

SYMPOSIUM ET11

Emerging Materials and Device Concepts for Flexible, Low-Cost Photovoltaic Technologies
November 26 - November 30, 2018

Symposium Organizers

Lan Fu, Australian National University
Alexander Sprafke, Halle-Wittenburg University
Rao Tatavarti, MicroLink Devices, Inc.
Lin Zhou, Nanjing University

Symposium Support

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* Invited Paper

SESSION ET11.01: Flexible PV
Session Chairs: Lan Fu and Erik Garnett
Monday Morning, November 26, 2018
Hynes, Level 3, Room 304

8:30 AM ET11.01.01

Highly Flexible Perovskite Solar Cells with Low Cost Electrodes and Charge Selective Materials Peng Li and Zijian Zheng; The Hong Kong Polytechnic University, Hong Kong, China.

The organic-inorganic halide perovskite solar cells (PSCs) have witnessed efficiency soar from initial 3.8% to current-record 22.7% in the past less than ten years, representing one of the most promising active photo absorber candidates to reduce the materials cost in the photovoltaic devices. It is however often overlooked that the majority of the materials cost in the PSCs come from transparent electrodes (e.g. ITO, FTO, etc), charge-selective carriers (e.g. PTAA, Spiro-MeOTAD) or metal contacts (e.g. Au, Ag), instead of the perovskite photo absorber itself. On the other hand, sufficiently thin perovskite film spontaneously inspires tremendous research interests and efforts in flexible application scenario in the emerging era of wearable electronics, imposing foldable, stretchable and even squeezable photovoltaic devices in huge demand.

Therein, we propose a perovskite solar cell system employing ultrathin substrate, low-cost copper front and back electrodes as well as inexpensive metal oxides charge-selective materials to enable highly flexible PSCs. All the materials can either be prepared with affordable synthesis cost on avalanche quantity basis or readily obtained in the commercial market. To be more specific, Cu mesh hybridized with doped PH1000 serving as bottom transparent electrode replaces costly transparent conductive oxides while top Cu electrode further reduces metal cost. NiOx as the hole transporting layer eliminates the use of expensive polymer PTAA yet maintains comparable high open-circuit voltage. Inorganic ZnO partially and in principle could completely fulfill the role of fullerene type electron transporting material of PCBM. As such, the whole PSC system embraces dramatically reduced material cost in corresponding components by several order of magnitudes. More interestingly, the ultrathin polymeric substrate endows the perovskite solar cells with terrific flexibility and accordingly robust application potentials.

8:45 AM ET11.01.02

Flexible Crystalline Silicon Photovoltaics with Vertically Aligned Microwires Inchan Hwang, Han-Don Um and Kwanyong Seo; Ulsan National Institute of Science and Technology, Ulsan, Korea (the Republic of).

Flexible photovoltaics (FPVs) are one of the most promising research fields in the solar energy industry because they can be utilized as a continuous power source for wearable and portable electronic devices. Thin crystalline silicon (c-Si) has attracted much attention as a potential means for FPVs because of its excellent flexibility while retaining the advantages of c-Si PVs of high efficiency and stability. For highly efficient thin c-Si FPVs, it is important to maximize light absorption while maintaining the flexibility characteristics. In general, the conventional c-Si photovoltaics have increased light absorption by applying surface structures. However, the surface structures without consideration of the flexibility would limit the flexibility of the FPVs because induced stress during bending cannot be uniformly dispersed. In this study, vertically aligned microwires (MWs) on a 50 μm -thick thin c-Si substrate are designed for novel FPVs. Increasing the length of the MWs enhances the optical properties of the thin c-Si without affecting its flexibility. To maximize the efficiency of the thin c-Si FPVs with MWs, tapered MWs and a localized back-contact structure are devised. This device shows a maximum efficiency of 18.9%. In addition, the proposed thin c-Si FPV with MWs shows high stability without any change in efficiency, even with 1000 bending cycles with a bending radius of 12 mm. Thus, we successfully demonstrate battery-free flexible electronic devices integrated with our thin c-Si FPVs with MWs.

9:00 AM *ET11.01.03

BIPV—A Bad Idea or Tomorrow's Mainstream Application? Sarah R. Kurtz; University of California, Merced, Merced, California, United States.

In 1994, PowerLight introduced a building-integrated photovoltaic (BIPV) product, touting it as saving money (avoiding the cost of installing a conventional roof) while integrating PV into an attractive roof. At the time it was introduced, the mainstream opinion was that the future of PV would be building integrated and that utility-scale applications were a non starter. Today, utility-scale PV accounts for more than half of the world PV installations and BIPV is a niche market (with most rooftop systems being “building applied” rather than “building integrated.”) Was BIPV a bad idea?, or was BIPV an idea whose time had/has not come? Many things have changed since 1994; could BIPV be poised to become a mainstream application? Tesla and other companies are introducing BIPV products today. Will they be more successful? The talk will review many things that have changed (including power electronics, products with lower temperature coefficients, demonstration of PV as an accepted technology so that it's not such a risk to builders, the value of generating solar electricity near load centers, etc.), suggesting that there may be a new opportunity for BIPV. Then, the talk will review how a shift back

to a goal of large-scale deployment of BIPV and related products changes the research agenda.

9:30 AM ET11.01.04

All Dielectric Light Trapping Scheme for Enhancing the Efficiency of Ultrathin Flexible Gr/Si Solar Cell [Sonal Das](#)¹, Mohammad Jobayer Hossain², Kristopher Davis^{2,3} and Tania Roy^{1,3,4}; ¹NanoScience Technology Center, University of Central Florida, Orlando, Florida, United States; ²The College of Optics and Photonics, University of Central Florida, Orlando, Florida, United States; ³Department of Materials Science and Engineering, University of Central Florida, Orlando, Florida, United States; ⁴Department of Electrical and Computer Engineering, University of Central Florida, Orlando, Florida, United States.

Graphene/silicon (Gr/Si) Schottky junction solar cells have attracted much attention due to the ease and low cost of fabrication, along with the lucrative properties of high electron mobility, transparency and mechanical flexibility of graphene as a transparent conducting electrode. Utilizing its inherent mechanical flexibility, graphene can be integrated with thin flexible crystalline Si substrates opening up a new regime of applications in flexible and wearable electronics. Reducing Si absorber thickness below 50 nm offers advantages of reduced material cost, along with mechanical flexibility and light weight. But Si at such thicknesses suffers from low photon absorption in the solar spectrum. To compensate for the low light absorption in such thin substrates, light management schemes become essential. Light trapping in Gr/Si solar cells is enabled by engineering the Si surface to form nanopillars, nanowires etc., which decreases the reflection loss and allows more light to couple in to the Si substrate. The structured Si absorber increases surface area and surface recombination, which is detrimental to the solar cell efficiency. Thus, it is imperative to use a light trapping scheme devoid of Si structuring to enhance the photo-conversion efficiency.

We present an all-dielectric light-trapping scheme on planar Gr/Si Schottky junction solar cells with the use of bottom layer of titania spheres and top layer of silica spheres. An optimal Si thickness coupled with an optimized light trapping scheme leads to efficient electron-photon harvesting. The photo-conversion efficiency of a 200 nm thick nanosphere-decorated Gr/Si solar cell improves to 9%, which is 1.3x higher than the pristine cell's PCE of 7%. FDTD simulations are performed for optimizing the diameter of nanoparticles in each of the layers. The ratio of size of nanoparticles in the top to bottom layer plays a crucial role in advanced light management. An optimized structure of silica spheres, having diameter larger than that of titania spheres, suppresses reflection over wide angles of incidence and increases absorption in active Si layer over AM1.5G solar spectrum. The non-absorbing dielectric spheres can be easily realized by the well-known Stober technique. Additionally, the photovoltaic characteristic of the laminated solar cell shows negligible change after several bending cycles having bend radius ranging from 5 mm to 10 mm. After continuous bending and straightening, the ultra-thin solar cell can retain its performance, revealing the excellent stability and flexibility of the device. Such simple, low-cost light trapping schemes are universal in nature, devoid of recombination losses and are potentially viable for any solar cell technology.

References

1. Li, B. et. al., Graphene-On-Silicon Schottky Junction Solar Cells. *Adv. Mater.* 2010, 22, 2743 - 2748.
2. Petersen, K. E., Silicon as a mechanical material. *Proc. IEEE* 1982, 70, 420 - 457.

9:45 AM ET11.01.05

Silicon-Hybrid Multi-Junction Photovoltaic Devices for (Photo-)Electrochemical Applications Thierry de Vrijer, Johan Blanker, Paula Perez Rodriguez, Miro Zeman and [Arno H. Smets](#); Delft University of Technology, Delft, Netherlands.

Photovoltaic (PV) device configurations based on multi-junctions have the advantage of improved utilization of both photons in the solar spectrum and the energy of the photons. PV bottom junctions based on low-bandgap semiconductors allow to utilize the low energetic photons, whereas high-bandgap semiconductors in the top PV junctions allow to efficiently utilize the photon energy for high voltage generation. As a consequence multi-junctions PV devices are a straightforward approach to achieve higher solar-to-electricity conversion efficiencies (η). In addition, multi-junctions are interesting building blocks for new solar-to-fuel approaches based on PV/photo-electrochemical (PEC) or PV/electrochemical (EC) configurations. Multi-junctions PV devices offer high flexibility in delivering the high voltages of 1.6-3.2 V required to split water or reduce carbon-dioxide.

In this contribution we report on the optimization of a large variety of hybrid multi-junction PV devices. The devices are based on 1) a large portfolio of photovoltaic materials and 2) various types of PV device architectures, like: amorphous silicon (a-Si:H), amorphous silicon-germanium (a-SiGe:H), and nano-crystalline silicon (nc-Si:H) p-i-n junctions; CIGS/CdS hetero-junctions; organic photovoltaic (OPV) devices; and monocrystalline silicon wafer/a-Si:H based hetero-junction solar cells (c-Si HJ). Every type of multi-junction device configurations exhibits its own advantage, like high conversion efficiencies, cost-effective module topologies, limited usage of materials, easy up-scalable processing methods for large areas, high water resistant PV materials to allow flexible and cheaply encapsulated modules and high voltage (and current) material devices for monolithically integrated PEC-PV concepts.

The results of various types of devices will be presented: a-Si:H/CIGS 2-junctions, a-Si:H/OPV 2-junctions, and a-Si:H/a-Si:H/OPV 3-junctions, nc-Si:H/c-Si 2-junction and a-Si:H/nc-Si:H/c-Si 3-junction and a-Si:H/a-SiGe:H/c-Si 3-junctions.

The general design rules of these hybrid PV devices to accomplish high conversion efficiencies are discussed, like tackling the crucial electrical and optical loss mechanism. First, a detailed study on a wide variety of tunnel-recombination junctions for hybrid devices will be presented. Secondly, to realize conditions close to current matching a wide variety of light management concepts are discussed, like: modulated surface textured substrates and interfaces to establish a compromise between ideal light trapping and processing of high quality PV materials; bi-functional intermediate layers that act as reflector layers and tunnel recombination junctions; and minimizing the parasitic absorption losses of supporting layers. The current state-of-the-art hybrid PV devices will be presented.

Finally, examples of the application of these multi-junction devices in solar-to-fuel and water purification applications will be presented.

10:00 AM BREAK

SESSION ET11.02: Nano Technology Application to PV I
Session Chairs: Elisa Antolín and Huiyun Liu
Monday Morning, November 26, 2018
Hynes, Level 3, Room 304

10:30 AM *ET11.02.01

What Can Nano Really Do for Solar? [Erik Garnett](#)^{1,2}; ¹AMOLF, Amsterdam, Netherlands; ²University of Amsterdam, Amsterdam, Netherlands.

Over the past decade there has been extensive research into using nanostructures for solar cells. Although many interesting optical and electrical phenomena have been observed, nanostructured solar cells still have not exceeded (or even reached) the same efficiency level as their bulk counterparts.

The goal of this talk is to describe the ways in which nanoscience can theoretically improve solar cells and outline the remaining fundamental and applied research necessary to realize such theoretical gains in practice.

The talk will consist of two parts. First, ways in which nanoscience can help reach the standard Shockley-Queisser efficiency limit (34%) will be discussed. In particular, new methods for making a variety of relevant monocrystalline nanomaterials will be presented along with the accompanying nanophotonic nanoscale contact mechanisms that improve efficiency. Besides enhancing the intrinsic performance, such monocrystalline materials also present ideal model systems for nanoscale characterization, which can help in identifying and mitigating remaining loss mechanisms. Furthermore, a new characterization technique will be described which allows for fair performance comparison between nanoscale macroscopic solar cells. Second, concepts for going beyond the 34% efficiency limit will be discussed. These include implementing directional emitting nanostructures that can reduce photon entropy loss as well as new designs for multijunction solar cells that take advantage of the unique properties of nanomaterials.

11:00 AM ET11.02.02

Design and Simulation of Bifacial III-V Nanowire Arrays on Silicon [Anastasiia Fedorenko](#), Mohadesch A. Baboli, Parsian Mohseni and Seth Hubbard; Rochester Institute of Technology, Rochester, New York, United States.

Cost-competitive Si-based hybrid photovoltaic systems featuring high photoconversion efficiency can be realized through multijunction designs by combining Si and III-V materials. The manufacturing cost of III-V-on-Si solar cells can be further reduced by transitioning from thin-film to nanowire-based devices. III-V-on-Si multijunction solar cells using 1.75 eV GaAsP nanowires on the front side of bulk Si solar cell and 0.5 eV InGaAs nanowires on the rear side can theoretically exceed 50% conversion efficiency owing to an increase in absorption and improved carrier collection in nanowire structures compared to the planar devices. Wide-bandgap GaAsP top nanowire array, however, can suffer from low short-circuit current density lowering the overall efficiency of the multijunction cell. Thus, an optimization of the dimensions of nanowires relatively to their spatial distribution in the arrays is the key to achieving absorption enhancement providing high short-circuit current output to promote current matching between the subcells. Finite-difference time-domain (FDTD) simulation was used to model the absorption in periodic arrays of GaAsP nanowires on Si substrates dependent on the diameter, length, and spacing (center-to-center distance, or pitch) of the nanowires. Based on this study, the highest ultimate efficiency of 26% of the top 1.5 μm -thick nanowire array was achieved for the array with the nanowire diameter of 300 nm and pitch of 500 nm, thus showing an enhancement by about 5% compared to the planar GaAsP absorber with the same thickness. The peak total absorption of the arrays with different pitch was found to be associated with the diameter-to-pitch ratio of 0.6. Distinct resonance modes were resolved in the low-dimension nanowires. Additionally, front-side nanowires were shown to exhibit waveguiding properties in the absorption range of the underlying cells. The final presentation will include physics based simulation of devices utilizing GaAsP nanowire arrays on active Si substrates.

11:15 AM ET11.02.03

Optical and Electrical Properties of RF-PECVD Germanium Spin Coated with 40nm Silver Nanoparticles Khadija M. Jumaa¹, Aamenah Siddiqui¹, Ghada H. Dushaq², Mahmoud Rasras² and [Ammar Nayfeh](#)¹; ¹Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates; ²New York University Abu Dhabi, Abu Dhabi, United Arab Emirates.

Germanium is one of the promising semiconductors for photovoltaic applications such as solar cells, due to its high electron and hole mobility [1], and its high absorption in the infrared region. Several researchers have demonstrated Ge-based solar cells [2], in fact, Germanium-based solar cells already account for more than 80% of satellite applications [3]. Recently, good quality Ge-on-Si films fabricated using RF-PECVD (at $T < 600^\circ\text{C}$) were demonstrated [4]-[6], paving the way for their use in photovoltaic applications. From optical perspective, Ge has a high refraction index and 60% normal incidence reflection which leads to high surface reflection and hinder its use in solar cells without employing anti-reflective coatings (ARC). The use of metal nanoparticles, such as silver, is a low-cost and viable alternative to other ARC materials to improve the optical and electrical properties of Ge-on-Si films for solar cell applications. Metal nanoparticles are strong scatterers of light at wavelengths near their resonant frequency [7]. This work studies the effect of spin coating of 40nm silver nanoparticles on 700nm of Ge-on-Si films grown using RF-PECVD. The optical and electrical properties of the films after spin coating with 10ml and 20ml of 40nm silver nanoparticle colloidal solution are studied and compared to the film properties with no nanoparticles present. The concentration of silver nanoparticles in the aqueous buffer solution is 0.02mg/ml, provided by Sigma-Aldrich. In this work, Ossila Spin coater was used for spinning 40nm silver nanoparticles on RF-PECVD deposited 700nm Ge-on-Si films [4]-[6], where the spinning was performed for 45 seconds at 2000rpm. Three samples of Ge films were used, one sample is left as a reference sample and the other two are coated with 10ml and 20ml of the silver nanoparticles colloidal solution, respectively, which was dispersed using a pipette. Using ImageJ software for image analysis the spinning led to the deposition of ~ 480 nanoparticles/ mm^2 (0.047%) surface coverage and ~ 3280 nanoparticles/ mm^2 (0.328%) coverage, the samples were then characterized for optical reflectance and sheet resistance.

