc. Nafion, with high proton conductivities and proven stability is the most commonly used proton conductors. However, operation condition of the Nafion membranes and derivatives was limited under 100°C due to the presence of water being an essential condition for its high proton conductivity. Thus, solid-state anhydrous proton conductors are being sought.

The organic ionic plastic crystals (OIPCs) have emerged as a novel solid-state ionic conductor, with unique plastic phase that ensure good mechanical flexibility and improved contact between electrodes and electrolyte. [1] In addition, intrinsic ionic conductivity, non-flammability, good thermal stability and wide electrochemical windows are all desirable properties obtained by OIPCs. [1-2] Forsyth and MacFarlane groups have developed knowledge of the proton transport behaviour in electrolyte materials which are important for the design and development of novel

solid electrolytes for electrochemical device application.

In this work, we investigate thermal properties, phase behavior, ionic conductivity and proton transport behavior of the protic organic salts DMEDAH Tf and DMEDAH₂ Tf₂, in order to achieve a fundamental understanding of the relationship between chemical structure/composition of protic organic salt based electrolyte and their proton conductivity.

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High-Performance Perovskite Solar Cells Based on Carbon Nanotubes Incorporated TiO₂ Nanofiber Photoelectrodes

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One dimensional (1D) semiconducting oxides are unique structures that have been widely used for photovoltaic (PV) devices due to their capability to provide a direct pathway for charge transport. In addition, carbon nanotubes (CNTs) have played multifunctional roles in a range of PV cells because of their fascinating properties. Herein, the influence of CNTs on the PV performance of 1D titanium dioxide nanofiber (TiO₂ NF) photoelectrode based perovskite solar cells (PSCs) is systematically explored. Among different types of CNTs, single-walled CNTs (SWCNTs) incorporated in TiO₂ NF photoelectrode PSCs showed a significant enhancement (~40%) in the power conversion efficiency (PCE) as compared to the control cell fabricated with TiO₂ NFs-only. Highly conductive SWCNTs incorporated in TiO₂ NFs provided a fast electron transfer within the photoelectrode, resulting in an increase in the short-circuit current (J_{sc}) value. On the basis of our theoretical calculation, the improved open-circuit voltage (V_{oc}) of the cells can be attributed to a shift in energy level of the photoelectrodes after the introduction of SWCNTs. Furthermore, we found that the incorporation of SWCNTs into TiO₂ NFs reduces the hysteresis effect and improves the stability of the PSC devices under ambient conditions (>60% humidity). The best performing PSC device constructed with SWCNT structures achieved a PCE of 14.03%.

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Tuning Photon Up-conversion with New Molecular Geometries

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Photon upconversion based on triplet-triplet annihilation (TTA) is a promising light wavelength-tuning route to enhance the efficiency of all solar cell devices by converting long wavelength (low-energy) light to short wavelength (high-energy) light.¹ However, most efficient TTA upconversion

is achieved in solution to allow the fast diffusion of chromophores. This is extremely impractical for real-world applications. Therefore, we are investigating materials design for solid-state upconversion. Conventional solid-state upconversion systems suffer from limited excited state energy mobility and the aggregation or phase separation of chromophores. In addition, two or more emitter molecules should be close enough (< 1 nm) to

realize efficient TTA, and further efficient upconversion.² Moreover, materials design demands intense absorption of the excitation light, long triplet lifetime and high upconversion quantum yield for TTA upconversion. A series of new molecular geometries with multiple emitters are designed and aim to realize efficient TTA upconversion through intramolecular energy

transfer in diffusion-free system. Furthermore, the relationship between molecular geometry and TTA upconversion efficiency will be investigated, and efficient solid state upconversion solar cell devices will be developed ultimately.

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Development of nanoparticle-based Electrolytes for Thermal Energy Harvesting

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Thermogalvanic cells, which are also known as thermocells, are a method for conversion of thermal energy directly to electricity. ¹ Research on thermocells is mostly limited to using liquid electrolytes. ²⁻⁴ In spite of reasonable performance of cells containing liquid electrolytes, resulting from the high ion conductivity, their application in thermocells suffers from potential leakage, volatility and flammability problems. These problems can be addressed by solidification of the electrolyte, but the application of solid electrolytes in thermocell technologies has not yet been thoroughly investigated. The development of a safe electrolyte with no leakage problems can provide an opportunity for commercialisation and application e.g. in industrial sectors.

Here we report the development of solid nanoparticle-based electrolytes for thermocell technologies. Different types of nanoparticles were used for solidification of the liquid electrolytes, and the effect of this solidification on the performance of the thermocell was investigated.

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Synthesis of Phosphorene and Its Use in Solar Cells

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Phosphorene, a single- or few-layered semiconductor material obtained from black phosphorus, has attracted significant attention over the past few years and has shown great promise in many applications including transistors, batteries and photovoltaics (PV) due to its unique properties.¹⁻³ However, the successful and controllable synthesis of high quality few layer phosphorene is still challenging. In this project, we systematically investigated the effect of different ultrasonication methods for the production of solution processable phosphorene in various organic solvents. As a result, we found that high-quality, few-layer phosphorene can be produced by a liquid exfoliation method under ambient conditions in N-Methyl-2-pyrrolidone (NMP) solvent. Importantly, few-layer phosphorene in NMP exhibited excellent stability in ambient conditions, demonstrating that this material is potentially useful in a range of applications including solar cells.