The optical and electrical properties of Ge-on-Si films with and without silver nanoparticles were analyzed. The reflectance was measured using LAMBDA1050UV/Vis/NIR Spectrometer. Results showed that presence of nanoparticles reduced the amount of the reflected light due to plasmon effect which enhances the light absorption in the visible and near-infrared region. The sample with no nanoparticles had the highest sheet resistance (200 Ω /Sq) whereas the sample with ~ 480 and ~ 3280 nanoparticles/ mm^2 appeared to have lower sheet resistance of 60 and 1.5 Ω /Sq, respectively, which is $>95\%$ less than the reference sample, showing promising film properties for device applications. Moreover, this finding validates the potential of using spin coated nanoparticles as a low-cost alternative to conventional ARC layers for photovoltaic applications.

11:30 AM ET11.02.04

Greenhouse Effect in Photovoltaic Cells to Enhance Efficiency Beyond the Shockley-Queisser Limit [Andrei Sergeev](#), Harry Hier, Kimberly Sablon and Christopher M. Waits; Army Research Laboratory, Adelphi, Maryland, United States.

The fundamental Shockley - Queisser (S-Q) model assumes chemical equilibrium between photocarriers and emitted photons (the same chemical potentials) and establishes a maximum solar conversion efficiency, which is limited by endoreversible thermodynamics. In this work we propose and investigate a new converter design, which mimics the greenhouse operation and increases the conversion efficiency, potentially above the Shockley - Queisser (S-Q) limit, due to suppression of radiative emission.

To overcome the S-Q limit, at least one of the conditions (i-v) that lead to the S-Q limit should be modified: (i) All above-bandgap photons are absorbed; (ii) All below-bandgap photons are lost; (iii) Every above-bandgap photon excites one electron-hole pair, (iv) All photocarriers reach thermal equilibrium with the lattice; (v) Photocarriers and emitted photons reach the chemical equilibrium. While various solar cell concepts related to (ii) - (iv) conditions have been actively studied (intermediate band cell, multi-exciton generation, hot carrier solar cell), the PV devices with chemical nonequilibrium between photocarriers and emitted photons (condition (v)) were not considered yet.

The proposed photonic-enhanced PV converter device mimics the greenhouse effect. The converter has a reflective interference "greenhouse" filter placed in front of a semiconductor cell and a reflective mirror on the back of the cell. The front filter is transparent for high energy photons, but traps low energy

photons emitted by photocarriers accumulated near the semiconductor bandgap. Thus, the high energy band-edge of the greenhouse filter establishes the photonic bandgap above the semiconductor bandgap. The photons with energy above the photonic bandgap are absorbed and create electron – hole pairs. Most of the excess energy is gained by the photoelectron, while the hole has energy close to the edge of the valence band. For this reason, the kinetics of photoelectrons is more manageable than the kinetics of photo-generated holes. To optimize the kinetics of photoelectrons, the semiconductor PV cell should be the n-p single junction diode with a p-doped base. In the optimized operating regime of the greenhouse converter, the chemical potential of photoelectrons near semiconductor bandgap can substantially exceed the chemical potential of photoelectrons above the photonic bandgap established by the filter. Such chemical nonequilibrium may be realized due to strong interaction of photoelectrons with holes. As a result, the photoelectrons depopulate the states with energies above the photonic bandgap. Reduced photoelectron population of states above the photonic bandgap reduces the emission and improves conversion efficiency above the S-Q limit, up to 44%.

The work was supported by U.S. Army Research Laboratory.

11:45 AM ET11.02.05

SiGeSn as a Candidate Material System for use in Thin-Film Multi-Junction Solar Cells Phoebe Pearce¹, Nicholas Ekins-Daukes^{2,1} and Andrew Johnson³; ¹Department of Physics, Imperial College London, London, United Kingdom; ²School of Photovoltaic and Renewable Energy Engineering, University of New South Wales, Sydney, New South Wales, Australia; ³IQE, Cardiff, United Kingdom.

Materials with a circa-1 eV bandgap are necessary in the optimal design of multi-junction solar cells, with one of the optimal bandgaps in many designs for two, three and four-junction cells being close to 1 eV. The lack of suitable high-quality photovoltaic absorbers with a circa-1 eV bandgap and lattice constant matching that of Ge, (In)GaAs and In_{0.5}Ga_{0.5}P, commonly used in multi-junction solar cells, has meant recent research interest in various candidate material systems which can meet these requirements, including dilute nitrides, antimonides and bismides. A novel material system for use as a 1 eV absorber is the ternary Group IV alloy silicon-germanium-tin (Si_xGe_{1-x-y}Sn_y). By adding relatively small amounts of Si and Sn to Ge, both the bandgap and lattice constant can be tuned. With an Si:Sn composition of around 3.7:1, the lattice constant of the resulting alloy remains equal to that of Ge, while the bandgap can be tuned by varying the Si and Sn fractions in this ratio. It is possible to achieve a circa-1 eV direct transition at relatively low (x ≈ 0.1) Si and Sn fractions. At these compositions, the material remains slightly indirect, with its indirect bandgap around 0.8 eV. It is expected that the V_{OC} of solar cells incorporating SiGeSn will be reduced compared to a material with a fundamental direct gap at 1 eV, since carriers can thermalize to the lowest available band edge; however, current-matching considerations mean it is still beneficial to absorb primarily across the 1 eV transition, which also allows thin layers to be used. Single and triple-junction (InGaP (1.9 eV)/InGaAs (1.4 eV)/SiGeSn (≈ 1 eV)) devices incorporating SiGeSn have previously been demonstrated, and 0.95-1.05 eV direct transitions (and corresponding indirect gaps around 0.7-0.8 eV) have been observed in samples grown through CVD through optical photoluminescence and spectroscopic ellipsometry measurements. Further material and optical characterization will be presented, including X-ray diffraction, photoluminescence, photoreflectance, and spectroscopic ellipsometry, for a range of SiGeSn compositions lattice-matched to Ge. With knowledge of the fundamental material properties, the usefulness of SiGeSn for thin-film device architectures, e.g. in a triple-junction InGaP/InGaAs/SiGeSn solar cell, or as a bottom junction in a two-junction device, can be assessed through device modelling based on measured data. For each architecture, the optimal composition of SiGeSn within the range which can be grown can be determined. Because the aim is to use the 1 eV direct edge for absorption, rather than the lower indirect edge, a relatively thin layer of SiGeSn (several microns) can be used in these architectures, as opposed to e.g. Ge or Si-based tandems.

SESSION ET11.03: Perovskites

Session Chairs: Nicholas Ekins-Daukes and Rao Tatavarti
Monday Afternoon, November 26, 2018
Hynes, Level 3, Room 304

1:45 PM *ET11.03.01

High Throughput Analysis of Novel Semiconductor Materials for Photovoltaics Thomas Unold¹, Hannes Hempel¹, Justus Just², Pascal Becker¹ and Jose Marquez Prieto¹; ¹Dept. Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; ²Lund University, Lund, Sweden.

Future large scale application and employment of photovoltaic technologies calls for options for new compound semiconductor absorber materials that enable low-cost, earth-abundant, stable and high efficiency devices. The large phase space of multinary materials, caused by the compositional degrees of freedom, traditionally calls for tedious and time-consuming exploration of different compositional regions using multiple sample preparation and characterization runs. Accelerated development of multinary semiconductors can be achieved by deliberately generating compositional gradients to access a large compositional (combinatorial) variations within single deposition runs. Thus deposited films are analyzed by high-throughput characterization yielding maps of fundamental photovoltaic parameters such as absorption coefficient, luminescence-quantum yield, carrier lifetime, carrier mobilities and doping. Correlating these parameters with high-resolution composition mapping by spatially resolved X-ray fluorescence allows to quickly access promising regions in composition space, which can be further refined by additional variation of experimental conditions. We will discuss the application of such methods to kesterite-type materials Cu₂Zn(Sn,Ge)Se₄ as well as inorganic halid perovskites CsPbI₃, both prepared by combinatorial coevaporation techniques.

2:15 PM ET11.03.02

Structural and Optical Characterization of NaSbS₂- A Promising Solar Absorber Winnie Leung¹, Christopher Savory¹, Robert Palgrave¹ and David O. Scanlon^{1,2,3}; ¹Department of Chemistry, University College London, London, United Kingdom; ²Harwell Science and Innovation Campus, Diamond Light Source Ltd., Didcot, United Kingdom; ³University College London, Thomas Young Centre, London, United Kingdom.

There is an increasing demand to develop higher efficiency photovoltaics materials with desirable properties such as a band gap between 1.1 eV to 1.5 eV, high abundance and biocompatibility. Although CdTe and CIGS are the most commonly used and commercially available photovoltaic materials in solar cells, there are major drawbacks including the scarcity of tellurium and high toxicity of cadmium would hinder the potential of such materials and impact the environment. In order to overcome such challenge, earth-abundant photovoltaics are of increasing interest to become a better substitute and the new rising star in photovoltaic applications.

NaSbS₂ has been found to have desirable features for an efficient solar absorber material, such as an experimental band gap value of 1.5-1.8 eV and a large absorption coefficient within the visible light range¹. Recently, Rahayu *et al.* have demonstrated a strong absorption of light in NaSbS₂ coated SSCs

(semiconductor-sensitized solar cells) which leads to a high photovoltaic efficiency of 2.30%. Employing NaSbS₂ in photovoltaics is a relatively new and less explored area, however, non-toxicity and a high earth abundance, together with the desirable features of NaSbS₂ could make it an ideal candidate for photovoltaic applications.

In this study, we will investigate NaSbS₂ using different characterization techniques such as PXR, UV-Vis, XPS and EDX as well as ab initio calculations using hybrid Density Functional Theory to give a detailed analysis of the properties and potential applications of NaSbS₂.

References

1. V. Bazakutsa, N. Gnidash, A. Kul'chitskaya and A. Salov, *J. Sov. Physics*, **1975**, 18, 472-475
2. S. Rahayu, C. Chou, N. Suriyawong, B.A. Aragaw, J. Shi and M. Lee, *APL Mater.* **4**, **2016**, 116103

2:30 PM ET11.03.03

Tailoring the Structure and Defects of Non-Toxic Nanocrystalline Bi₂S₃ Solar Cells Maryam Masroor Shalmani and Pratap M. Rao; Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

Solar cells can satisfy the increasing demand for energy worldwide, but the toxicity of semiconductors used in solar cells can overshadow their utility as a renewable source of energy. Bi₂S₃, with a desirable band gap of 1.3 eV, and as a non-toxic n-type semiconductor can be a favorable replacement for toxic semiconductors containing Pb, Cd or Te. However, nanocrystalline Bi₂S₃ films synthesized by various techniques such as successive ionic layer adsorption and reaction (SILAR) have not reached high solar energy conversion efficiencies hitherto, and have primarily been studied as sensitizers for photoelectrochemical applications. Here, we report the synthesis and characterization of non-toxic all-inorganic solid-state Bi₂S₃ photovoltaic solar cells by SILAR. We enhanced the solar energy conversion efficiency of the nanocrystalline Bi₂S₃ solar cells by optimizing the structure of the electron and hole transport layers, and by tailored annealing treatments that modify the size of the Bi₂S₃ nanocrystals and decrease their defect concentrations.

2:45 PM ET11.03.04

Efficient Solid-State Infrared-to-Visible Upconversion Integrated in a Microcavity Mengfei Wu, Ting-An Lin, Michelle C. Sherrott, Vladimir Bulović and Marc Baldo; Energy Frontier Research Center for Excitonics, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Optical upconversion that turns infrared light into visible light could improve the efficiency of solar cells by capturing sub-bandgap photons. A solid-state device consisting of a monolayer of lead sulfide colloidal nanocrystals and a thin film of rubrene with a luminescent dopant can convert infrared photons at $\lambda \sim 1 \mu\text{m}$ into visible photons at $\lambda \sim 610 \text{ nm}$ via sensitized triplet-triplet annihilation [1]. Such a bilayer device, limited by low infrared absorption in the nanocrystals, requires 12 W cm⁻² of incident intensity at $\lambda = 808 \text{ nm}$ to attain maximum upconversion efficiency [1]. Depositing a silver back reflector with an optical spacer on top of the active bilayer enhances the optical field, and hence absorption, in the nanocrystal layer due to interference, boosting the upconverted emission by an order of magnitude and lowering the threshold intensity to 1.1 W cm⁻² when pumped at $\lambda = 980 \text{ nm}$ [2]. Here, to further increase the optical field, we deposit the above interference-enhanced device on top of a distributed Bragg reflector (DBR). Such a structure places the nanocrystal layer in a microcavity whose resonance can be tuned to the pump wavelength by adjusting the thicknesses of the DBR layers and the optical spacer. We observe another order-of-magnitude increase in the upconverted emission, and a threshold intensity as low as 20 mW cm⁻² at $\lambda = 980 \text{ nm}$, similar to the flux available in the AM1.5 solar spectrum. The microcavity-integrated device demonstrates the possibility of efficient solid-state upconversion under sunlight and its application to solar cells.

[1] Wu, Congreve, Wilson *et al.*, *Nat. Photon.* **10**, 31-34 (2016)

[2] Wu *et al.*, *Appl. Phys. Lett.* **110**, 211101 (2017)

3:00 PM BREAK

SESSION ET11.04: Organic Photovoltaics I
Session Chairs: Lan Fu and Jinwei Gao
Monday Afternoon, November 26, 2018
Hynes, Level 3, Room 304

3:30 PM *ET11.04.01

Studies of Carrier Generation, Separation and Transport in Mixed-Dimensional Heterojunctions by Scanning Photocurrent Microscopy Lincoln J. Lauhon; Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States.

The novel properties that emerge in low-dimensional materials and their heterojunctions have inspired exploratory research into both conventional and unconventional devices. Regardless of the application in question, Herbert Kroemer's famous statement that "...the interface is the device" remains a useful guide to understanding the potential for new or improved functionality and highlights an important challenge for characterization. In particular, the correlated structural and functional characterization of interfaces is necessary to understanding the potential landscape that regulates the behavior of excitons and charge carriers. This talk with focus on the photoresponse of unconventional mixed-dimensional heterojunctions in which charge carrier separation can be exploited for photodetector and photovoltaic applications. I will review our application of time and energy resolved scanning photocurrent microscopy (SPCM) to devices in thin film geometries that two-dimensional (2D) materials with nanowires, nanotubes, and organic semiconductors that are well studied for photovoltaic applications. {Allen, 2009 #42; Hyun, 2011 #25; Howell, 2013 #155; Jariwala, 2013 #161; Yoon, 2013 #160; Howell, 2015 #175; Jariwala, 2016 #193} SPCM encodes local information about the materials and junction in the device response, enabling the application of finite element device modeling to extract intrinsic materials parameters as well as understanding of extrinsic factors influencing performance.

Henning, A.; Sangwan, V. K.; Bergeron, H.; Balla, I.; Sun, Z. Y.; Hersam, M. C.; Lauhon, L. J. Charge Separation at Mixed-Dimensional Single and Multilayer MoS₂/Silicon Nanowire Heterojunctions. *ACS Applied Materials & Interfaces* **2018**, 10, 16760-16767. Yoon, K.; Lee, J. H.; Kang, J.; Kang, J.; Moody, M. J.; Hersam, M. C.; Lauhon, L. J. Metal-Free Carbon-Based Nanomaterial Coatings Protect Silicon Photoanodes in Solar Water-Splitting. *Nano Lett* **2016**, 16, 7370-7375. Jariwala, D.; Howell, S. L.; Chen, K. S.; Kang, J. M.; Sangwan, V. K.; Filippone, S. A.; Turrissi, R.; Marks, T. J.; Lauhon, L. J.; Hersam, M. C. Hybrid, Gate-Tunable, van der Waals p-n Heterojunctions from Pentacene and MoS₂. *Nano Lett* **2016**, 16, 497-503. Howell, S. L.; Jariwala, D.; Wu, C. C.; Chen, K. S.; Sangwan, V. K.; Kang, J. M.; Marks, T. J.; Hersam, M. C.; Lauhon, L. J. Investigation of Band-Offsets at Monolayer-Multilayer MoS₂ Junctions by Scanning Photocurrent Microscopy. *Nano Lett* **2015**, 15, 2278-2284.

4:00 PM ET11.04.02

Environmental Friendly Processing of Water/Alcohol Based Nanoparticle Inks for Organic Solar Cells Chen Xie, Ning Li and C. Brabec; University of Erlangen-Nuremberg, Erlangen, Germany.

Low-cost fabrication through industrial printing or roll-to-roll coating techniques at low temperatures is the central strategy of organic photovoltaics to gain market readiness. One pivotal challenge to transfer organic photovoltaic (OPV) from lab to fab is to establish methods allowing to replace environmental hazardous solvents by using non-halogenated, eco-friendly and green solvents without losing efficiency.

To achieve the environmental friendly processing in OPV, here we report on application of light-harvesting material-based nanoparticle (NP) inks for water/alcohol processing. A low bandgap polymer diketopyrrolopyrrole–quinquethiophene (PDPP5T-2) and the methanofullerene PC₇₁BM were processed into three types of nanoparticles: pristine fullerene NPs, pristine polymer NPs as well as mixed polymer:fullerene NPs, allowing the formation of bulk heterojunction (BHJ) composites with different domain sizes. Mild thermal annealing is required to melt the nano-spheres and enable the formation of interconnected pathways within mixed phases. This BHJ is accompanied by a shrinkage of film, whereas the more compact layers show enhanced mobility. We find consistently reduced recombination and better performance for mixed NP, containing both, the polymer and the fullerene within a single NP. The optimized solar cell processed by ultra-small NPs delivered a power conversion efficiency (PCE) of about 3.4%. This is among the highest values reported for aqueous processed OPVs, but still lacks performance compared to those being processed from halogenated solvents. Incomplete crystallization are identified as main roots for reduced efficiency.

We further demonstrate a novel, robot based, high throughput procedure performing automatic poly(3-hexylthio- phenylene-2,5-diyl) (P3HT) and indene-C60 bisadduct (ICBA) nanoparticle ink synthesis in non-toxic alcohols. A novel methodology to prepare particle dispersions for high-efficient OPVs by manipulating the particle size and solvent system was studied in detail. The ethanol dispersion with a particle diameter around 80-100 nm exhibits reduced aggregation and sedimentation yielding a power conversion efficiency of 4.52%, which is the highest performance reported for water/alcohol processed OPV devices.

By achieving both the water and alcohol processing of high efficient organic solar cells, we believe that the aqueous/alcoholic printing of organic NP inks will be a trendsetting strategy for the reliable and eco-friendly production of OPVs.

4:15 PM ET11.04.03

Aggregation Strength Tuning in Difluorobenzoxadiazole-Based Polymeric Semiconductors for High-Performance Thick-Film Polymer Solar Cells Chen Peng; Department of Materials Science and Engineering, South University of Science and Technology of China, Shen Zhen, China.

High-performance polymer solar cells (PSCs) with thick active layers are essential for large-scale production. Polymer semiconductors exhibiting temperature-dependent aggregation property offer great advantages towards this purpose. In this study, three difluorobenzoxadiazole (fBX)-based donor polymers, **PfBX-T**, **PfBX-TT**, and **PfBX-DTT**, were synthesized, which contain thiophene (T), thieno[3, 2-*b*]thiophene (TT), and dithieno[3,2-*b*:2',3'-*d'*]thiophene (DTT) as the π -spacers, respectively. Temperature-dependent absorption spectra reveal that the aggregation strength increases in the order of **PfBX-T**, **PfBX-TT**, and **PfBX-DTT** as the π -spacer becomes larger. **PfBX-TT** with the intermediate aggregation strength enables well controlled disorder-order transition in the casting process of blend film, thus leading to the best film morphology and the highest performance in PSCs. Thick-film PSC with an average power conversion efficiency (PCE) of 8.91% and the maximum value of 9.10% is achieved using **PfBX-TT**:PC₇₁BM active layer with a thickness of 250 nm. The neat film of **PfBX-TT** also shows a high hole mobility of 1.09 cm² V⁻¹ s⁻¹ in organic thin-film transistors. When **PfBX-DTT** and **PfBX-T** are incorporated into PSCs utilizing PC₇₁BM acceptor, the average PCE decreases to 6.54% and 1.33%, respectively. The performance drop mainly comes from reduced short-circuit current, as a result of non-optimal blend film morphology caused by a less well controlled film formation process. A similar trend was also observed in non-fullerene type thick-film PSCs using IT-4F as the electron acceptor. These results show the significance of polymer aggregation strength tuning towards optimal bulk heterojunction film morphology using fBX-based polymer model system. The study demonstrates that adjusting π -spacer is an effective method, in combination with other important approaches such as alkyl chain optimization, to generate high-performance thick-film PSCs which are critical for practical applications.

4:30 PM ET11.04.04

Minimal Driving Energy and Reduced Recombination Yield Record Low Voltage Losses in Cascade Organic Solar Cells Vasileios C. Nikolis¹, Johannes Benduhn¹, Dieter Neher², Donato Spoltore¹ and Koen Vandewal³; ¹TU Dresden, Dresden, Germany; ²University of Potsdam, Berlin, Germany; ³Hasselt University, Hasselt, Belgium.

High photon energy losses (E_{loss}) constitute a major performance limiting factor for organic solar cells (OSCs), limiting significantly their open-circuit voltage (V_{OC}) and power conversion efficiency (PCE). Reduction of E_{loss} , while keeping a high external quantum efficiency (EQE), can lead OSCs into significantly higher power conversion efficiencies (PCE).

In this work, we report a multilayer cascade device architecture which increases V_{OC} through the insertion of discontinuous interlayers between electron donor (D) and electron acceptor (A). We systematically study the influence of adding various interlayers in a sequentially deposited α -6T/interlayer/SubNc/SubPc cascade OSC, resulting in a V_{OC} which increases from 0.98 V to 1.16 V. We show that this remarkable V_{OC} -increase of 0.18 V is due to the suppression of non-radiative recombination, as a consequence of a reduced physical contact between α -6T (D) and SubNc (A). The EQE of electroluminescence (EQE_{EL}) of 0.9 E-4 for our highest voltage device is one of the highest for OSCs and corresponds to non-radiative losses of 0.23 eV, which are the lowest reported for OSCs. Hence, we achieve E_{loss} of 0.58 eV from the optical gap (E_{opt}) to V_{OC} and 0.61 eV energy losses from the low energy peak of the EQE spectrum to V_{OC} . Most importantly, the low energy (700 nm) EQE peak remains high at 79%, despite a minimal driving force for charge transfer of less than 10 meV.

Our work shows that low E_{loss} can be efficiently combined with a high EQE in organic photovoltaic devices.

8:30 AM *ET11.05.01

2D Material-Based Layer Transfer to Revolutionize Photovoltaic Energy Generation Jeehwan Kim; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Because of substantially low cost of Si wafers, Si-based photovoltaics (PV) has been dominating although maximum power conversion efficiency of III-V solar cells is substantially higher than that of Si solar cells. To address this issue, wafer-recycling technique has been developed for the past few decades. However, the cost of recycling process has been much higher than that of the wafer. Thus, the room to improve leveled cost of energy has been limited. In today's talk, I will introduce MIT's novel wafer-recycling technique, so called a 2D material-based layer transfer process. We discovered that single-crystalline III-V PV layers can be epitaxially grown on graphene-coated III-V substrates, where the graphene is sufficiently thin such that crystalline orientation of III-V films can be guided by the substrate beneath graphene. The slippery graphene surface allows the III-V PV layers to be released from the substrate while the III-V substrate can be constantly reused. I will discuss how this technology revolutionizes photovoltaic technology by maximizing efficiency of solar cells while maintaining the production cost.

9:00 AM ET11.05.02

Improved Light Harvesting with a Printed Light Guiding Nano-Structure to Increase the Performance of Flexible CZTS-Monograin Photovoltaic Modules Martin Ursprung¹, Lukas Plessing¹, Dieter Nees², Dirk Bontinck³ and Dieter Meissner^{1,4}; ¹CrystalSol GmbH, Vienna, Austria; ²Materials, Institut für Surface Technologies and Photonics, Joanneum Research Forschungsgesellschaft mbh, Weiz, Austria; ³Allnex, Drogenbos, Belgium; ⁴Materials and Environmental Technology, TTÜ, Tallinn, Estonia.

CrystalSol has developed a novel PV-module structure and a manufacturing process for both, the semiconductor powder as well as the PV-modules. The core innovations are a light absorbing layer made of a single crystalline semiconductor powder and a low cost and scalable roll-to-roll production process. The crystals are made of copper, zinc, tin, sulfur and selenium (CZTS) and are manufactured separately before module production. This unique technology combines the advantage of a single crystalline absorber with a vacuum free low cost printing process.

The weight of the membrane is about 0.5 kg/square meter up to 1 kg/square meter depending on the encapsulation used. It can be rolled with a radius of less than 5 cm and tailored to the customer's needs. As a result of intense research an efficiency of 9.5 % has been reached.

The CrystalSol membrane layout is based on semiconductor grains, which are deposited as a monolayer. The photoactive material - the grains - covers about 80 % of the provided area thus incident light falling into the gaps between the grains, is not utilized.

In this paper a light-guiding structure is presented, which deflects the light towards the CZTS-grains enabling a higher share of incident light absorption and therefore an increase in photocurrent of up to 6.5 % which results in a 6.7 % gain in module performance. The foil deflects roughly 40 % of the incident light perpendicular to the line structure, whereby longer wavelengths show a wider deflection angle than shorter wavelengths. This structure was developed within the framework of the project Nano_Outside by JR (roll-to-roll-UV-nanoimprint lithography – R2R-UV-NIL), allnex (UV-curable resins) and CrystalSol (flexible PV-modules). The project is funded by the Austrian Research Promotion Agency (FFG). The concept was first tested with printed nanostructures and developed further by using R2R-UV-imprinting on a self-adhesive PET foil, which could easily be applied to the CrystalSol modules. The UV-imprint-resin is based on urethane acrylates and designed to meet the requirements of the R2R-UV-NIL processes being strong adhesion to polymer substrates, high curing speed and imprint fidelity as well as excellent outdoor – i.e. abrasion and weathering – stability for the application on PV-modules.

The optimization of the nanostructure manufacturing, its impact on the PV-performance, as well as an outdoor stability assessment of the structure will be demonstrated.

9:15 AM ET11.05.03

Thermo-Mechanical Lift-Off of Thin-Film Photovoltaics—High Specific Power, Low Cost Deborah McGott^{2,1}, Mike Kempe², Stephen Glynn², Nick Bosco², Colin A. Wolden¹ and Matthew O. Reese²; ¹Colorado School of Mines, Golden, Colorado, United States; ²National Renewable Energy Laboratory, Golden, Colorado, United States.

Thin-film photovoltaics (PV), such as cadmium telluride (CdTe) and $\text{CuIn}_x\text{Ga}_{1-x}\text{Se}_2$ (CIGS), offer extremely low manufacturing costs ($< \$0.50/\text{W}_p$) and have achieved device and module efficiencies that rival multi-crystalline silicon. However, despite being comprised of just a few microns of active material, thin-film modules are among the heaviest due to their double glass construction. This increases costs and prohibits their use in applications where flexibility and specific power (power-to-weight ratio) are critical factors. One approach to overcome this issue is to synthesize the solar cells directly on flexible substrates such as stainless-steel foils or polyimide. While success has been obtained using this approach, it can often introduce additional weight (stainless steel) and/or processing steps (polyimide).

Here, we describe an innovative technique to lift off thin-film solar cells that are grown under standard processing conditions from their glass substrates in a clean, reproducible manner. In this two-step process, we first laminate a commercially available polymeric backsheet to the solar cell, then submerge the stack in a cold bath ($T \leq -30^\circ\text{C}$) to thermally shock the system. This causes the polymer to contract quickly and pull the polycrystalline film cleanly off of its substrate at an interface that is weakened by a monolayer accumulation of 2-D material (CdCl_2 in CdTe and MoS_2 in CIGS). To enable clean lift-off of diverse thin-film architectures, a theoretical framework is developed and key process control parameters are identified. Focusing on CdTe devices, we show that the lamination temperature and device architecture control the quality of lift-off, while the rate at which the film stack is removed is controlled by the temperature of the cold bath.

Crack-free CdTe devices are removed and successfully re-contacted, recovering up to 80% of the original device efficiency. The areal density of these devices is $\sim 0.4 \text{ kg m}^{-2}$, a reduction of over an order of magnitude relative to their initial weight on glass. The broader applicability of this technique is then demonstrated by lifting off large areas ($>50 \text{ cm}^2$) of CIGS solar cells. The ability to lift these two major thin-film technologies off post-growth will allow for pre-existing high-volume manufacturing lines and their cost-structure to be leveraged, thus providing an alternative pathway toward inexpensive, flexible PV with high specific power.

9:30 AM ET11.05.04

Ligand Exchange of Copper Indium Gallium Sulfide Nanoparticles for Minimization of Carbonaceous Impurities in High Efficiency Solution Processed Photovoltaics Ryan Ellis, Jacob Fields and Rakesh Agrawal; Purdue University, West Lafayette, Indiana, United States.

Solution processing is an attractive method of producing high efficiency copper indium gallium selenide (CIGSse) photovoltaics with significantly lower manufacturing costs, higher throughput, and greater large scale uniformity compared to traditional vacuum-based deposition technologies. A relatively benign colloidal nanoparticle route has shown great promise, reaching power conversion efficiencies up to 15%. However, further improvements are hindered by carbonaceous impurities originating from high boiling point organic ligands commonly used in nanoparticle synthesis. These ligands are

difficult to remove via thermal treatment and often leave carbonaceous impurities in the final photovoltaic device as a distinct “fine grain layer” which can increase series resistance and could contribute to interfacial recombination. As such, the exchange of native ligands with volatile and non-contaminating ligands is of great interest to reduce carbonaceous impurities. For a successful ligand exchange for photovoltaic device fabrication, the exchange must remove the majority of native ligands, be thermally labile and not leave impurity elements, retain the stoichiometry of the as-synthesized nanoparticles, exhibit excellent colloidal stability at high mass concentrations, and not inhibit liquid selenium assisted sintering of the absorber layer. In this work, we screen a wide variety of ligand exchange reactions for removal of native oleylamine ligands on copper indium gallium sulfide nanoparticles using a variety of amines, thiols, pyridines, and inorganic sulfide ligands to simultaneously meet the aforementioned criteria necessary for photovoltaic device fabrication. The screening revealed that alkylamines preferentially etched indium and gallium from the nanoparticles, thiols and functionalized pyridines were not readily thermally labile, and inorganic sulfides and pyridine were individually unable to remove the entirety of native ligands. Using these observations, a novel two-step ligand exchange was developed in which an initial microwave-assisted solvothermal ligand exchange was performed with pyridine to remove the bulk of native ligands, followed by an inorganic sulfide exchange to remove pyridine, additional native ligands, and to significantly enhance the colloidal stability of the nanoparticles in a variety of polar solvents. The two-step approach was uniquely able to meet all of the aforementioned criteria necessary for successful photovoltaic device fabrication. Along with the careful selection of solvents for ink formulation, ligand exchanged inks were employed for the fabrication of solution processed absorber layers, demonstrating high efficiency, fine grain free CIGSSe photovoltaics using a highly scalable and benign ink. The novel ligand exchange and subsequent photovoltaic device fabrication methods used hold wide applicability for the removal of carbonaceous impurities in nanoparticle based solution processed chalcogenide photovoltaics.

9:45 AM ET11.05.05

Effect of Solution pH and Post-Annealing on the Optical Bandgap of the Copper Oxide Thin Films Grown by SILAR Method Farhad Syed¹, Alauddin Hossain², Md. Abdul Majed Patwary³, Rumana Akter², Nazmul Islam Tanvir¹, Shanta Majumder², Muhammad Shahriar Bashar⁴ and Mohammad Atiqur Rahman²; ¹Industrial Physics Division, Bangladesh Council of Scientific and Industrial Research, Dhaka, Bangladesh; ²Department of Chemistry, Comilla University, Kotbari, Bangladesh; ³Optoelectronics Laboratory, Department of Science and Advanced Technology, Saga University, Saga, Japan; ⁴Institute of Fuel Research and Development (IFRD), Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh.

Copper oxide is one of the most studied p-type materials for solar cell and other optoelectronic devices due to its direct band gap, high optical absorption in the visible region and suitable band alignment with its n-type counterpart materials such as ZnO, TiO₂ etc. Cuprous oxide (Cu₂O) thin films have been grown on both microscope glass slides and Fluorine-doped Tin Oxide (FTO) substrates by SILAR technique. The pH level of the bath solution and concentration of NaOH solution were systematically varied. The films were deposited in the pH range 3.45 - 7.35 as well as 1M and 2M NaOH solution to control the texturing and phase purity of the as-deposited films. The effect of post-annealing temperatures (75-350 °C) on the as-deposited films was also studied and found to be crucial to control the optical band gap and electrical properties of the films. The XRD measurement showed that the as-deposited films were single phase Cu₂O with (111) preferred orientation and found to be changing with increasing pH and annealing temperature. The (111) texturing of the annealed Cu₂O films were found to be increasing and stable phase up to 200 °C and completely converted to cupric oxide (CuO) phases when the temperature reached to 350 °C. The estimated optical band gap and the sheet resistivity of the as-deposited and annealed samples were found to be in the range (2.35 – 1.43) eV and (154.22 –393.9) × 10⁴ Ω/square respectively. The prepared film shows fiber-like and dense grain surface morphology observed from their SEM images. The performance of copper oxide films was tested by estimating LED modulated ON/OFF ratio into a photoelectrochemical cell and was found to be reasonable to integrate them into optoelectronic devices.

10:00 AM BREAK

SESSION ET11.06: Organic Photovoltaics II

Session Chairs: Lan Fu and Jia Zhu
Tuesday Morning, November 27, 2018
Hynes, Level 3, Room 304

10:30 AM *ET11.06.01

Bio-Inspired Metallic Networks as Flexible Transparent Conductors—From Lab to Pilot Scale Jinwei Gao¹, Jun-Ming Liu² and Krzysztof Kempa³; ¹South China Normal Univ, Guangzhou, China; ²Nanjing University, Nanjing, China; ³Boston College, Chestnut Hill, Massachusetts, United States.