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Study of Synthesizing 2,5-dimethylfuran (DMF) from Nature Cellulose for Alternative Fuel Usage

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Nowadays, the need for energy kept increasing along with human mobility level, particularly on transportation. Therefore, the demand of fossil fuel such as gasoline as the prominent energy source is also increasing. However, the availability of fossil fuel is limited. This should immediately be addressed by changing fossil fuel with environmental-friendly fuel that produces the relatively same energy as fossil fuel does. Lately, there has been many alternative fuels that could be used. One of which is 2,5-dimethylfuran (DMF). DMF can be synthesized from the hydrogenolysis of 5-hydroxymethylfurfural (HMF) which can be obtained from glucose which is a monomer of cellulose so that it can be obtained from organic waste such as dead plants, woods, or unused bamboos. From literatures that we have studied, glucose conversion into HMF is possible with a mixed solvent of γ -valerolactone (GVL) and water with weight ratio of GVL:water = 9:1 using Sn- β (Si:Sn = 400) and Amberlyst-70 (Amb-70) as the catalysts. A high HMF yield of 59% is obtained from glucose at 130°C after 20 minutes. HMF hydrogenolysis into DMF is possible with the use of bimetal RuSn/C catalyst in the presence of lactones. DMF yield of 46% is obtained from HMF at 200°C. DMF produces 31,1 MJ/L of energy whereas fossil fuel produces 35 MJ/L which makes it a viable option for alternative fuel. More importantly, hydrogenolysis of HMF into DMF can be done without the conversion of the solvent.

Keywords: synthesis, cellulose, hydrogenolysis, 5-hydroxymethylfurfural, 2,5-dimethylfuran, γ -valerolactone, SnRu/C

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Hydration generation from ethylene diamine bisborane along with different ionic liquids

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Hydrogen Fuel is considered globally as the new face of energy sector and EthylenediamineBisborane (EDAB) is known to releases 10 wt% of Hydrogen. COSMO-SAC (CONductor like Screening MOdel Segment Activity Coefficient) model was used to select the Ionic liquids (IL) for dehydrogenation experiment. The ILs with the lowest Infinite dilution activity coefficient (IDAC) were selected, as the lower the IDAC- higher the solubility of EDAB in IL. The following ILs are 1-ethyl-3-methyl imidazolium acetate ([EMIM][OAc]), 1-butyl-3-methyl imidazolium acetate ([BMIM][OAc]), 1-butyl-1-methylpyrrolidinium methyl carbonate ([Bmipr][CH₃CO₃]), Trihexyl(tetradecyl)phosphonium bis (2,4,4-trimethylpentyl) phosphinate ([TDTHP][Phosph]) and Trihexyl(tetradecyl)phosphonium dicyanamide ([TDTHP][DCA]). The experiments were carried out at a vacuum of 4×10^{-2} mbar (gauge pressure) and at temperature of 95 °C and 105 °C. The highest Equivalent of Hydrogen (3.96) was released from [BMIM][OAc]. Further analysis of the residue was done for better understanding about the role of IL as catalyst and EDAB as consummate for hydrogen production.

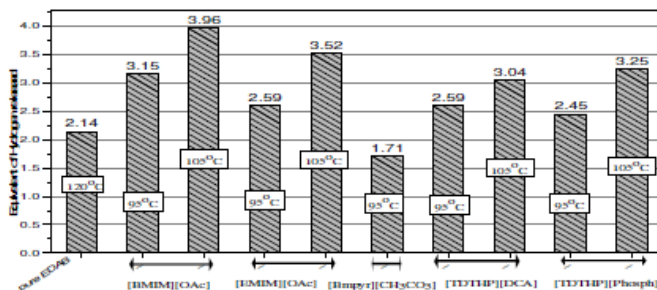


Figure 1: Comparative studies of equivalent of hydrogen released from all EDAB/IL complexes

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Performance Enhancement in Organic Solar Cells with Gold Nanoparticle Clusters

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Plasmonic metal nanoparticles hold great promise to improve light absorption and charge generation of organic photovoltaics. Unfortunately, power conversion efficiency of the organic photovoltaics with plasmonic nanoparticles is still limited as randomly separated nanoparticles hardly exploit the effective plasmonic enhancement by interparticle coupling. Here we demonstrate single-junction high performance organic photovoltaics using gold nanoparticle clusters with controlled morphology as a plasmonic component. Near-field coupling at the interparticle gaps of nanoparticle clusters gives rise to strong enhancement in localized electromagnetic field, which led to the significant improvement of exciton generation and dissociation in the active layer of organic solar cells. A power conversion efficiency of 9.48% is attained by employing gold nanoparticle clusters at the bottom of the organic active layer. This is one of the highest efficiency values reported thus far for the single active layer organic photovoltaics [1].