Transparent conductors (TC) are critical materials for modern optoelectronic applications ranging from light emitting diodes, to displays (including touch-screen and flexible), to solar cells, wearable electronics. In lighting and solar applications TC must be highly conducting in order to lower the ohmic losses. In display applications, microscopic transparency and lack of haze is required, as well as there is a need for mechanical flexibility in the case of flexible displays and wearable electronics. A chemical stability is also a must. These new requirements put pressure on the current standard material, indium tin oxide (ITO), which has overall good electro-optic performance and chemical stability, but is resistive, brittle and quite expensive. Recently, a new generation of TC materials emerged as a possible replacement for ITO, which can be tailored to satisfy all the above requirements. This talk will review such materials including our metallic networks, which have been inspired by nature. In one example, we developed the quasi-fractal hierarchical TC based on the self-cracking network combined with nanowires. This network TC has record high conductivity and simultaneously excellent transparency, and thus is ideal for lighting and solar applications. We have shown, that it is the plasmonic refraction of nanowires, which allows for the network increased transparency beyond the classic, shading limit. In addition, this network TC is mechanically flexible, and can be made inexpensively with wet chemical processing only. A version of this network can be used in displays, due to its low haze and low network visibility. We have very recently developed a roll-to-roll pilot production line of the self-cracking network on flexible plastic substrates with width of ~ 400 mm.

11:00 AM ET11.06.02

Exciton Binding Energy and Dielectric Effect in Small Molecular and Polymeric Photovoltaic Materials Ho-Wa Li, Liu Taili and Sai-Wing Tsang; City University of Hong Kong, Hong Kong, Hong Kong.

Owing to the low dielectric constant of organic materials, organic photovoltaic (OPV) is regarded as an excitonic solar cell that excitons are generated upon photo-excitation. Such intrinsic small dielectric constant (ϵ) in organic materials results in large exciton binding energy (E_b). That becomes a key detrimental factor limiting the further improvement in organic photovoltaic cells. Increasing the material dielectric constant seems to be a straight-forward

strategy to reduce the strong coulombic attraction of the photo-generated electron-hole pairs. Despite the matter of importance, there are limited reports in measuring the E_b and ε in organic photovoltaic materials and the correlation between the dielectric constant and the exciton binding energy is unclear. Here, we extend our demonstration by using quantum efficiency measurement [1] and electro-absorption to access the transporting gap and exciton binding energy in pristine organic photovoltaic materials for polymeric donor, fullerene and non-fullerene small molecular acceptors. It is found that E_b varies from 0.3 eV to 1.2 eV in those prototypical materials and it apparently follows a second power law with the inverse of the dielectric constant of the materials, i.e. $E_b \propto 1/\varepsilon^2$. Instead of widely assumed first-order dependence, this second order dependent relationship is firstly reported. Interestingly, we have also found that the binding energy is more dependent on the molecular-molecular interaction rather than the intrinsic properties of single molecule. In this presentation, we will also demonstrate how the higher dielectric material benefits the exciton dissociation at donor/acceptor interface.

[1]: Ho-Wa Li, Zhiqiang Guan, Yuanhang Cheng, Taili Liu, Qingdan Yang, Chun-Sing Lee, Song Chen, Sai-Wing Tsang, On the Study of Exciton Binding Energy with Direct Charge Generation in Photovoltaic Polymers, *Adv. Electron. Mater.*, 2016, 2 (11), 1600200.

11:15 AM ET11.06.03

Improving the Photovoltaic Performance and Mechanical Stability of Flexible All-Polymer Solar Cells via Tailoring Intermolecular Interactions Minjun Kim, Hong Il Kim, Seung Un Ryu, Cheol Woong Park and Taiho Park; Pohang University of Science and Technology, Pohang, Korea (the Republic of).

Naphthalene diimide (NDI)-based polymers are significantly promising electron accepting materials in all-polymer solar cells (all-PSCs) due to strong light absorption at the near infrared region and high electron mobility. Most NDI-based polymers have a large crystal structure through thermodynamically self-assembled aggregates, which lead to the low intermixing with polymer donor, resulting in large-scale phase separation in all-polymer blend films. The undesirable all-polymer blend morphologies cause inefficient exciton dissociation and charge transport between polymer donor and polymer acceptor, limiting the photovoltaic performance as well as mechanical resilience in all-PSCs. The low crystalline polymer acceptor with highly interconnected networks can provide an effective approach to high electron mobility and finely phase-separated blend morphology. Herein, we introduced a copolymer of NDI and (*E*)-1,2-bis(3-fluorophenyl)ethene (FTVT) (PNDI-FTVT) as a polymer acceptor with a low crystalline structure and high electron mobility (μ_e). The blend film incorporating PNDI-FTVT exhibits well-mixed morphology without a large-scale phase separation. Moreover, PNDI-FTVT forms inter-junctions between polymer donor and polymer acceptor through strong π - π stacking via fluorine induced dipole-dipole intermolecular interactions, improving the chain interconnectivity to construct better charge transport pathway. PNDI-FTVT based flexible all-PSC exhibited increased photovoltaic performance compared to PNDI-TVT based flexible all-PSC (3.86% \rightarrow 5.90%) and excellent mechanical stability in the flexible all-PSC, maintaining 72% of its initial performances (5.90% \rightarrow 4.26%). This is the highest efficiency in the field of flexible all-PSCs and the first demonstration of the photovoltaic operation in bending test.

11:30 AM ET11.06.04

Inclusion of Hybridised Silicon Nanospheres into Photovoltaic Devices Using Semiconducting Polymers Jonathon Mitchell; Koriyama, Japan.

Hybridised silicon nanospheres formed by simplified plasma-enhanced chemical vapour deposition (PECVD), without seed particle injection or microwave plasma are fabricated in a variety of dimensions and with differing physiochemical properties, such as selective doping, via a modified Multi-Layer PECVD technique. Although the nanospheres can be directly incorporated onto a suitable substrate and within a dielectric during deposition, ex-situ processes have shown additional purpose can be ascribed to the nanosphere surface. By reducing the necessity of colloidal suspension or centrifugation steps, the nanospheres can be produced in functionalised states, for wavelength selection, light trapping and nanoscale dopant inclusion without negatively compromising the conductivity or passivation of the underlying structure. This can be attributed to the homogeneous H-Si distribution with no evidence for surface or bulk aggregation.

Suspension in poly-vinyl alcohol or ethyl acetate was utilised first for liquid phase analysis, then subsequently, for printing onto a selection of substrates, including crystalline silicon (c-Si) and semiconducting polymer. For silicon, monocrystalline with both planar and lightly textured surfaces were utilised. Semiconducting polymers based on naphthobisoxadiazole (PNOz4T), and Benzo[1,2-b:4,5-b']dithiophene (BDT) incorporating thieno[3,4-c]pyrrole-4,6-dione (TPD) as a main chain and oligo(thienylenevinylene) side chain were tested.

Non-peripherally alkyl-substituted phthalocyanines like octahexylphthalocyanine (C6PcH₂) were examined as a top-layer for their higher carrier mobility compared to a-Si:H layers, and present a suitable matrix for allocation of the nanospheres, due to its hexagonal disordered columnar mesophase at approximately 170°C. An amorphous In₂O₃ front contact layer comprised of a transparent conducting oxide (TCO) and transparent oxide semiconductor (TOS) are shown to be effective in enhancing the short circuit current density of the assembled device.

When incorporated into the polymer-silicon membrane, the hybridised silicon nanospheres provide a solution to non-brittle light trapping or wavelength selection for flexible photovoltaic devices.

SESSION ET11.07: Nano Technology Application to PV II

Session Chairs: Magnus Borgstrom and Yun Liu

Tuesday Afternoon, November 27, 2018

Hynes, Level 3, Room 304

1:30 PM *ET11.07.01

GaAsP Nanowires and Nanowire Solar Cells Jia Xu, Yunyan Zhang and Huiyun Liu; University College London, London, United Kingdom.

Aiming to achieve high-efficiency solar cells (SCs) and in the meantime driving down the cell cost has become the main challenge for photovoltaic researchers. Semiconductor nanowires (NWs), a special one-dimensional columnar structure with confining the carriers in two dimensions, has potential utilization to fabricate next-generation SCs due to its good strain tolerance, which can accommodate large lattice and thermal expansion coefficient mismatch between the nanowire and substrate. The band gap of the ternary material GaAsP can cover wavelengths ranging from green (550 nm) to near infrared (860 nm) at room temperature, which is one of the most promising III-V compound semiconductors for nanowire-based photovoltaic. While the silicon provides a cheap substrate, combining GaAsP nanowire with such silicon substrate is a feasible way to reduce the cost and increase the efficiency of SCs for the nanowire removes the issues related to strain at the GaAsP/Si interface. A two-junction tandem SC, consisting of a 1.7-eV GaAsP NW junction and a 1.1-eV Si junction, has been predicted to have a theoretical efficiency of 33.8% at 1 sun AM1.5G and 42.3% under 500 suns AM1.5D concentration respectively. Application of such a high-efficiency 1.7-eV/1.1-eV two-junction device in water splitting has potential to achieve high efficiency with 27.0%.

Here, we present the high-quality core-shell self-catalyzed GaAsP NWs grown on both un-patterned and patterned substrate by means of solid-source Molecular Beam Epitaxy (MBE) technique, which shows almost stacking-fault-free zinc blend crystal structure. We demonstrate their potential application on photovoltaic devices by single-NW solar cells achieved a single NW world record efficiency of 10.2%. We further investigate the application of GaAsP NWs and the effect of InGaP passivation in the water splitting and present a wafer-scale solar-to-hydrogen conversion efficiency of 0.5% for water splitting. These results open up new perspectives for integrating III-V nanowire photovoltaics on a silicon platform by using self-catalyzed GaAsP core-shell NWs. All of the enabling technology for fabricating the GaAsP SCs has already been developed.

2:00 PM ET11.07.02

Light Management in III-V Photovoltaics Using Back Surface Reflectors [Julia D'Rozario](#)¹, George Nelson¹, Rao Tatavarti² and Seth Hubbard¹; ¹Rochester Institute of Technology, Rochester, New York, United States; ²MicroLink Devices Inc., Niles, Illinois, United States.

Surface texturing has been used as an effective method to manage and trap light in photovoltaic devices. For GaAs solar cells, this can result in highly efficient devices that require less semiconductor material. In this work, light trapping techniques have been employed through textured back surface reflectors (BSR) in order to increase photon path length in GaAs solar cells which have been grown by metal organic chemical vapor deposition (MOCVD). The textured BSRs enable any unabsorbed photons to reflect off the back surface and reabsorb in the active region of the solar cell. This work focuses on the impacts from three different BSR designs which have been developed through lithography and wet chemical etch processes. All three textures were fabricated in an AlGaAs contact layer with 10% Al and 90% Ga. The first texture is a flat reflector which will allow a path length enhancement of 2. The second texture is a triangular grating and allows higher reflectance due to the increase in surface angles from the triangular geometry. The last texture is a random design and has been developed through a maskless wet chemical etch. This gives rise to a cheaper and faster method compared to the triangular grating which requires lithography processes and equipment. Compared to the flat and triangular textures, the random texture has resulted in a significantly increased optical path length due to the wide range of surface angles that allow light to be scattered in directions that result in total internal reflections from the front surface. These designs have been developed on GaAs solar cells with a range of base thickness and also using low bandgap nanostructures. The benefits from the different textures will be presented and can be seen by the increase in generated output current and voltage from the devices.

2:15 PM ET11.07.03

The Potential of Singlet Fission Photon Multiplier as an Alternative to Silicon-Based Tandem Solar Cells [Moritz H. Futscher](#)¹, Akshay Rao² and Bruno Ehrler¹; ¹AMOLF, Amsterdam, Netherlands; ²University of Cambridge, Cambridge, United Kingdom.

For large-scale implementation of photovoltaics, further improvement in the power-conversion efficiency is needed. Conventional silicon solar cells lose a large part of incident sunlight energy via thermalization of excited charge carriers. Singlet fission, a spin-allowed charge-carrier multiplication process which converts one singlet exciton into two triplet excitons is a promising way to reduce such thermalization losses. One way to harvest triplet excitons is by transfer of their energy into quantum dots that then emit photons into the silicon solar cell underneath. Thereby, the efficiency of the silicon solar cell can be increased by modulating the broadband solar spectrum.

We develop a model to simulate such a "photon multiplier", and how it enhances silicon solar cells under realistic conditions. This model includes the relevant physical parameters such as the energy of the singlet and triplet exciton, the full width at half-maximum of the quantum dot emission, and losses due to parasitic absorption and non-perfect wave guiding of the emitted photons. We simulate the performance potential of a photon multiplier in comparison to an optimized perovskite/silicon tandem solar cell under realistic conditions. We find that the photon multiplier is more stable against changes in the solar spectrum than tandem solar cells. We furthermore find that the better the silicon base cell, the lower the efficiency gain of a tandem solar cell compared to the silicon solar cell alone, while the efficiency gain of a photon multiplier increases with increasing efficiency of the silicon solar cell. For current record silicon solar cells, the photon multiplier can boost the efficiency by up to 4.2% absolute under realistic conditions.

2:30 PM ET11.07.04

Flexible and Light Weight GaAs Solar Cells with Micro-Pattern and Back Reflectors Kamran Forghani, David Rowell, Chris Stender and [Rao Tatavarti](#); MicroLink Devices Inc., Niles, Illinois, United States.

III-V multijunction solar cells have the highest record efficiency for any type of photovoltaic devices: E.g. about 38% for AM1.5 1-sun and 33% for AM1.5 1-sun, as reported for 3 junction cells utilizing epitaxial-lift-off (ELO) [1].

Application of backside reflecting mirror for solar cells will enhance the performance by multiple photo-recycling events. The increase in optical absorption, not only helps to boost the performance but also helps to thin the cell, making them radiation-hard for space applications. We present our finding on back patterned GaAs solar cells. Single junction GaAs solar cells with two different configurations of up-right on rigid n-type substrate, as well as inverted flexible ELO cells were investigated. Several different patterns were applied and their effect on the overall cell short circuit current (Jsc) and quantum efficiency was studied. A more than 4% increase of the Jsc was observed in the backside patterned devices. The Jsc as function of light incident angle will also be presented, indicating an improved photo-response at smaller incident angles as compared to the planar control samples.

[1] Alex Kirk et al., Recent Progress in Epitaxial Lift-Off Solar Cells, IEEE PVSC Proceeding (2018)

2:45 PM ET11.07.05

Epitaxial Growth of SiGe on Si Substrate by Printing and Firing of Al-Ge Mixed Paste [Shogo Fukami](#)¹, Yoshihiko Nakagawa¹, Kazuhiro Gotoh¹, Yasuyoshi Kurokawa¹, Masahiro Nakahara², Marwan Dhamrin² and Noritaka Usami¹; ¹Nagoya University, Nagoya, Japan; ²Toyo Aluminium KK, Gamo-Gun, Japan.

The germanium substrate used for the bottom cell of tandem III-V solar cells is one of the most expensive components of this device structure. To make these devices cost-competitive with silicon, it is necessary to find an alternative material having a narrow gap which is suitable for the bottom cell. Silicon-germanium (SiGe) has a lattice constant and band gap close to Ge while also being relatively low cost and environmentally friendly. Also, because SiGe is an all-proportional solid solution whose composition can be freely controlled, its lattice constant and bandgap can be precisely controlled. However, conventional SiGe fabrication methods such as solid phase crystallization or chemical vapor deposition require long growth times or toxic gases. Thus, we focus on liquid phase epitaxial (LPE) growth utilizing the melting point depression phenomena of Ge and Si by Al [1]. In this paper, we investigated methods for LPE growth of SiGe on Si(100) substrate by printing and firing Al-Ge mixed paste and the influence of epitaxial growth by heat treatment under various conditions.

We applied Al-Ge mixed paste which its thickness is about 30 μm on Si(100) substrate by screen printing and dried. LPE was performed using an Al-Ge mixed paste screen-printed on a Si(100) substrate and then annealing above Al-Ge eutectic temperature (420 °C) in the air or the Ar atmosphere. And we annealed at 700, 800 and 900 °C to investigate the influence of annealing temperature on the growth of SiGe. After annealing, the residue at the top of the Si substrate surface was etched with a solution of phosphoric acid (H₃PO₄: CH₃COOH: HNO₃: H₂O=16:1:1:2). The obtained SiGe was characterized by X-ray diffraction reciprocal space mapping (XRD-RSM), Scanning Electron Micrographs (SEM) and energy dispersive X-ray spectroscopy (EDX).

From the SEM and EDX images, in case of annealing at 800 °C in the air, wave-like oxide film was confirmed at SiGe/Si interface. It is assumed that the oxide film interfered with the growth of SiGe. On the other hand, at 800 °C in the Ar atmosphere, we succeeded in forming abrupt heterointerface with thick SiGe. The results of XRD-RSM indicated that only the Si peak was observed before annealing. After annealing, a peak derived from SiGe appeared in addition to the Si peak. The SiGe peak shape was widely distributed since the composition distribution of SiGe occurred. The peak obtained from XRD-RSM by annealing at 700 °C in the Ar atmosphere showed that Ge fraction in SiGe was 7.56 %, which is higher than at 800 and 900 °C. It is assumed that Ge fraction in SiGe decreased by annealing at higher temperature due to more dissolution of Si substrate. These results suggest that the average composition and composition distribution in the SiGe can be controlled by changing paste composition and heat treatment history.

[1] M. Dhamrin *et al.*, presented at PVSEC26, Singapore, 2016

3:00 PM BREAK

SESSION ET11.08: Thin Films II
Session Chairs: Jeehwan Kim and Kyle Montgomery
Tuesday Afternoon, November 27, 2018
Hynes, Level 3, Room 304

3:30 PM *ET11.08.01

Packing Photovoltaic Power Conversion in Solar Cells—Where is the Limit? Jean Francois Guillemoles^{1,4}, Stephane Collin^{3,1,4}, Laurent Lombez^{1,4}, Yoshitaka Okada² and Maxime Giteau²; ¹CNRS, IPVF, Palaiseau, France; ²RCAST, NextPV, Tokyo, Japan; ³C2N, CNRS, Palaiseau, France; ⁴NextPV, CNRS, Tokyo, Japan.

There are many benefits to be using lighter and thinner cells: they range from opening new application opportunities, increasing the technology sustainability, and possibly increasing efficiency and lowering the costs. Such possibilities were demonstrated by us and others on thin films, like CIGS and perovskite, but also on III-V compounds that have been made into flexible solar cells with potential for high efficiency and record power to mass ratio. As it turns, highest performance for solar cells goes with high power processing per unit volume, provided that absorption of incoming light is kept high. This is seen for instance in concentrated PV, but can also be done by reducing the thickness of the active material, provided efficient light management schemes are developed, such as the multi-resonant approach.

The presentation will highlight recent results obtained with high efficiency approaches to flexible solar cells, starting with thin film technologies and aiming at ultimate efficiencies such as III-V and Hot Carrier solar cells.

4:00 PM ET11.08.02

Investigation into the Selenization of Solution Processed Silver Zin Tin Selenide (Ag₂ZnSnSe₄) Thin-Film Solar Cells Xianyi Hu¹, Dana Sulas³, Steve Johnston³, Darius Kuciauskas³, Carol A. Handwerker¹ and Rakesh Agrawal²; ¹Materials Engineering, Purdue University, West Lafayette, Indiana, United States; ²Chemical Engineering, Purdue University, West Lafayette, Indiana, United States; ³National Renewable Energy Laboratory, Golden, Colorado, United States.

Although CZTS solar cells have been fabricated with a maximum power conversion efficiency (PCE) of 12.6%, no further improvement has been demonstrated since 2013 due to intrinsic defects. It has been proven that the high density of Cu_{Zn} or Zn_{Cu} anti-site defects limits performance. These defects create band tails and dramatically decrease the open circuit voltage (V_{oc}) of devices. To eliminate these intrinsic defects, Ag has been used to substitute for Cu, which increases the formation energy of anti-site defects due to its larger radius and single valence. Our group did partial substitution of Cu with Ag and showed improved minority carrier life time. Gershon *et al.* developed photovoltaic devices based on an n-type Ag₂ZnSnSe₄(AZTSe) absorber layer by co-evaporation and achieved ~ 5% PCE, suggesting the potential of this material.

To establish a more cost-effective method for large-scale fabrication of AZTSe, compared with vacuum deposition, solution-processing is needed. Here, we report a systematic investigation into the selenization process from mixed AZTS and ZnS nanoparticle films into large grain selenide films. We study key factors, such as selenization time, temperature, heating rate as well as Se vapor pressure utilizing a rapid thermal processor. Our results demonstrate that AZTSe has a narrow processing window to obtain phase-pure films with uniform composition and few pin-holes. We find that the heating rate plays an essential role in eliminating the formation of SnSe₂. Due to the fast sintering rate of the Ag-contained sulfide nanoparticles, selenization temperature and time have to be balanced to fabricate uniform, continuous, large grains. In addition, Se vapor condenses on the surface of nanoparticle film to enhance liquid-phase assisted grain growth of AZTSe films. To achieve a more uniform microstructure of AZTSe films and better adhesion between films and substrate, we deposit an intermediate layer on the surface of the film. We demonstrate that this layer helps with nucleation at the beginning of the selenization. We characterize the AZTSe films with photoluminescence and show a single, sharp peak at 1.3 eV without a defect emission shoulder in contrast to CZTSe.

We propose a selenization mechanism based on the microstructure evolution and phase transformations that we observed and compared with CZTS. Ultimately, we establish a strategy to obtain AZTSe films consisting of continuous grains with uniform composition and few pin-holes, which is essential for the future production of AZTSe solar cells.

4:15 PM ET11.08.03

An Insight into the Effect of Band Alignment at Grain Boundaries on Photovoltaic Performance in CIGS and CZTS Thin-Film Solar Cells Wenjie Li; Shenzhen Institute of Advanced Technology, Shenzhen, China.

The efficiency of CZTS solar cells is still not so high compared with other thin films such as CIGS. The underlying mechanism for the difference is a long-standing question that has remained elusive in spite of tremendous research efforts in the past. For polycrystalline thin film semiconductor, highly populated grain boundaries in the material will certainly have big influences on the photo-generated electron-holes. In this work, a conducting probe atomic force microscopy has been applied to study the electronic structure of CIGS and CZTS thin films with capability of nm-scale resolution. To exclude the surface effect, grain boundaries in the bulk were examined through cross-sectional SPM measurements and compared for both CIGS and CZTS. Different electronic structure of the grain-interior (GI) and grain boundary (GB) have been identified in both CIGS and CZTS thin films. We find that the band alignment between GI and GB in CIGS and CZTS is different, which can well explain the different device performance in two type of solar cells. With good Schottky contact between the AFM tip and semiconductor, a local electrical and photovoltaic performance can be measured and the conduction

band and valence band offset between GB and neighboring GI can be obtained. In CIGS, we can clearly find that the conduction band bent downward for about 200 meV and the valence band bent downward for about 340 meV at the GB, which makes the GB and GI in CIGS to form a type-II structure that benefits the electron-hole separation to give high photovoltaic performance. For CZTS, it is found that the conduction band bent downward, while the valence band bent upward which is in opposite to the case in CIGS. The GB and GI in CZTS behaves like a type-I hetero-structure that will trap both electron and hole inside the GB to produce strong recombination.

Many experiments had demonstrated that air annealing process can improve the CZTS device efficiency with increased open-circuit voltage and fill factor. Our experiments of cross-sectional SPM measurements revealed that, for grain boundaries in the bulk, after air annealing, the downward bending valence band of GB turned to be upward bending, while the conduction band of GB turned from downward bending to upward bending. This resulted in the formation of electron and hole barrier at GBs which reduced the recombination, which can well explain the increased efficiency. However, the air annealing induced GB states behaved as barriers which can block the transport of electron and holes. Better GB passivation techniques are still in need.

4:30 PM ET11.08.04

Improved Voc Deficit in Kesterite $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ Solar Cells via Grain Boundary Passivation at the p-n Junction Interfaces Cheng-Ying Chen^{1,2}, Naili Saidatin^{1,2,3}, Chih-Yang Huang^{1,2,4}, Bandyah Sri Aprillia^{1,2,3}, Ruci-San Chen³, Jih-Shang Hwang⁴, Kuei-Hsien Chen^{2,1} and Li-Chyong Chen¹; ¹National Taiwan University, Taipei, Taiwan; ²Institute of Atomic and Molecular Science, Academia Sinica, Taipei 106, Taiwan, Taipei, Taiwan; ³Graduate Institute of Applied Science and Technology National Taiwan University of Science and Technology, Taipei, Taiwan; ⁴Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan, Keelung, Taiwan.

Kesterite based $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe) have emerged as potential alternatives for CdTe and CIGSSe absorbers due to the use of non-toxic and earth-abundant elements and providing desirable optoelectronic properties similar to those of CIGSSe. To raise the performance of CZTSSe based solar cells, much effort has been applied to improving the quality of absorbers, band alignments/passivation at p-n junction, front and back interfaces/contacts. [1,2,3,4]

The present investigation mainly addresses the open circuit voltage (Voc) issue in kesterites based $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ solar cells by simply introducing an interfacial alkaline earth fluoride (several nm MgF_2) between the absorber (*i.e.*, CZTSSe) and the buffer layer (*i.e.*, CdS) after sulfo-selenization processes without post-annealing. In statistical studies (10 cells), the alkaline earth fluoride increases power conversion efficiency V_{oc} from 7.5% to 8.8%, short circuit current density (J_{sc}) from 30.7 mA/cm² to 32.6 mA/cm² and from 440 mV to 470 mV, possibly resulting from the MgF_2 induced electric field passivation at grain boundaries. [2]. Finally, a 9.4 % efficient CZTSSe solar cell with V_{oc} of 470 mV, J_{sc} of 32.96 mA/cm² and fill factor (FF) of 60.7 % was obtained.

The morphology, elemental composition, and distribution of the absorber layers are being examined by scanning Kelvin probe microscopy measurement, X-ray diffraction (XRD), X-ray fluorescence spectrometry (XRF), scanning electron microscopy (SEM), Raman spectroscopy, Nanoscale secondary ion mass spectrometry (nanoSIMS), and nano Auger electron spectroscopy (AES).

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4:45 PM ET11.08.05

Towards High Open-Circuit Voltage in Two-Dimensional Transition Metal Dichalcogenide Photovoltaics Cora Went¹, Joeson Wong¹, Phillip Jahelka¹, Deep M. Jariwala^{1,2}, Joseph S. DuChene¹ and Harry A. Atwater¹; ¹California Institute of Technology, Pasadena, California, United States; ²University of Pennsylvania, Philadelphia, Pennsylvania, United States.

Two-dimensional transition metal dichalcogenides (2D TMDs) are promising candidates for ultrathin photovoltaics because they have direct bandgaps that lie in the visible range, their absorption coefficients are one to two orders of magnitude higher than conventional semiconductors, and their interlayer van der Waals interaction eliminates the constraint of lattice matching in heterostructure design. While our group has demonstrated high internal quantum efficiency in 2D TMD photovoltaics (1), high open-circuit voltage remains a challenge (2). Here, we study open-circuit voltage in 2D TMD photovoltaics by fabricating both vertical and lateral photovoltaic devices with monolayer TMD absorber layers and contacts with asymmetric work functions (e.g. silver and platinum). In both vertical and lateral geometries, we compare the effects of transferred and directly evaporated metal contacts on the device's open-circuit voltage. To transfer metal contacts, we modify a procedure that has been shown to create contacts to 2D materials with atomically smooth interfaces and no Fermi level pinning (3). Metals are patterned onto a smooth sacrificial substrate (*i.e.* silicon dioxide) using photolithography, peeled off that substrate using polyvinyl alcohol (PVA), and transferred onto a TMD device using a viscoelastic stamp. The devices are characterized, then passivated by immersion in solutions of the superacid bis(trifluoromethane)sulfonimide in acetonitrile to achieve near-unity photoluminescence quantum yield, as previously reported (4,5). Using photoluminescence mapping, photocurrent spectroscopy, and Kelvin probe force microscopy, we characterize these devices to analyze the effects of 1) vertical vs. lateral device geometry, 2) superacid-treated vs. untreated absorber layers, and 3) transferred vs. evaporated metal contacts on the open-circuit voltage of our photovoltaic devices. Our results demonstrate a pathway towards high open-circuit voltage in 2D TMD photovoltaics, and we outline specific design considerations for future high-efficiency devices.

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8:30 AM ET11.09.01

Metalorganic Vapor Phase Epitaxy of Large CdTe Grains on 2D Substrates through Chemical and van der Waals Mixed Interactions Xin Sun¹, Dibyajyoti Mohanty¹, Zonghuan Lu¹, Yu Xiang¹, Yiping Wang¹, Lihua Zhang², Kim Kisslinger², Jian Shi¹, Lei Gao³, Morris Washington¹, Gwo-Ching Wang¹, Toh-Ming Lu¹ and Ishwara Bhat¹; ¹RPI, Clifton Park, New York, United States; ²Brookhaven National Laboratory, Upton, New York, United States; ³University of Science and Technology Beijing, Beijing, China.

High-quality heteroepitaxy of CdTe is challenging due to lattice mismatches of CdTe with many substrates. Herein, we demonstrate the epitaxial growth of single crystalline CdTe films on mica using metalorganic chemical vapor deposition, regardless of large in-plane lattice mismatch between CdTe(111) and mica. X-ray and electron diffractions suggest that CdTe is epitaxially aligned with mica: out-of-plane CdTe(111)//mica(001) and in-plane CdTe [-12-1]//mica [010]. Full-width-at-half-maximum (FWHM) of X-ray rocking curve and FWHM of X-ray azimuthal in-plane angular dispersion of CdTe are shown to be 0.11° and 0.38°, respectively, better than most CdTe films reported. Electron backscattering diffraction shows that CdTe grains are tens of μm in size and, if twin boundaries are excluded, in excess of 250 μm in size. In contrast to the belief that overlayer growth on mica is purely through van der Waals interaction, our first-principles calculations unveil that van der Waals interaction only contributes to 20% of the total interfacial energy, and 80% of the interfacial energy comes from chemical interaction. Furthermore, we demonstrate that epitaxial CdTe films can be achieved on other 2D substrates, such as graphene. Compared to on mica, however, the films grown on graphene are characterized with larger orientation dispersions along out-of-plane and in-plane directions and smaller grains. Our first-principles calculations indicate a van der Waals interaction dominating interface between CdTe and graphene. We thus conclude that the nature of interface interactions dictates crystal quality of CdTe films on different 2D substrates. The demonstrated epitaxy of II-VI semiconductors on 2D van der Waals substrates suggests potential for flexible optoelectronic devices.

8:45 AM ET11.09.02

Effect of Stacking Disorder and Metastable Polymorph on Charge Conduction in Earth-Abundant Cu₂ZnSn(S, Se)₄ Ji-Sang Park, Sunghyun Kim and Aron Walsh; Imperial College London, London, United Kingdom.

Cu₂ZnSn(S, Se)₄ based solar cells have attracted a much attention in achieving terra-watt scale photovoltaic. The solar conversion efficiency of Cu₂ZnSn(S, Se)₄ solar cells, however, is generally lower than Cu(In, Ga)Se₂ solar cells because of low open-circuit voltage, usually termed as the open-circuit voltage deficit. While the problem has not been solved yet, the spatial fluctuations of band edge have been suggested as the culprit which results in the band tailing and the lower efficiency. The spatial fluctuations can be caused by the formation of anti-site defect pairs which form electrostatic dipoles, or lower bandgap polymorphs.

Indeed the formation of the lower bandgap polymorph (e.g. stannite) can be understood as the periodic formation of anti-site defect complexes. In multi-cation materials such as Cu₂ZnSn(S, Se)₄, the octet rule can be satisfied when anti-site defects are formed on two-dimensional planes in certain ways. Metastable polymorphs can be obtained from kesterite crystal structure by applying such operations globally, and the metastable polymorphs are shown to have lower band gap from the hybrid density functional theory (DFT) calculations [1]. If the operation is locally applied, then it results in the formation of so-called anti-site domain boundaries, and their formation has been experimentally proven in Cu₂ZnSnS₄ nanocrystal. In this work, we performed hybrid DFT calculations and found that these defects in Cu₂ZnSn(S, Se)₄ lower the conduction band locally, and thus act as electron captures [2].

On the other hand, studies of other solar cell absorber materials show that stacking faults are formed abundantly in zinc-blende-derived materials. We calculated the formation energy of the stacking faults (e.g. intrinsic stacking faults) and analyzed their effect on the electronic structure as well. We found that Stacking fault defects in Cu₂ZnSn(S, Se)₄ are more easily formed than the anti-site domain boundaries [2]. In contrast to the anti-site domain boundaries, the stacking faults increase the conduction band and thus electron barriers are locally formed, hamper the electron conduction.

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9:00 AM *ET11.09.03

Nanowires for Tandem Junction Solar Cells Magnus Borgstrom; Lund University, Lund, Sweden.

Semiconducting nanowires have been recognized as promising materials for high-performance electronics and optics where optical and electrical properties can be tuned individually, where the nanowires due to excellent light absorbing properties [1] have been suggested for future high efficiency solar cells [2, 3]. Especially, the geometrical shape of the NWs offers excellent light absorption.

In order to further optimize the performance of NWPV, and integrate them on Si in a tandem junction configuration, nanowires with dimensions corresponding to optimal light harvesting capability are necessary. We developed nano imprint lithography for patterning of catalytic metal particles with a diameter of 200 nm in a hexagonal pitch of 500 nm, for which synthesis was redeveloped since the metal particles were found to move during annealing, destroying pattern fidelity before nucleation. By use of electron beam induced current measurements we learn how to improve the photocurrent generation profile in the nanowires by reducing native defects incorporated during synthesis, either by tuning the V/III ratio or by compensation doping, resulting in a certified efficiency of 15 % for a 12 % surface coverage of nanowires. We intend to transfer these grown nanowires to a Si platform (existing PV), either by direct growth on Si PV, or by nanowire peel off in polymer, followed by transfer and electrical contacting, or by aerotaxy and alignment for transfer to Si. The optimal band gap in combination with Si is about 1.7 eV, where we identify GaInP and GaAsP as materials for development of nanowire pn junctions by doping, the heart in a solar cell.

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9:30 AM ET11.09.04

Tailoring the Defect Properties of Chalcogenide Systems for Photovoltaic Applications [John Buckeridge](#), Alex M. Ganose and David O. Scanlon; University College London, London, United Kingdom.