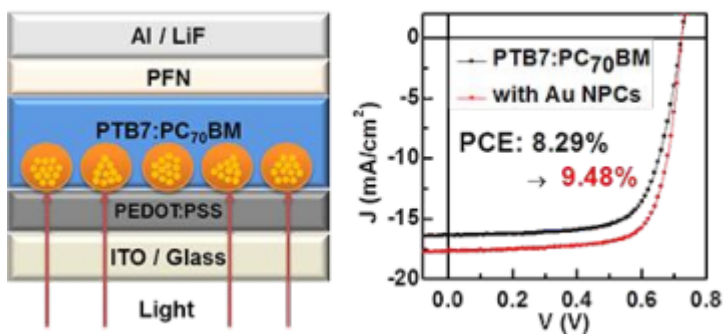


Fig. 1 Device schematic and its J-V characteristics

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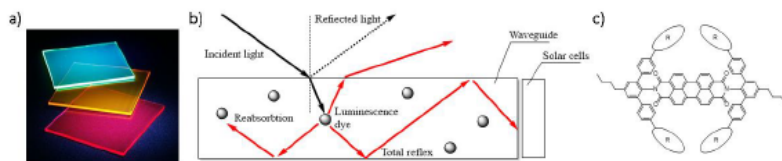
New Organic Dyes for Luminescent Solar Concentrators

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A typical luminescent solar concentrator (LSC) usually consists of a piece of planar transparent glass or plastic sheet (the waveguide) that can harvest solar light from the front surface and concentrate the light to the edges. The output light then is collected by solar cells sitting on the edges. The benefits of LSCs are that: (1) they can significantly reduce the area demand of solar cells; (2) the light harvesting and power converting modules are separated; (3) it is a legitimately transparent light harvesting device. The LSCs are normally covered or embodied with some fluorescent dyes which can capture the incident photons and reemit them inside the waveguide. The emitted light then is transported to the edges via total internal reflection. The fluorophore plays quite an important role in the light harvesting process: it needs to have an absorption spectrum which matches the solar flux, the emission spectrum must match the solar cell absorbance, and high photon-to-photon conversion efficiency is required. Perylene diimide (PDI) derivatives, as good candidates to the LSC fluorophores, meet all the above criteria. The only problem is that the PDI-based fluorophores are usually in a planar molecular configuration, which potentially leads to intermolecular aggregation and, consequently, aggregation-induced quenching. To avoid this problem, we designed and synthesized a series of new PDI-based fluorophores with bulky substituents that can keep the fluorescent perylene moieties sufficiently apart. This allowed us to load the fluorophores in high concentration and harvest more light without suffering from aggregation quenching.



a) The LSC device; b) the waveguiding process and c) the bulky-PDIs

3D Printer Based Slot Die Coater as a Lab-to-Fab Translation Tool for Solution Processed Solar Cells

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Perovskite solar cells have emerged as the most promising third-generation solar cells with a rapid increase in the record efficiencies. The next challenge in this field will be translating the lab-scale to a large-scale production process, which will preferably include a cost-competitive roll-to-roll printing process. The Commonwealth Scientific and Industrial Research Organisation (CSIRO) is a national science agency of Australia. As a key member of the Victorian Organic Solar Cell Consortium (VICOSC), CSIRO has played a leading role in the development of large scale printed organic solar cells. During the development of a roll-to-roll printing process, an efficient lab-to-fab translation tool was designed to optimize the printing process on a small scale. A 3D printing platform was used for the research tool, which is able to provide automated control of x,y,z-positioning, coating speed, acceleration and temperature. This degree of control allows us to mimic and develop the actual printing conditions appropriate to a real roll-to-roll manufacturing process. Optimisation of this scalable fabrication process has lead to printed perovskite cells with power conversion efficiencies as high as 12% which compare favourably with literature performances for lab-scale devices. The process has been further modified and transferred to a pilot-scale roll-to-roll printer. Recent progress on the translation process for perovskite solar cells will be presented.

Highly concentrated inorganic-organic ionic liquid electrolyte for extensive sodium metal plating and stripping

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Seamlessly incorporating renewable energy into our ever evolving smart grid requires implementation of efficient and inexpensive rechargeable batteries. Sodium energy storage technology has recently been investigated due to the considerable low cost and great abundance of the element Sodium in the Earth's crust. In addition, a Sodium technology may provide a specific energy of 3630 Wh kg⁻¹ (namely Na-O₂) comparable to current lithium-ion cells (typically 100 – 270 Wh kg⁻¹).[1] We herein further investigate Ionic liquids including high salt concentrations and their effects on charge-discharge cycling and the morphological and compositional changes of the anode surface.

By characterising the surface of sodium electrodes after they have undergone plating/stripping, we reveal the effects polarization may have on a Na metal battery. For high performance batteries, the solid-electrolyte interphase is expected to exhibit smooth morphology,[2] devoid of dendritic structures,[3] ionically conduct the ingress and egress of Na⁺ whilst also passivating the NaO from further reaction with electrolyte species.[4]

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Lifetime Assessment of Printed Photovoltaic Devices

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Organic-based solar cells fabricated on plastic substrates are attracting worldwide attention due to advantages such as flexibility, large-scale printability, lightweight, and potential utility for new products. However, exposure of these devices to atmospheric oxygen and water vapour is known to cause rapid device degradation. Encapsulation using materials having ultra-low permeability to these atmospheric constituents is required to achieve sufficient operational lifetimes for commercial applications. We have found that pre-entrained moisture in the encapsulation materials, and post-encapsulation ingress of moisture/oxygen through adhesive layers and around electrical contacts are significant lifetime-limiting factors. Encapsulation architectures were developed using a variety of flexible barrier films and adhesives to address these issues, and the lifetime of encapsulated large-area (active area $\sim 50 \text{ cm}^2$) fully-printed OPV modules were assessed under various storage conditions. Fracture tests were conducted on encapsulated modules exposed to continuous 1-sun illumination to investigate the effects on inter- and intra-layer adhesion and cohesion. New encapsulation architectures were found to significantly enhance the durability of printed OPV modules, with results showing modules exhibiting a shelf-life of more than 5 years under ambient conditions and durability of more than 3 years under exposure to outdoor conditions.

Key words: Organic photovoltaics, Perovskite solar cells, encapsulation, barrier films, stability, lifetime

Exergetic Evaluation of Small DI Diesel Engine

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Exergy analysis method has been widely used in the design simulation and performance assessment of various types of engine for identifying losses. This study is done by coupling 1st law and 2nd law of thermodynamics which gives a clear picture on fuel consumption, brake thermal efficiency, exergy efficiency and different exergy terms with the varying load. In this investigation, the energy and exergy analysis are employed to analyze the quantity and quality of energy in 4-stroke single cylinder direct injection small diesel engine using diesel as fuel. The tests are carried out for various loads in a speed range of 1300-2400 rev/min.

The experimental data are collected using steady state tests which enable measurements of air, fuel flow rates and relevant temperatures. Balances of energy and exergy rates for the engine are determined and various performance parameters (loss exergy, exergy accompanying due to heat, exhaust exergy, brake thermal efficiency etc.) are calculated for each load level and compared with each other. The parameters analyzed are the energy and exergy of fuel input, exhaust gas and exergy destruction, entropy generation. Side by side, the effect of the variation of load on peak pressure, exergy efficiency, entropy generation and various exergy terms are also discussed. Emission analysis is also done along with the exergy analysis. Experimental result show that the exergy efficiency is higher.

PAPERS

Effects of thermal treatment and bio-oil extraction on the pyrolysis of mallee wood

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Abstract: Pretreatment of biomass prior to pyrolysis is an important way to modify the structure and property of biomass, which could in turn change the yield and quality of bio-oil from the pyrolysis of biomass. The controlled thermal pretreatment of big wood particles combined with grinding was effective to give the high yield of bio-oil with improved aromatic contents. The pretreatment (bio-oil extraction) of fine wood particles prior to pyrolysis remarkably decreased the carbonyl groups (reactive functionalities) content in the bio-oil from the pyrolysis of the pretreated wood.

Introduction

Pyrolysis is a potential technology converting biomass into biofuels [1-2]. However, the overall pyrolysis rate of large biomass particles can be significantly slowed down by the intraparticle mass and heat transfer limitations [3]. However, the pulverisation of large wood particles into fine particles is an energy-intensive process. Thus, grinding pyrolysis, a new technology has been developed for the efficient

pyrolysis of the large wood particles [4]. This study aims to investigate the effects of the thermal pretreatment and subsequent grinding of mallee wood and the extraction of mallee wood with bio-oil on the yields and properties of the bio-oil from the pyrolysis of treated biomass at 500 °C.

Method

To investigate the combined effects of thermal treatment and grinding, mallee wood cylinders (ca. 10 mm of length and ca. 8 mm of diameter) were prepared for the thermal treatment, and then the treated cylinders were milled into 90-300 µm of particles as the feedstock in the subsequent pyrolysis. The direct pyrolysis of wood cylinders and particles (90-300 µm) were performed for comparison. To investigate the effects of solvent (bio-oil) extraction of wood on its pyrolysis behaviour, wood particles with the size range of 180-425 µm before and after bi-oil extraction were pyrolysed for comparison. The thermal treatment and the pyrolysis of mallee wood cylinders were carried out in a fluidised-bed reactor.

Results and discussions

As is shown in Fig. 1a, for the big wood particles, the thermal treatment at low temperatures (e.g. 200 °C) followed by ex-situ grinding of mallee wood cylinders can give bio-oil yields much higher than the direct pyrolysis of wood cylinders, but the positive effect became small with the increase in the thermal treatment temperature (e.g. from 200 °C to 320 °C). The low temperature pretreatment might have activated the biomass structure for further pyrolysis. The intensified charring reactions took place during the treatment of cylinders at high temperature (e.g. 320 °C) reduced the

yield of bio-oil. It demonstrates that the thermal treatment would improve the grindability of big biomass particles and the subsequent grinding could significantly reduce the mass transfer limitation for the release of volatiles could be easily released, resulting in the high bio-oil yield.

The extraction of fine particles with bio-oil at room temperature (Fig. 1b), the yields of heavy bio-oil did not significantly change during the subsequent pyrolysis. It indicates that the extraction of wood particles with bio-oil prior to pyrolysis has limited effects on the production of heavy bio-oil.