Bismuth chalcogenides are promising new candidates for cheap, nontoxic and highly effective solar absorber layers in photovoltaic systems. The majority of those studied so far, however, have shown poor efficiencies well below industry standards. We investigate the suitability of these materials for solar energy applications using relativistic first-principles computational techniques, focussing on two of the most promising systems: BiSI and BiSeI. We find that both compounds possess desirable optoelectronic properties, with band gaps well within the visible range combined with strong optical absorption, resulting in high predicted device performance. Our analysis of their defect chemistry indicates that deep traps are likely to form, which may account for the observed poor performance of the materials. Nevertheless, we show that, by varying the experimentally accessible synthesis conditions, it is possible to avoid the formation of such killer defects, which would allow much higher efficiencies to be achieved. Furthermore, we apply similar analysis to study other III- (and V-) chalcogenides and determine their suitability for photovoltaic applications, building up a family of promising mixed-anion materials with similar optoelectronic properties.

9:45 AM ET11.09.05

Development of New High-Band Gap Photoabsorbers for Low-Cost Tandem Solar Cells with Different Thermal Budgets [Andrea Crovetto](#), Brian J. Seger, Ole Hansen, Peter Vesborg and Ib Chorkendorff; Technical University of Denmark, Kgs. Lyngby, Denmark.

One of the current key challenges in both photovoltaics and solar-driven water splitting is to identify an efficient, stable, and low-cost material to be used as a high-band gap (1.6-2.0 eV) photoabsorber in tandem device configurations. In this contribution, we will report on our group's development of three different emerging, inorganic, high-band gap solar absorbers with thermal budgets from 150°C to 1000°C, which may satisfy different applications. The first material is BiI₃ (thermal budget of 150°C, record efficiency 1.0%), which is straightforward to make and may be used for tandem solar cells on flexible plastic substrates [1]. The second material is Cu₂BaSnS₄ (thermal budget of 550°C, record efficiency 2.0%), which is a promising alternative to the more extensively studied Cu₂ZnSnS₄, due to its more appropriate band gap for tandem solar cell applications and to its lower density of tail states [2]. The third material is LaYS₃ (thermal budget of 1000°C, no efficiency reports). To our knowledge, LaYS₃ the first chalcogenide perovskite to have been synthesized in thin film form, as well as one of the first photoabsorbers discovered by computational screening that were actually synthesized [3]. Those three materials are currently being investigated in our group. They share the following favorable optoelectronic properties: 1) appropriate band gap (1.7-2.0 eV) as a top absorber in a tandem solar cell; 2) strong photoluminescence, and 3) small shift between band gap energy and photoluminescence peak energy. We will present our results on alternative growth methods for the two previously synthesized absorbers (iodization of metallic Bi for BiI₃; sulfurization of oxide films for Cu₂BaSnS₄), as well as the main optoelectronic properties of the novel LaYS₃ absorber. Finally, we will discuss the solar cell performance obtained from the three absorber materials, with particular emphasis on the different device architecture limitations arising from the different thermal budgets of the three materials.

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10:00 AM BREAK

SESSION ET11.10: Nano Technology Application to PV III

Session Chairs: Magnus Borgstrom and Lin Zhou

Wednesday Morning, November 28, 2018

Hynes, Level 3, Room 304

10:30 AM *ET11.10.01

Interface-Enhanced Bulk Photovoltaic Effect in Metal Oxides [Yun Liu](#); The Australian National University, Canberra, Australian Capital Territory, Australia.

Photovoltaic (PV) is a process converting light energy to electrical energy. A high efficient PV effect relies on two factors: (i) a high photocurrent and (ii) a built-in electric field enabling the separation of the photogenerated electrons and holes. In traditional PV devices, electron-hole pairs are generated by light absorption in narrow bandgap semiconductors, and then separated through the depletion field in the heterojunction. The maximum voltage of these devices, however, equals to their bandgap, and thus the power conversion efficiency is restricted by Shockley-Queisser limitation. To break this limitation and obtain higher voltage, ferroelectric (FE) materials, due to their non-centrosymmetric structures that can induce stable depolarization electric fields and generate much higher photovoltage than their bandgap (named as bulk PV effect), have received a renewed attention in the PV application. Despite the high voltage the FE materials can exhibit, the photocurrent of most of the FE materials is really low because of their wide bandgaps resulting in the low conductivity and the deficient absorption of the solar energy. In this talk, we will present several strategies to improve bulk PV effect of materials, especially focusing on structurally distorted and chemically varied narrow bandgap metal oxide semiconductors, in which high performance ferroelectric properties are achieved without significantly changing their intrinsic electronic and photoelectronic properties. It is found that such a very thin (<10nm) functional metal oxide layer, deposited on a strain layer, shows an excellent bulk photovoltaic effect with a photocurrent 10³-10⁴ times higher than that of conventional ferroelectric materials and comparable to state-of-the-art multilayered multiferroics.

11:00 AM ET11.10.02

Optimizing the Properties of Transparent Electrodes Based on Silver Nanowire Networks for Integration into Organic Solar Cells [Joao A. Resende](#)¹, Thomas Sanniccolo¹, Afzal Khan², Nicolas Charvin³, Ali Nouridine³, Dorina Papanastasiou¹, Viethuong Nguyen^{1,5}, Sara Aghazadehchors^{1,4}, David Munoz-Rojas¹, Carmen Jimenez¹, Ngoc Duy Nguyen⁴, Lionel Flandin³ and Daniel Bellet¹; ¹LMGP, Grenoble, France; ²Department of Physics, Univ. of Peshawar, Peshawar, Pakistan; ³Univ. Grenoble Alpes, Université Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, Grenoble, France; ⁴Université de Liège, CESAM/Q-MAT, Liege, Belgium; ⁵CEA-INES, LITEN, Le Bourget-du-Lac, France.

The demand for low-cost and flexible photovoltaic systems is rapidly increasing, creating a need for a new generation of transparent electrodes. In the

specific case of organic photovoltaics (OPV), flexible transparent electrodes compatible with cheap roll-to-roll technologies would allow the wide-spread of large-scale OPV, offering a technology with non-toxic, low-weight and flexible modules available in different shapes and colors. Although indium-tin-oxide (ITO) constitutes the state-of-the-art transparent conductive material for solar cells, it exhibits drawbacks such as brittleness, thus preventing its application in flexible devices. To replace ITO, metal-based nanowire networks have been considered as a promising alternative solution that exhibits high potential in OPV. In the case of randomly deposited silver nanowire (AgNW) networks, outstanding properties are obtained with sheet resistance values below 10 Ω /sq, optical transparency of 90% and mechanical stability under bending tests when deposited on flexible substrates. Still, for an accomplished integration into organic solar cells, a large number of other requirements have to be considered.

In this work, we report the impact of electrical homogeneity and stability of silver nanowire networks aiming for integration into organic photovoltaics. Single probe mapping of the electric potential was found to be a relevant and simple technique for extracting the bias-dependent equipotential lines in networks in order to analyze the corresponding electrical homogeneity of the electrode. Thus, the lower tortuosity of the electrical equipotential lines on dense AgNW networks, the higher the electrical homogeneity of the electrode. With respect to the application of AgNW networks into solar cells, the electrical homogeneity is indeed likely to have a substantial influence on the efficiency of the device, in such a way that inhomogeneities might increase series resistance, leading to a lower form factor in the J-V curve. In addition, collection efficiency is expected to be higher for homogeneous networks. Furthermore, we created a nanocomposite electrode by encapsulating the AgNW networks with a protective Zinc Oxide (ZnO) layer, using the atmospheric pressure spatial atomic layer deposition (AP-SALD). The obtained nanocomposite shows improved adhesion as well as increased thermal and electrical stability, with only a small reduction in optical transparency. By controlling the key characteristics of this nanocomposite, as the network density or the thickness of the ZnO protective layer, one can tune physical properties that are critical in photovoltaics, such as surface roughness, charge collection efficiency and the work function of the electrode. The composites have been fabricated using low-temperature process steps and upscaling methods that are compatible with organic photovoltaic technologies as roll-to-roll as well as with other low-cost, high throughput, processing methods.

11:15 AM ET11.10.03

Head-to-Head Linkage Containing 4-alkoxy-5-(3-alkylthiophen-2-yl)thiazole-Based Polymeric Semiconductors for Polymer Solar Cells with Small Voltage Loss [Xin Zhou](#), Chen Peng, Jianwei Yu, Han Guo and Xugang Guo; Southern University of Science and Technology, Shenzhen, China.

Head-to-head linked bithiophene-type unit with advantages of good solubility and high planarity has been proven as a successful building block for polymeric semiconductors. However, since the strong electron-donating nature of alkoxy chain, bithiophene-based polymers suffer from elevated frontier molecular orbitals (FMOs), which are unfavorable to stability of semiconductors and lead to small open-circuit voltages (V_{oc}) in polymer solar cells (PSCs). Herein, we report the design, synthesis and characterization of a new head-to-head linked building block 4-alkoxy-5-(3-alkylthiophen-2-yl)thiazole (TRTzOR). Compared to our previous work, 3-alkoxy-3'-alkyl-2,2'-bithiophene (TRTOR), TRTzOR retains high planarity through the intramolecular noncovalent S-O interaction, while its FMOs have been considerably lowered for the substitution of electron-deficient thiazole for the electron-rich thiophene. Copolymerized with the benzothiadiazole and its fluorinated derivatives, TRTzOR-based polymer showed a wider absorption range extending to 950 nm and tune FMOs down by 0.2–0.3 eV, versus TRTOR-based analogous polymers. Thus, TRTzOR-based polymeric donor enlarges the V_{oc} of polymer solar cells by 0.1 eV. Moreover, a much smaller energy loss as low as 0.61 eV was realized. Our study demonstrates thiazole substitution is an effective approach to tuning energy levels for higher open-circuit voltages in PSCs. The exceptional small energy loss indicates that head-to-head linkage TRTzOR motif is a promising building block for organic semiconductor.

11:30 AM ET11.10.04

IMPULSE-OPV—Integrated Molecular Plasmon Upconverter for Low-Cost, Scalable and Efficient Organic Photovoltaics [Jonas S. Lissau](#) and Morten Madsen; SDU NanoSYD, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark.

Upconversion of low-energy photons transmitted by traditional single-threshold solar cells is a promising approach to overcome their theoretical efficiency limit. Due to their relatively high-energy absorption threshold organic solar cells have a particular high loss of low-energy photons and consequently a high potential for improvement by photon upconversion.

In IMPULSE-OPV, we apply photon upconversion via triplet fusion in organic molecules to improve the efficiency of organic solar cells. This approach can be synthetically tuned to match the spectral requirements of the solar cell technology. In addition, molecular photon upconversion benefits from spin-allowed broadband absorbing transitions, which facilitates reasonable upconversion efficiency under solar flux [1].

Specifically, we investigate in this work systems based on palladium(II) 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine as a triplet sensitizer and rubrene as a triplet-triplet annihilator. After light absorption and intersystem crossing the resulting triplet state is transferred to rubrene. The molecular upconverter is embedded in a polyurethane matrix which allows for efficient triplet energy migration via molecular diffusion. Two rubrene triplet states can annihilate (triplet fusion) to produce a high-energy singlet state which decays by emission of an (upconverted) high-energy photon.

To further boost the photon upconversion efficiency, metal nanostructures tailored for plasmon resonance at the absorption band of the upconverter are integrated. This work therefore provides a route for production of low-cost, scalable, and efficient organic solar cells via photon upconversion.

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11:45 AM ET11.10.05

Metal Decorated Nano-Composite Effects to Enhance the Performance of Inverted Thin-Film Organic Solar Cells [Genevieve T. Mola](#); University of KwaZulu-Natal, Pietermaritzburg, South Africa.

The efficient generation and transportation of charge carriers are the major factors that influence the performance of thin film organic solar cells (TFOSC). We have successfully synthesized and employed tri-metallic nanocomposite (Ag:Zn:Ni) in the preparations of TFOSC with the view to address some of the challenges with respect to charge generation and transportation. The nanocomposites were dispersed in the solution phase of the photoactive layer of the solar cells. As consequence, notable influence of the nanocomposite was evident on the power conversion efficiency of the devices due to local surface plasmon resonance (LPSR). Several synthesis methods have been employed in the preparations of various bi and tri-metallic nanoparticles which include chemical, physical and biosynthesis methods such as chemical reduction, microwave and laser ablation [1,2,3,4,5]. Among these techniques, the chemical reduction method is the most preferred one because of its simplicity and low cost preparation. Moreover, the chemical reduction method offers the ability to control size and distribution of the nanoparticles by optimizing the experimental parameters. In this work, we have synthesized and characterized of silver:zinc:nickel (Ag:Zn:Ni) tri-metallic nanoparticles which are eventually explored for first time to influence the photovoltaic performance of bulk-heterojunction organic solar cells. The synthesis of the nanocomposite, device preparation and characterization are discussed in terms of changes in optical, electrical and morphological properties.

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SESSION ET11.11: Oxides

Session Chairs: Seth Hubbard and Aaron Ptak
Wednesday Afternoon, November 28, 2018
Hynes, Level 3, Room 304

1:30 PM *ET11.11.01

Interfacial Solar Steam Generations—Materials, Structures and Applications Jia Zhu; Nanjing University, Nanjing, China.

Nanomaterials with carefully tailored properties can be used to manipulate the flow of phonons, electrons and photons, to enable unconventional solution for solar energy conversion. In this talk, I will present our recent progress in interfacial solar steam generations.

We report a plasmon-enhanced solar desalination device. This most efficient and broad-band plasmonic absorber is fabricated through self-assembly of metallic nanoparticles onto a nanoporous template by one step deposition process. Because of its efficient light absorption and strong field enhancement, it can enable very efficient and effective solar desalination by using low cost aluminum nanoparticles. Inspired by the transpiration process in plants, we report an artificial transpiration device with a unique design of two dimensional water path. With efficient two dimensional water supply and suppressed heat loss, it can enable an efficient (80% under one-sun illumination) and effective (four orders salinity decrement) solar desalination device. The energy transfer efficiency of this artificial transpiration device is independent of water quantity and can be achieved without extra optical or thermal supporting systems, therefore significantly improve the scalability and feasibility of this technology. In addition, interfacial solar steam generations can enable effective sterilization and efficient generations of electricity.

2:00 PM ET11.11.02

Synthesis and Characterization of c-Axis Oriented Zinc Oxide Thin Films and Its Use for the Subsequent Hydrothermal Growth of Zinc Oxide Nanorods Farhad Syed¹, Nazmul Islam Tanvir¹, Muhammad Shahriar Bashar² and Munira Sultana²; ¹Solar Energy Conversion and Storage Research Section, Industrial Physics Division, BCSIR Labs, Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh; ²Institute of Fuel Research and Development (IFRD), Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh.

Oriented ZnO seed layers were deposited by simple drop casting of zinc acetate dihydrate(ZAD) solution on glass substrates at room temperature followed by a post-heat treatment at 250 °C. X-ray diffraction (XRD) analyses revealed that ZAD solutions with concentration 0.0025 – 0.0100 M produced amorphous type thin films, whereas 0.020 M ZAD solutions produced ZnO seed layers with a preferential c-axis texturing. The Scanning Electron Microscopy (SEM) analysis evident that the morphology of ZnO seed layer surface is compact and coherently carpets the underlying glass substrate. ZnO nanorods were then grown by hydrothermal method atop the oriented ZnO seeded and non-seeded substrates. The presence of ZnO seeding layers was found to significantly affect the surface morphology and crystallographic orientation of the resultant ZnO NRs films. The optical band gap of ZnO seed and ZnO NR were estimated to be in the range of 3.40 – 3.95 eV and 3.20 – 3.25 eV respectively by using UV-VIS-NIR diffuse reflection spectroscopy. The room temperature photoluminescence analyses revealed that nanostructured ZnO films exhibit a sharp near-band-edge luminescence peak at ~380 nm consistent with the estimated optical band gap and the ZnO nanorod arrays are notably free from defect-related green-yellow emission peaks.

2:15 PM ET11.11.03

Slow Transient Photoconductivity in ZnO Explained from Light-Induced Trap Filling Jason A. Rohr^{1,2}, Mohamed Abdellah³, Liam Appelson¹, Anna Cieslak⁴, Janusz Lewinski^{4,5}, Jacinto Sa^{3,4} and Steven Konezny^{1,2}; ¹Department of Chemistry, Yale University, New Haven, Connecticut, United States; ²Energy Sciences Institute, Yale University, West Haven, Connecticut, United States; ³Department of Chemistry, Uppsala University, Uppsala, Sweden; ⁴Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland; ⁵Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland.