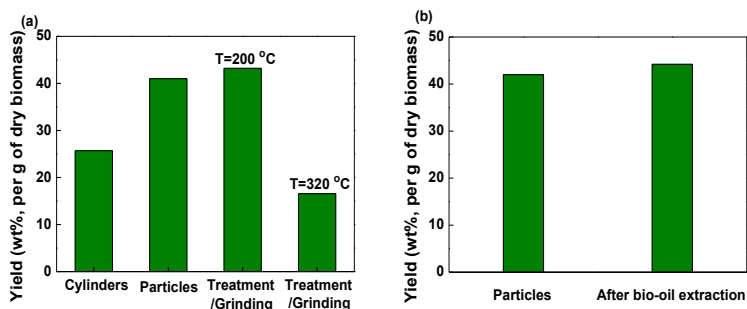


Fig. 1. The yields of heavy bio-oil from the pyrolysis of mallee wood. (a) The pyrolysis of thermally pretreated (200 °C and 320 °C) and ground mallee wood, untreated mallee wood cylinders and particles; (b) The pyrolysis of untreated mallee wood particles and mallee wood particles extracted with bio-oil (some data in Fig. 1a have been used in another paper [5]).

Fig. 2a and b show the effects of thermal treatment and bio-oil extraction on the formation of aromatics in bio-oil from the pyrolysis of untreated and treated mallee wood. Compared with the direct pyrolysis of wood cylinders, the thermal pretreatment at low temperature (e.g. 200 °C) and grinding could favour

the formation and release of species containing aromatic ring systems during pyrolysis. Grinding was essential to improve the release of aromatics. However, when the thermal treatment temperature was increased to 320 °C, the formation of aromatics in bio-oil decreased. It indicates that the reactions during the thermal treatment of mallee wood cylinders significantly influenced the production of aromatics during the subsequent pyrolysis. While, for the fine wood particles, the extraction of wood with bio-oil did not affect the formation and release of aromatic structures during the subsequent pyrolysis.

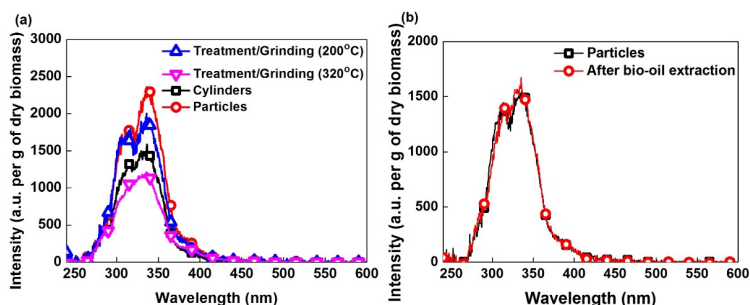


Fig. 2. Constant energy (-2800 cm^{-1}) synchronous spectra of bio-oils from the pyrolysis of mallee wood. (a) The pyrolysis of thermally pretreated (200 °C and 320 °C) and ground mallee wood, untreated mallee wood cylinders and particles; (b) The pyrolysis of untreated mallee wood particles and mallee wood particles extracted with bio-oil (some data in Fig. 2a have been used in another paper [5]).

The effects of thermal treatment and bio-oil extraction on the carbonyl groups in bio-oil from the pyrolysis of untreated and treated mallee wood are depicted in Fig. 3. The extraction of wood with bio-oil prior to pyrolysis can significantly reduce the formation and release of hydroxyl unsaturated ketones/aldehydes

(1651 cm^{-1}) as bio-oil components during pyrolysis while the effects of thermal pretreatment were much smaller. For other carbonyl groups in bio-oil such as the unconjugated alkyl aldehydes/esters, carboxylic acids and aromatics (1740, 1713 and 1607 cm^{-1}), both the thermal treatment and bio-oil extraction showed limit effects on the production of these compounds during pyrolysis.

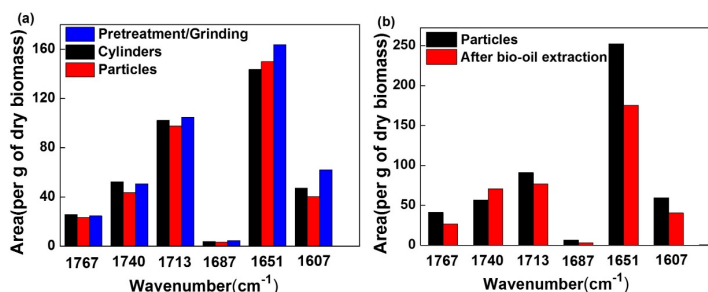


Fig. 3. Band areas from the spectral deconvolution of the FT-IR spectra of bio-oils from the pyrolysis of mallee wood. (a) The pyrolysis of thermally pretreated (200 °C) and ground mallee wood, untreated mallee wood cylinders and particles; (b) The pyrolysis of untreated mallee wood particles and mallee wood particles extracted with bio-oil (some data in Fig. 3a have been used in another paper [5]).

Conclusions

The thermal treatment and ex-situ grinding was an effective pretreatment method for the large wood particles. The controlled temperature of thermal pretreatment (to improve grindability) followed by grinding can improve the bio-oil yield during pyrolysis, which could also favor the formation of aromatics in bio-oil. These data would help to better understand the fundamental aspects of the grinding pyrolysis

technology. However, for the fine particles, the extraction of wood with bio-oil prior to pyrolysis could not improve the production of bio-oil, but did modify the concentration of some reactive functionalities in the bio-oil products, which possibly improve the stability of bio-oil product.

Acknowledgement

This project received funding from ARENA as part of ARENA's Emerging Renewables Program.

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Direct Current Micro Grid Bus Voltage Regulation for Photovoltaic and Wind Integrated Systems

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Abstract

The rise in energy demand in the grid distribution network and grid isolated areas, the renewable energy sets with micro grid setup trendy to meet the challenge. The electricity generation from renewable sets specifically from photovoltaic cells and wind turbine is of stochastic nature. Since, the demand regulation of voltage output in order to meet the standard load requirements. Therefore an integration of these

renewable sets in a direct current micro grid (DCMG) setup has been proposed. This is considered due to practicability and economic viability to transform voltage output in DC and maintain the DC bus voltage at 12V. The simulation of two sources have been considered and maintained at a level of 12V under various conditions. The appropriate dc load has been deployed for DCMG system performance measurements. The results show that the dc voltage level has been maintained satisfactorily at the dc-bus for both loads and sources. Thus, the proposed model is significant for integrating multiple renewable energy sets for dc supply under isolated dc micro grid setup.

Introduction

In present era, the socio–economic development of any country is proportional to the energy usage. Due to flexibility, ease in transportation and control, electrical energy has dominance over other forms and its utilization is considered as the sign of development for any country or state. Despite of vast technology revolution still majority of the remote areas in developing countries have no access to this essential energy form due to long distance from the utility grids.

One of the possible solutions of aforesaid issue is to adopt the distributed efficient renewable energy trends of power generation to meet the basic needs of any country. Implementation of these endless clean energy resources also plays a valuable contribution to reduce the greenhouse gas emissions, hence reduce the global warming and conserve the earth for coming generations. However, a power generating unit based on single renewable energy source (wind, solar, etc) is not effective in terms of efficiency and reliability.

The formation of a hybrid energy system by combining different renewable energy resources is a feasible alternative solution [1-3]. Hybrid systems include the combination of various renewable energy resources such as solar, wind, fuel cells, hydro, diesel, etc to offer the advantages of high stability and reliability. Electrical power at comparatively economic rates can be supplied to the remote areas by means of these hybrid systems [4]. The design of the hybrid renewable energy systems must be optimal in terms of their operation, cost, and control and element selection, to reliably and economically obtain the electrical power from these systems. Many topologies of the hybrid system are

available based on the type of the renewable energy source and the converters interfacing the source with DC bus. Design of a stand-alone low voltage dc hybrid wind-solar system based on converters and cascaded controller was proposed by [4] and refers it best for the battery charging, water pumps and desalination applications. Simulation study of the separate photovoltaic, wind, hydro and their hybrid systems was carried by [5] to observe their behavior. A possible configuration of wind-solar-battery hybrid was presented by [6] with separate dc and ac bus system architectures.

It is seen that the researchers have set trend to use the wind and solar energies as basic components of the hybrid systems. It is expected because of their free of cost availability in bulk with high potentials and efficiencies [7]. This is the reason that the photovoltaic cells and wind turbine generators are the most common and popular methods for electrical power generation now a days [8]. The proposed model in this research work as well is a hybrid wind-solar system based on the basic electronic components with main focus on the cost-effective design which works at very low voltage of

approximately 5 volts. Proposed system is viable for isolated applications like small dc appliances and as a battery charging circuit.

Proposed Hybrid Wind–Solar System

The proposed hybrid system based on basic low–cost electronic components which uses solar and wind power to efficiently and reliably power a small dc load. The proposed model, shown in figure 1, comprises of the following components;

Solar Panel (0–22 volt)

Wind Generator set (0–12 volt)

Zener Diodes (as voltage regulators and for over–voltage protection)

Operational Amplifier (as comparator)

Transistors (as switches)

Diodes (for protection against reverse current flow between the sources)

Light Emitting Diodes (as the projected load)

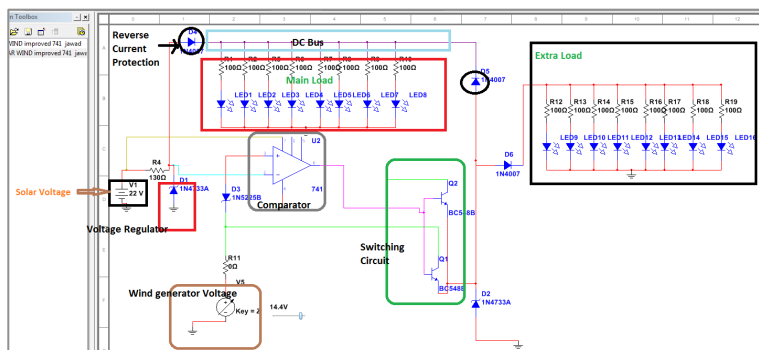


Figure 1: Circuit diagram of the proposed system

System Description

During the day, solar voltage remains nearly constant whereas the voltage generated from the wind generator is variable. So, for the designed system voltage from photovoltaic system is taken as the reference value for the comparator. When the voltage from wind system goes high to that of solar system, the output of the comparator will be high and activates the switching transistors. The output of the comparator is required to just provide the base current to the transistors, which is very small. The transistors are used here to switch on or off the wind generator's output while the solar voltage is directly connected to the load through the regulator and the reverse current protection diodes.