Zinc oxide (ZnO) nanoparticles have been studied extensively as gas sensors, as an alternative electron transport material to titanium dioxide in dye-sensitized solar cells, and as a potential photocatalyst for solar driven water splitting. This is primarily due to their low cost, material abundance, potentially large surface area as mesoporous films, low toxicity, relatively large charge-carrier mobilities, and their capability to be doped either n- or p-type. However, important fundamental mechanistic questions remain unanswered. The chemical nature of charge-carrier traps, and the observed transient behavior of the conductivity of ZnO thin films after UV light exposure, also known as persistent photoconductivity, are still as much the subject of debate as it has been over the last three decades. We offer new insight based on a combination of temperature-dependent conductivity measurements, in the 8 to 310 K range, and mid-infrared transient absorption spectroscopy measurements. Using these techniques we are able to isolate the effects from light and temperature. At low temperature, the conductivity increases as transport tends from being trap limited to trap filled when exposed to UV light as the fraction of filled traps increases. At higher temperatures, the dark current, post UV exposure, slowly decreases as it returns to trap-limited behavior as charge carriers are reemitted from the traps. At practical device temperatures and light conditions, the observed conductivity is governed by both trapping and detrapping kinetics that establish an equilibrium density of occupied trap levels. We show that the conductivity can be modeled within this framework by assuming a combination of inter-particle tunneling, light induced trap filling and temperature-dependent detrapping kinetics. This model can be used to extract the trap depths, which can be assigned to the defects limiting the transport. Our findings not only give insight into the conduction mechanism of

ZnO particle films, but into any conduction mechanism exhibiting persistent photoconductivity, such as other nanostructured metal oxides and amorphous metal chalcogenides.

2:30 PM BREAK

3:30 PM ET11.11.04

Optical Properties of Magnesium-Zinc Oxide for Thin-Film Photovoltaics Applications Mohammed Razzoqi, Prakash Koirala, Adam Phillip, Geethika K. Liyanage, Michael Heben and Robert W. Collins; Department of Physics and Astronomy, and Wright Center for Photovoltaics Innovation and Commercialization, The University of Toledo, Toledo, Ohio, United States.

Magnesium-zinc oxide ($Mg_xZn_{1-x}O$; MZO) is a window layer material of great interest in thin film photovoltaics technologies such as CdTe and $CuIn_{1-x}Ga_xSe_2$. Recent numerical modelling and experimental data have shown that replacing the CdS window layer in CdTe devices with an MZO layer improves the band alignment at the front contact, which in turn reduces recombination [1,2] and leads to improved solar cell open circuit voltage and fill factor [3]. Although the window layer performance is critically dependent on its optical properties, such characterization of MZO films after the various steps throughout device fabrication has not been reported to date. Specifically, information is lacking on the evolution of the optical properties as a function of time during thermal treatments in different environments. Whereas the SnO_2 high resistivity transparent (HRT) layer traditionally used in CdTe devices is known to be thermally stable, it is not clear the extent to which the properties of as-deposited MZO are affected by subsequent device processing. Here, we use spectroscopic ellipsometry (SE) to determine the optical properties of the MZO at various stages of CdTe device processing and apply this information to guide device fabrication. In these experiments, $Mg_xZn_{1-x}O$ films with Mg contents from $x = 0$ to $x = 0.25$ were sputtered at room temperature on soda lime glass (SLG). This provides a range in the MZO bandgap energy from $E_g = 3.3$ eV to $E_g = 3.7$ eV, respectively. The room temperature complex dielectric functions of the MZO films on SLG were measured immediately after deposition and again after heating for 4 hours at 250 °C, the same thermal cycle used for sputtering an overlying CdTe film. In subsequent studies, the optical properties of the annealed SLG/ $Mg_xZn_{1-x}O$ have served as a database for analyzing complete PV stacks using a multilayer model consisting of SLG/TEC-15/ $Mg_xZn_{1-x}O$ /CdTe. The capabilities of SE are explored in particular for determining the magnesium content x simultaneously with the film structure for correlations of both composition and thickness with the device performance.

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3:45 PM ET11.11.05

Integrated Photon Management in Multijunction Photovoltaics Seth Hubbard¹, George Nelson¹, Stephen J. Polly¹, Julia D'Rozario¹ and Rao Tataavarti²; ¹Rochester Institute of Technology, Rochester, New York, United States; ²Microlink Devices, Niles, Illinois, United States.

Photon management can be used in III-V solar cells to increase absorption in the active region of the device. This can allow addition of low bandgap nanostructures such as quantum wells, without the need for excessive strain balancing. It can also be used to harden space cells against high-energy, damaging particles. In this work, a model was first developed integrating simulations from electromagnetics and device physics software packages to evaluate absorption enhancement in, and performance of, III-V solar cells with both flat and textured back surface reflectors as well as front side scattering structures. Models predicted that a nanostructured GaAs cell with a pyramid-textured back surface reflector (BSR) could enhance absorption of in the nanostructures by over 30 times that of a conventional upright design of the same thickness. The model also found that integrated light management could be used to radiation harden InGaP/GaAs/Ge space cells by thinning the GaAs subcell to less than half of the conventional thickness. In addition, simulation was compared to experiment focusing on the GaAs middle cell using combinations of textured back reflectors as well as partially reflective epitaxial DBR mirrors. For epitaxial DBR mirrors, internal and external quantum efficiency, as well as performance under 1-sun illumination shows nearly complete recovery of performance to optically thick conditions, while using half the thickness of GaAs absorber. As well, pyramidal and random back surface texturing has shown that optical path lengths much greater than 2 can be realized in practice. These results have been used to verify and refine the developed simulations and as well predict realistic end of life enhancements for typical space radiation conditions.

SESSION ET11.12: Poster Session
Session Chairs: Rao Tataavarti and Lin Zhou
Wednesday Afternoon, November 28, 2018
8:00 PM - 10:00 PM
Hynes, Level 1, Hall B

ET11.12.01

ZIF-67 Derived Nanostructures of Co/CoO and Co@N-Doped Graphitic Carbon as Counter Electrode for Highly Efficient Dye-Sensitized Solar Cells Hongyu Jing, Suzhen Ren, Yantao Shi, Xuedan Song, Yonglin An and Ce Hao; State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, China.

Here we present a facile one-step approach of using ZIF-67 as a sacrificial template for the synthesis of counter electrode (CE) catalyst of dye-sensitized solar cells (DSCs). Via controlling the carbonization temperature under N_2 atmosphere, porous nanocomposites of Co, CoO and N-doped graphitic carbon are synthesized. Structural characterizations indicate that some cobalt nanoparticles are well embedded in an N-doped graphitic carbon matrix (a core-shell structure named as Co@NGC) while the other cobalt and cobalt oxide nanoparticles are exposed on the external surface (named as Co/CoO). Especially, the nanostructure of Co@NGC is more chemically stable than Co/CoO against etching of strong acid, for example, hydrochloric acid (HCl, 0.1 M). The performance of DSC using ZIF-67-850 (pyrolyzed at 850 °C) as CE yields a photoelectric conversion efficiency (PCE) of 7.92%, which is close to that of Pt CE (8.18%) in the liquid I_3^-/I^- redox couple electrolyte. The excellent performance of ZIF-67-850 can be ascribed to the synergetic effects between the Co and CoO coupled with the nitrogen doped graphitic carbon. The cost-effective porous Co/CoO and Co@NGC nanocomposites show great potential for application in the field of high performance CE in solar cells.

ET11.12.02

Effect of Solvent and Substrate on the Surface Binding Mode of Carboxylate-Functionalized Aromatic Molecules [Janna Domenico](#)¹, Michael E. Foster², Erik D. Spoecke³, Mark Allendorf⁴ and Karl Sohlberg¹; ¹Department of Chemistry, Drexel University, Philadelphia, Pennsylvania, United States; ²Department of Materials Physics, Sandia National Laboratories, Livermore, California, United States; ³ Department of Electronic, Optical, and Nano Materials, Sandia National Laboratories, Albuquerque, New Mexico, United States; ⁴Department of Energy and Transportation Technology Center, Sandia National Laboratories, Livermore, California, United States.

The efficiency of dye-sensitized solar cells (DSSCs) is strongly influenced by dye molecule orientation and interactions with the substrate. Therefore, understanding the factors controlling the surface orientation of sensitizing organic molecules will aid in the improvement of both traditional DSSCs and other devices that integrate molecular linkers at interfaces. Herein, we employ DFT calculations and ab initio molecular dynamics simulations to investigate the effect of substrate, solvent, and protonation state on the orientation of linker molecules relevant to DSSCs. In the absence of solvent, we predict that most carboxylic acid-functionalized molecules prefer to lie flat (parallel) on the surface, due to van der Waals interactions, as opposed to binding at a tilted orientation with respect to the surface that is favored by covalent bonding of the carboxylic acid group to the substrate. Once solvation effects are considered, however, most molecules are predicted to orient perpendicular to the surface. This approach can be extended to help understand and guide the orientation of metal-organic framework (MOF) thin-film growth on various metal-oxide substrates. Finally, a two-part analytical model is developed that predicts the binding energy of a molecule by chemical and dispersion forces on rutile and anatase TiO₂ surfaces, and quantifies the dye solvation energy for two solvents. The model is in good agreement with the DFT calculations and enables rapid prediction of dye molecule and MOF linker binding preference on the basis of the size of the adsorbing molecule, identity of the surface, and the solvent environment. Results suggest that linker orientation can be controlled by choice of adsorbate, substrate, and solvent; this novel approach can be used to achieve a desired linker orientation and, by extension, MOF growth orientation in a MOF-based DSSC.

ET11.12.03

Solar Cell Degradation Due to Corrosion of Glass Substrates [Yuriy Kudriavtsev](#), [Angelica Hernandez](#), Rene Asomoza-Palacio, Miguel Avendaño and Marcela Guerrero; CINVESTAV, Mexico City, Mexico.

Thin film solar cells meet a great interest because of their low price and a relatively high efficiency. Many technologists use glass substrates to deposit thin films forming a photo-diode structure. In the most popular configuration of solar cells, photons transmit through the glass substrate and a special transparent ohmic contact before arriving in a p-n junction region. It is evident that glasses with a highest possible transmittance coefficient are necessary for the higher solar cell efficiency and the transmittance should be saved for the time of life of the cells. Borosilicate (b-s) and soda-lime (s-l) glasses are most popular substrates because of the mentioned reasons.

In our previous studies, we demonstrated that interaction of atmospheric water vapor with silicate glasses results to their corrosion. A radical difference in the corrosion mechanisms was observed for s-l and b-s glasses. Hydration of a near surface layer occurs in s-l glasses, whereas hydrogenation - in b-s glasses. Both the hydration and the hydrogenation processes are stimulated strongly by the temperature. Typical solar cells work at elevated temperatures, which can reach 90-100°C in a sunny day, so the glass substrate corrosion for a working solar cell due to such glass surface corrosion looks very possible. We realized an experimental hydration of s-l and b-s glasses in a 100% water vapor atmosphere at 90°C for two months to simulate the glass substrate corrosion. Experimental samples were cut from commercial polished substrates. SIMS depth profiling analysis was performed to define the thickness of hydrated and hydrogenated layers, formed in the s-l and b-s glass samples, respectively. Optical transmittance coefficients were measured for the hydrated samples in comparison with the original ones. We concluded a radical decrease of the transmittance of the s-l glasses, caused by hydrated layer formation. An insignificant decrease of the transmittance coefficient was observed for b-s glass.

We concluded that a special study should be realized directly to those of the glass substrates used for solar cell fabrication to avoid cells degradation due to glass surface corrosion.

ET11.12.04

Origins of Voltage Deficit in Earth-Abundant Kesterite Thin-Film Solar Cells [Samantha Hood](#)¹, Sunghyun Kim¹, Ji-Sang Park¹ and Aron Walsh^{1,2}; ¹Imperial College London, Kensington, United Kingdom; ²Yonsei University, Seoul, Korea (the Republic of).

The kesterite family of semiconductors are being widely studied for their application in thin-film solar cells. In particular, the material Cu₂ZnSnS₄ (CZTS) has a band gap (1.5 eV) well matched to the solar spectrum and is composed of non-toxic and earth-abundant elements. However, the performance of kesterite solar cells falls well below the Shockley-Queisser limit [1].

The origin of the low voltage of CZTS photovoltaics is a matter of debate, with several proposed mechanisms for the high rates of electron-hole recombination [2]. We will present our latest findings concerning the role of lattice vibrations (phonons) in both band gap fluctuations and defect-assisted non-radiative recombination [3]. In particular we emphasise the role of phonon anharmonicity in accelerating electron-hole recombination in this class of compounds, as well as the effect of multi-valency of the Sn atoms, which facilitates electron and hole localisation in the form of small polarons.

Our simulations have been supported with experiments performed as part of the STARCELL network (H2020 project no. 720907).

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ET11.12.06

Coumarin-Based Europium Complexes for Luminescent Solar Concentrators [Ahmad Alsaleh](#), Anita C. Jones and Neil Robertson; University of Edinburgh, Edinburgh, United Kingdom.

Solar energy is the most promising source to address the growing energy needs of the planet. Luminescent solar concentrators (LSCs) can collect light over a large area and concentrate it onto a small area of solar cells in order to enhance the performance of solar cells. The light is absorbed by a transparent sheet containing luminescent dyes and the emission is transported by total internal reflection to the edge of the plate where photovoltaic cells are positioned.¹ β -diketonate-based Europium (III) complexes are promising candidates for use as dyes in LSCs due to their high quantum yields, extended absorption window, minimal overlap between the absorption and emission spectra, and narrow emission band.² We will report a study of β -diketonates coumarin-based Lanthanide complexes aimed at optimising their luminescence characteristics by ligand design. Coumarins are well-known organic dyes³ that have served as antennae for LSC applications.² We will report the preparation and photophysical properties of two Europium complexes, [Eu(L)₃X₂] where,

X=DPEPO, L=7-methoxy or 7-diethylamine coumarin derivative, and investigation of their incorporation in several polymer films.

Acknowledgment

We are grateful to Dr. Álvaro Cañete M. (Pontificia Universidad Católica de Chile) for the gift of the coumarin ligands.

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ET11.12.07

Fast Hall™—A New Method for Measuring Low Mobility Thin-Film Materials Jeffrey R. Lindemuth; Lake Shore Cryotronics, Inc., Westerville, Ohio, United States.

The Hall effect is the primary method to measure carrier density, mobility and carrier type in materials. The most common method for measuring the Hall effect in semiconductors uses a DC magnetic field. The community has developed a well-defined protocol for removing spurious voltages in the measurement. Reversing the magnetic field and subtracting the measured voltages will remove any voltage that does not depend on the magnetic field. As research interest in studies of the transport mechanisms expands beyond semiconductors, with moderate to high mobility, the standard DC field method reaches its limit of applicability. We present a new measurement protocol based on the reverse-field reciprocity theorem. The reverse-field reciprocity theorem considers a four port network with current inputs and voltage measurements and an applied magnetic field. If a current is applied to two of the inputs (say 1 and 3) and a positive field B a voltage (V) is measured on terminals 2 and 4. This voltage can depend of the magnetic field $V_1(B)$. If the current and voltage leads are interchanged, current on terminals 2 and 4, voltage measured between 1 and 3, $V_2(B)$. The theorem states that $V_2(B) = V_1(-B)$. This is a very general result; the only requirement of the material is that it is electrically linear. This means that thermoelectric voltages require special treatment. In the above example, $V_1(B) - V_2(B)$ removes the offset voltage without physically reversing the magnetic field. Measurements using the Fast Hall™ method on InAs, IGZO, ZnO, pyrite, Graphene and GaAsSb have demonstrated excellent agreement between measurements using DC or AC field hall and Fast Hall. The Fast Hal method can preform up to 100 Hall measurements per second. The high speed of the measurements greatly reduces the effects of thermal drift and self-heating of the sample during the measurement. Thermal drift is one of the major contributions to noise in hall measurements of low mobility and thin film samples. The Fast Hall method increases measurement speed, extends the range of mobility that can be measured using DC field methods. The method is applicable to both single carrier materials and multi-carrier materials.

ET11.12.08

Air-Processed Defect-Free ZnO Nano-Particles for Solution Processed Photovoltaic Cells Yuhui Ma, Xiuwen Xu, Yuemin Xie, Menglin Li and Sai-Wing Tsang; Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong, Hong Kong.

Solution-processed ZnO nano-particles (ZnO-NPs) have been widely used as electron transporting layer (ETL) in developing high efficiency organic photovoltaic (OPVs) cells. However, the ZnO-NPs are known to be sensitive to oxygen and moisture in air with strong trap emission in the visible (400-700nm) region. Consequently, those reported high efficiency OPVs with ZnO ETL were fabricated in inert environment. This limits the large-scale industrial deployment of low-cost and high-efficiency photovoltaic cells. Here, we will demonstrate an approach to achieve defect-free ZnO NPs thin film processable in ambient air. It is found that the trap states in ZnO are rapidly induced by oxygen and moisture within a few seconds exposure in air. Interesting, this trap developing process is completing with the ultra-violet (UV) irradiation. There exists an operation widow that the trap states can be drastically reduced in very short period of UV irradiation time with less than 10s. However, they start growing gradually with continuous irradiation in longer time for more than 1min. Using the air-processed ZnO-NPs ETL with short time UV irradiation, it is found that different donor:acceptor OPVs can achieve high efficiencies comparable with those fabricated in inert environment. By eliminating the trap states, it mainly reduces the interfacial recombination with enhanced fill-factor and prolonged device lifetime. The un-encapsulated devices stored in ambient air can retain more than 80% of the initial efficiency.

ET11.12.09

Synthesis and Characterization of SnO₂ and TiO₂ Nanoparticles Doped with Li or Ni and Hybrid Composites Antonio Vázquez¹, María Taeño¹, David Maestre¹, Julio Ramírez Castellanos² and Ana Cremades¹; ¹Física de Materiales, Facultad de CC. Físicas, Universidad Complutense de Madrid, Madrid, Spain; ²Química Inorgánica I, Facultad de CC. Químicas, Madrid, Spain.