The comparator is an operational amplifier used in open loop configuration without any feedback and compares the voltage of the solar panel with that of wind generator's voltage. For the subject work, wind generator system is represented by means of variable dc source of 12 volts and solar system with fixed 22 volts dc source. The system consists of two loads; Main Load (M.L) and Extra Load (E.L), which are comprises of series-parallel combination of resistors and Light Emitting Diodes (LED's) and are used here as a small dc load. The extra load is included in the system to utilize the full potential of the two sources. At high wind speeds, the wind generator is capable of supplying power to both loads, whereas, the solar system alone supports the power requirements of main load only because of its insufficient capacity. Extra load do not operate at the times when the capability of the wind system is less (as expected at low wind speeds). Working of the extra load is proportional to the high wind speeds when the wind voltage is integrated into the system. Figure 2 presents the simplified working of the proposed system.

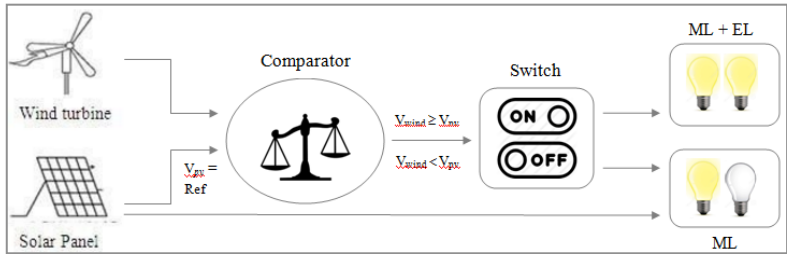


Figure 2: Diagrammatic representation of the functioning of the proposed system

The voltage regulators help to maintain the load voltage at approximately 4.5 volts. The overvoltage protection for the load is achieved by connecting the zener diode in parallel with the load. The selection of zener diode depends upon the rated load voltage and the maximum voltage that the load can sustain. So the zener diodes rated voltage should be between the loads rated and maximum sustainable voltage limits. For the protection against reverse current and back power flow between the sources, diodes are being used at the terminals of each load. At the times of unequal power share from the two sources, the reverse connected diodes will act in reverse biased condition; hence protect the sources from reverse current.

The following equations describe the different modes of operation of the proposed system;

Volts_{wind}	$\geq \text{Volts}_{solar}$	$P_T = P_{wind} + P_{solar}$	Main load + Extra load
	$< \text{Volts}_{solar}$	$P_T = P_{solar}$	Main load
Volts_{solar}	$<< \text{low or } = 0$	$P_T = 0$	----

Simulation Results

Simulation of the proposed system with measured values at various points of the circuit is shown in figure 3.

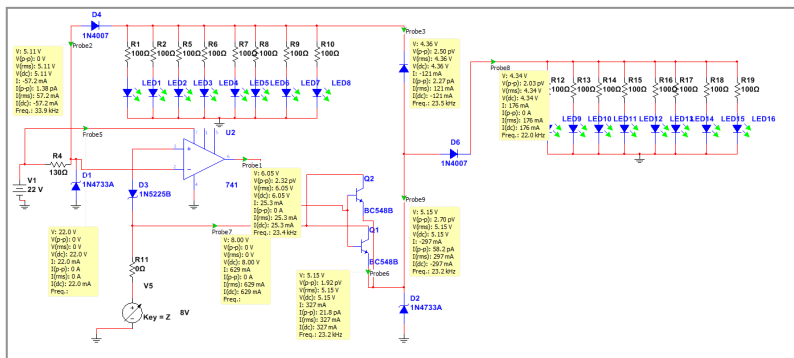


Figure 3: Simulation of the proposed system showing measured variables at various points

Case 1: $V_{Wind} \geq V_{Solar}$

At the times of high wind speeds, power output of the wind system is sufficient to be added into hybrid system. Under this condition, power supplied by both wind and solar systems is enough to fulfill the power

requirement of both loads. Hence both loads are in operation under this condition. Moreover, the voltages at load terminals are also improved. Table 1 presents the operating values at this condition.

Table 1: Measured values at $V_{Wind} \geq V_{Solar}$ condition

Voltage at Inverting (-ve) terminal of comparator $= V_{Solar}$	Voltage at Non-Inverting (+ve) terminal of comparator $= V_{Wind}$	Condition	Voltage at Main Load Terminals	Voltage at Extra Load Terminals	$P_{Total} = P_{Solar} + P_{Wind}$	Loads in Operation
4.70 V	4.70 V	$V_{Wind} = V_{Solar}$	3.91 V	3.77 V	0.54 W	Main Load + Extra Load
5.11 V	9.32 V	$V_{Wind} > V_{Solar}$	4.38 V	4.36 V	1.363 W	Main Load + Extra Load
5.12 V	13.3 V	$V_{Wind} > V_{Solar}$	4.39 V	4.37 V	1.4 W	Main Load + Extra Load

Case 2: $V_{Wind} < V_{Solar}$

At the times of low wind speed, wind system is not able to carry any load. Hence, solar system alone supplied its power to the system. Because of the insufficient capacity of the solar system only main load is in

operation. Voltages at the load terminals are also reduced to that of the voltages under case 1. Table 2 presents the operating values at this condition.

Table 2: Measured values at $V_{Wind} < V_{Solar}$ condition

Voltage at Inverting (-ve) terminal of comparator $= V_{Solar}$	Voltage at Non-Inverting (+ve) terminal of comparator $= V_{Wind}$	Condition	Voltage at Main Load Terminals	Voltage at Extra Load Terminals	$P_{Total} = P_{Solar} + P_{Wind}$	Loads in Operation
4.59 V	294 mV	$V_{Wind} < V_{Solar}$	3.79 V	139 mV	0.53 mW	Main Load
4.59 V	4.25 V	$V_{Wind} < V_{Solar}$	3.79 V	930 mV	0.62 mW	Main Load

Case 3: $V_{Solar} \ll \text{low}$ or $V_{Solar} = 0$

As the voltage generated from the solar system is set as the reference value for the comparator. In the night time, the voltages generated from the solar system are very low or almost equal to zero. At that time, the non-inverting (reference) terminal of the comparator is not activated and makes the complete system down. The wind system too does not contribute its part of the power share to the system because of the comparators incapability to trigger the base of the transistor switch. This condition can also be termed as the undesired condition for the developed system. Table 3 presents the operating values at this condition.

Table 3: Measured values at $V_{Solar} \ll \text{low}$ or $V_{Solar} = 0$ condition

Voltage at Inverting (-ve) terminal of comparator $= V_{Solar}$	Voltage at Non-Inverting (+ve) terminal of comparator $= V_{Wind}$	Condition	Voltage at Main Load Terminals	Voltage at Extra Load Terminals	$P_{Total} = P_{Solar} + P_{Wind}$	Loads in Operation
3.20 V	13.1 V	$V_{Solar} \ll \text{Low}$ $V_{Wind} > V_{Solar}$	2.48 V	930 mV	0.074 mW	No Load
3.20 V	265 mV	$V_{Solar} \ll \text{Low}$ $V_{Wind} < V_{Solar}$	2.48 V	139 mV	0.045 mW	No Load
0 V	5.09 V	$V_{Solar} = 0$ $V_{Wind} > V_{Solar}$	0 V	0 V	0 W	No Load

Thus, from the three discussed cases, it is seen that the high wind speeds not only make the developed system more reliable but also improve the systems stability by increasing and maintaining the voltages constant at load terminals. It can be considered as the ideal condition for the proposed system. The effect of increased wind generators output voltage on the voltages at main load and extra load terminals can be observed from the wave forms shown in figure 4 and

figure 5 respectively. Effect of voltage regulators, to not allow the voltage to be increased from set limit of 5 volt at load terminals, can also be observed from the following figures.

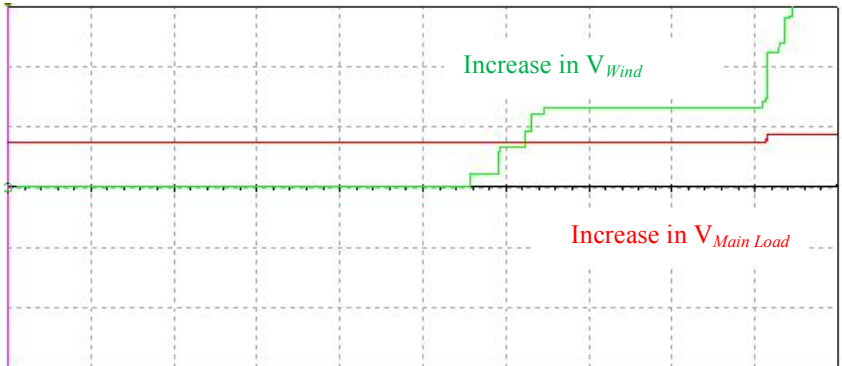


Figure 4: Effect of increased wind speeds on wind generators output voltage and voltage at main load terminals

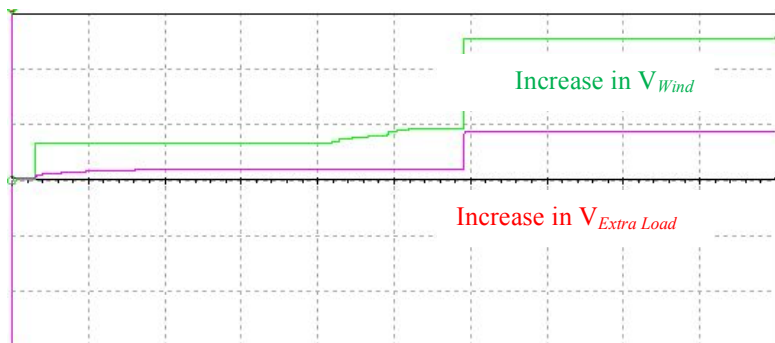


Figure 5: Effect of increased wind speeds on wind generators output voltage and voltage at extra load terminals

Conclusion

The proposed low cost hybrid wind–solar system works satisfactorily at various operating conditions and is suitable for small dc appliances applications. System offers poor performance at the time of low solar radiations which can be improved by some design modifications and adding the storage devices in the system. In future, the research can be carried out on designing the wind–solar hybrid systems for higher dc voltages, (i.e. at 12V, 24V etc) while keeping the systems cost low.

Acknowledgement

The authors are grateful to USPCAS – E Peshawar for project grant (USPCAS-E ARG-Dec15-042) and to carry out the research and Higher Education Commission (HEC) Pakistan for travel support. They would also like to acknowledge Mehran UET Jamshoro & UET Peshawar for joint carrying of the project.

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