Wide bandgap semiconducting oxides, such as SnO₂ and TiO₂, have demonstrated potential applicability in numerous fields such as optoelectronic devices, catalysis, gas sensing or energy storage, which can be improved by controlling the dimensions, morphology, doping and composition of these materials. Moreover, hybrid composites combining advantages of inorganic and organic compounds are emerging as low cost materials with promising application in photovoltaic and energy storage devices [1]. These hybrid composites can retain the advantages of their organic and inorganic counterparts and even exhibit new synergetic properties, hence gaining increasing research attention in the last years.

In this work, rutile SnO₂ and anatase TiO₂ nanoparticles have been synthesized by a co-precipitation method based on hydrolysis, using SnCl₂·2H₂O or Ti(OBu)₄, respectively, as precursors. For the synthesis of Ni or Li doped nanoparticles, stoichiometric amounts of NiCl₂·6H₂O or LiCl, respectively, were added as precursors. Large amounts of nanoparticles with high crystallinity, good homogeneity and dimensions ranging from 8 to 10 nm are obtained with this method. These nanoparticles have been initially characterized by x-ray diffraction (XRD), transmission electron microscopy (TEM), energy dispersive x-ray spectroscopy (EDS), Raman spectroscopy, X-ray absorption spectroscopy (XAS), photoluminescence (PL), and cathodoluminescence (CL). The presence of dopants induces changes in the dimensions of the nanoparticles, and in their structure of defects and optical and electronic properties. In this work, nanoparticles with reduced dimensions were achieved by Ni doping, while Li doping induces an enhancement of the luminescence, both for SnO₂ and TiO₂. Moreover, changes in the Raman signal, mainly in the E_g modes associated with O-Ti-O symmetric stretching vibrations in anatase TiO₂, and vibrations of O anions along the c axis in SnO₂, were observed.

In this work hybrid compounds made with PEDOT:PSS functionalized with the undoped or doped SnO₂ or TiO₂ nanoparticles, synthesized by hydrolysis, were deposited onto Si substrates at room temperature by spin-coating, thus involving low cost and rapidity, as compared with the commonly used vacuum-based techniques. The thickness of the composite layers fabricated in this work is around 120 nm, as measured by atomic force microscopy (AFM). The presence of inorganic SnO₂ or TiO₂ nanoparticles could add functionality to the hybrid composite and broaden its related applicability in photovoltaic devices [1], photocatalysis, optoelectronics and bioapplications, as some examples, due to charge transfer and variations in the local electronic structure of the hybrid material which can lead to improved performance.

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ET11.12.10

Improving Charge Extraction from Bismuth Oxyiodide Photovoltaics with 2D Metal Dichalcogenide Transport Layers Tahmida N. Huq^{1,3}, Rosie Baines¹, Robert L. Hoye^{2,1}, Pin-chun Shen⁴ and Judith L. MacManus-Driscoll¹; ¹Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom; ²Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom; ³EPSRC Centre for Doctoral Training in Graphene Technology, University of Cambridge, Cambridge, United Kingdom; ⁴Research Lab of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Bismuth oxyiodide (BiOI) has recently been shown to be a promising lead-free alternative to halide perovskites for photovoltaics. BiOI replicates the electronic structure of halide perovskites, and is predicted to show tolerance towards anti-site and vacancy defects. Notably, BiOI thin films have been found to be at least two orders of magnitude more air-stable than methylammonium lead iodide.^[1] Although record external quantum efficiencies of 80% have been achieved, the power conversion efficiency (1.8%) is limited by inefficient hole extraction in an ITO|NiO_x|BiOI|ZnO|Au device stack. This is due to downwards band-bending of BiOI at the NiO_x interface caused by poor energetic matching of the BiOI (work function of 5.1 eV) with NiO_x (work function of 4.8 eV). Higher work function materials are required to overcome this barrier. In this work, 2d molybdenum sulphide (MoS₂) is investigated as an alternative hole transport layer due to its work function tunability. Through plasma treatment, the work function is increased to >5.1 eV. We use photoemission spectroscopy to probe the MoS₂|BiOI interface, and our detailed studies reveal an upwards band-bending which can enable improved hole extraction. We explore the modification of chemical vapour transport BiOI growth conditions required as a result of the change in surface chemistry at the new hole transport layer interface. SEM microscopy and X-ray diffraction reveal that these modifications lead to an improvement in orientation and morphology (i.e. more compact and pinhole free) of the BiOI films, essential for shunt-free devices. Through these optimisations and subsequent characterisation, we are able to increase our understanding of the interfaces in the device stack which is crucial for achieving at least 4% efficient devices.

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ET11.12.11

Tomographic Imaging of PbSe Quantum Dot Superlattices for PV Applications Xiaolei Chu¹, Hamed Heidari¹, Alex Abelson², Caroline Y. Qian², Matt Law² and Adam J. Moule¹; ¹University of California, Davis, Davis, California, United States; ²University of California, Irvine, Irvine, California, United States.

Ordered PbS and PbSe quantum dot (QD) arrays have demonstrated multiple exciton generation in response to photo excitation by high energy photons. This inherently quantum material demonstrates a pathway to photovoltaic efficiency above the Shockley limit if ordered and defect free super-lattices of these QDs can be fabricated. Here we use high-resolution tomographic imaging of PbSe super-lattices to study the material order resulting from self-assembly and ligand exchange. Quantum dots are synthesized using long chain ligands to ensure a narrow size distribution. Superlattice arrays of long-chain ligand QDs self-assemble at liquid-liquid interfaces into ordered superlattice films with hexagonal packing. After the film has formed, in-situ ligand exchange is used to reduce the distance between QDs, leading to recrystallization of the super-lattice to a distorted simple cubic array. This array has structural defects including twinning between domains, point defects, and bridging between some neighboring QDs, that leads to a heterogeneous energy landscape. The super-lattice order, seen at the top interface of the film, is accessible using SEM imaging and is often very different from the arrangement of particles in the center of self-assembled films. We use tomographic reconstruction of STEM images to determine the position of QDs with nm precision and bridging between particles. We show how defects in the superlattice structure effects the charge localization.

ET11.12.12

Layered Hexagonal Oxy-carbides, M_{n+1}AO₂X_n (M=Sc, Y, La, Cr and Mo, A=Ca, X=C)—Novel Photovoltaic Ceramics Zhenyu Wang, Xin Chen and Chunming Niu; School of Electrical Engineering, Xi'an Jiaotong University, Xi'an, China.

Solar energy is increasingly becoming an integrated part in energy spectra worldwide and promises to greatly relieve the world from the shackle of the fossil fuels. Development of high performance solar cells depends on the discovery of new photovoltaic materials. The search for the new photovoltaic (PV) materials has been intensified since the invention of the perovskite solar cells.¹ The rapid development of computational methods and tools deepens our understanding of existing materials and provides an insightful guide for experiments.² And most importantly, it also makes more and more feasible to discover novel materials via computer simulations, such as solid state electrolytes, electrocatalytic materials, two-dimensional (2D) semiconductors, and perovskite solar cell materials.

In the recent years, advanced functional ceramics attract broad interests due to its outstanding mechanical properties, such as high strength and hardness, excellent wear resistance and good frictional behavior.³ Given excellent dimensional stability as well as the ability to withstand corrosive environments, the applications of functional ceramics in the semiconductor industry is desirable.

A family of layered hexagonal oxy-carbides and oxynitrides with the general formula, M_{n+1}AO₂X_n (MAOX) is discovered using first-principles DFT calculations, where n=1–3, M is an early transition metal, A is an alkaline earth metal in Group IIA or a late transition metal in Groups IB and IIB, X is C and/or N.⁴ The family can be divided into three sub-groups of 2121, 3122 and 4123 with n = 1, 2 and 3, respectively. Thermodynamically, the MAOX phases are very stable. Tuning the composition, MAOX can be metals, semimetals or semiconductors. In this report, we discuss five 2121 oxy-carbide MAOX semiconductors, M₂CaO₂C (M=Sc, Y, La, Cr and Mo). Their band gaps are from 0.39 to 1.14 eV. They have superior PV properties and their theoretical solar cell efficiencies are on par with GaAs. Particularly, the efficiency of Cr₂CaO₂C reaches 27.7% that is above 90% of the Schottky-Queisser (SQ) limit. Furthermore, amazingly, the five MAOX semiconductors possess outstanding strength and machinability, e.g., their Young's moduli are comparable to ceramics and MAX phases, and Poisson's ratios higher than MAX and even comparable to metals. MAOX semiconductors are promising multifunctional ceramics. The unique combination of the photovoltaic and mechanical properties suggests great potentials of MAOX semiconductors for advanced solar cell applications.

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ET11.12.13

Nanostructured Hybrid Semiconducting Materials as Efficient Photodetectors Dawit M. Gedamu¹, Ivy Asuo^{1,2}, Luis Felipe Gerlein¹, Ibrahima Ka¹, Riad Nechache¹, Suchismita Basu¹, Jaime Benavides-Guerrero¹ and Sylvain Cloutier¹; ¹École de technologie supérieure, Montreal, Quebec, Canada; ²inrs-ent, Varennes, Quebec, Canada.

Low cost high-speed photodetectors are in high demand for emerging technologies such as wearable, biochemical, biomedical or internet-of-things etc. The current photodetectors in the market are commonly based on silicon or semiconductor alloys which require costly and complex fabrication methods. Hybrid perovskite semiconductors recently emerged as one of the promising material systems for various optoelectronic applications because of low cost material synthesis in addition to an excellent material property such as high photon absorption, a small exciton binding energy (2 meV), tunable bandgap and versatile material properties. Despite the enormous progresses on employing HPs for solar energy-harvesting applications, very few have explored their potential for low-cost photodetectors.

In here we will demonstrate an efficient and stable nanostructured lead-halide perovskite-based photodetector using a perovskite nanowire networks as active layer deposited directly atop a micro-patterned fluorine-doped tin oxide (FTO) substrate by spin coating. The use of an intertwined perovskite nanowire network also greatly facilitates the fabrication and the scaling, while significantly improving the device performance due to a larger surface-to-volume ratio. Recently, we also developed a simple drop casting technique to integrate ZnO nanostructures in to lithographically patterned gold electrodes in a simple experimental strategy. The excellent photo detector capability in the UV range which is further broadened to NIR though the incorporation of PbS quantum dots will also be presented.

ET11.12.14

Graphene Electrodes for PbS Quantum Dot Photovoltaics M. Hadi Tavakoli Dastjerdi, Mohammad Mahdi Tavakoli, Nicole Moody, Jing Kong, Mounji Bawendi and Silvija Gradecak; Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

PbS quantum dots (QDs) have emerged as promising candidates for photovoltaic (PV) applications due to their direct and tunable bandgap and compatibility with solution processing. Zinc oxide (ZnO) nanowires (NWs) have been incorporated to enhance carrier extraction and graphene bottom electrodes have been used toward realization of flexible QD-based PV devices. However, the role of the nanowire geometry (*e.g.* density, length, or morphology) relative to the QD properties remains unexplored, in part due to challenges with controlled nanowire synthesis. Here, we use the precursor concentration as a handle to tailor ZnO NW growth and thereby PV characteristics resulting in power conversion efficiency beyond 10%. Lowering the precursor concentration results in the improvements of FF and V_{oc} likely due to: a) reduced nanowire areal density and thus a lower number of surface states, b) improved scattering of the incoming light resulting in increased optical path length and c) enhanced infiltration of NWs with QDs. Furthermore, we have achieved the first PbS QD PV device with graphene as top electrode by optimizing the transfer process of graphene sheets grown by chemical vapor deposition. Replacing the currently dominant, but expensive gold top electrode with transparent graphene not only reduces the cost of device fabrication, but also allows for illumination of the device through the top electrode. Our results have shown that this leads to increased density of photo-generated carriers, evidenced by >10% increase in J_{sc} .

ET11.12.15

Improve the Photo-Stability of Polymer Solar Cells by Controlling the Chemical Structure of Photoactive Materials Rasool Shafket^{1,2}, Vu Van Doan^{1,2}, Chang Eun Song^{1,2}, Hang Ken Lee¹ and Won Suk Shin^{1,2}; ¹Energy Materials Research Center, Korea Research Institute of Chemical Technology, Daejeon, Korea (the Republic of); ²Advanced Materials and Chemical Engineering, University of Science and Technology, Daejeon, Korea (the Republic of).

To commercialize the polymer solar cells many conditions should be satisfied such as efficiency, process and stability. Recently many scientists are interested in the stability of the polymer solar cells, but most of the researches are hovering at thermal stability. But real challenges are in photo-stability and the burn-in loss during exposed on the sun light is one of the biggest challenges to go to the market. Lost more than 40% of their initial efficiency in just 24 hours after exposing to 1 sun condition is common for polymer solar cell devices. This burn-in loss does not come from the decomposition of the photoactive materials but rather caused by the electro- and physical-properties of the photoactive materials. To overcome the burn-in loss, we tried two approaches. First one is inserting an appropriate interlayer for inverted solar cells. Second approach is design new photoactive materials which reduce the burn-in loss. Here we present the improved photo-stability results by applying elaborately designed photoactive materials.

ET11.12.16

Hydrogen Motility at Reduced-Dimension Interfaces in Proximity to Near Semiconductor-Metal Boundaries and Dislocations Jonathon Mitchell; Koriyama, Japan.

Understanding of the fundamental physical processes underlying key material properties in electronically active interfaces has increased importance with reduced-dimension devices like FET, MOS and photovoltaics. As in many of these devices, the inclusion of non-natives like Hydrogen, Nitrogen and Oxygen, are known to strongly affect the electronic and structural properties of many materials and have particular importance in semiconductors for binding defects, enhancement or suppression of electrical activity, long-term stability and operation. Acting as an isolated interstitial impurity, amphoteric hydrogen occupies different lattice sites and can counter the conductivity of extrinsic dopants. Nitrogen is largely impeded by an anomalous optical saturation effect, and similarly Oxygen can be impacted by variable voltage influencing dielectric permittivity and charge separation. However, the mechanisms involved are more complex than the simple application of a single hydrogen, nitrogen or oxygen to the semiconductor bond. Although tracking individual particles through the sub-lattice interface remains difficult, previous theoretical and simulation study of these interfaces has provided additional information which resolves current experimental observations. Utilising an adaptive moving-mesh in Eulerian space with Lagrangian point-aggregation for a large 904 site interface surface with bookkeeping in z-space, our model has compared the smoother particle hydrodynamics with real-time and cumulative particle transport solids. Essentially rendering a recursive output for predictive yield of electron charge transport at or near semiconductor-metal interfaces.

In this work we evaluated planar and also surfaces with sharp discontinuities from manufacture and handling, comparing the simulation to the intermediate and long-term interface properties. Non-Gaussian distribution agreed with the observed preferential diffusion probabilities and pseudo-spore motilities according to discontinuities including mecha-mechanical shearing, grain orientation, and chemical orientation of defect alignment. New information is obtained concerning the intergranular properties thermal characteristics, as well as the presence of distinct profiles seemingly dependent to some extent on the binding algorithm of the semiconductor between the bulk and extending through the interface. For MOS-like devices (including photovoltaic), oxygen and hydrogen both introduced long-term parasitic conductivity, while the response for nitrogen and hydrogen was suppressed. This describes the suitability of nitrogen based environment during the semiconductor fabrication prior to encapsulation on the long-term performance and reliability of thin, flexible devices.

ET11.12.17

Exploring γ -In₂(Se_{1-x}Te_x)₃ Alloys as Photovoltaic Materials Wei Li, Tianshi Wang and Anderson Janotti; Materials Science and Engineering, University of Delaware, Newark, Delaware, United States.

γ -In₂Se₃ (hexagonal crystal structure, space group $P6_7$) has a direct band gap of ~ 1.8 eV with high absorption coefficients near the band edge. Alloying with Te could allow for tuning the band gap, widening the wavelength range in the absorption spectra, adding great flexibility to device design. Using density functional theory with the HSE06 hybrid functional, we investigate the electronic and optical properties of γ -In₂Se₃ and γ -In₂(Se_{1-x}Te_x)₃ alloys. The calculated band gap of 1.84 eV for γ -In₂Se₃ is in good agreement experimental data, and the absorption coefficient is found to be as high as that in direct gap III-V semiconductors. We also find that incorporation of Te, forming γ -In₂(Se_{1-x}Te_x)₃ alloys, is an effective way to tune the band gap from 1.84 eV down to 1.23 eV, thus covering the optimal band gap for single layer solar cells. We determined the band alignments between γ -In₂Se₃ and γ -In₂(Se_{1-x}Te_x)₃, and their band edge positions with respect to vacuum level. Our results indicate that γ -In₂Se₃ has a tendency for displaying n -type conductivity.

ET11.12.18

Synthesis and Measurement of Optical and Transport Properties of Promising Metal Oxide Light Absorber CuBiW₂O₈ with 1.5 eV Band Gap [Lize Zhou](#)³, Guangjiang Li², Edan Bainglass¹, Pranab Sarker¹, Lyubov V. Titova², Muhammad N. Huda¹ and Pratap M. Rao³; ¹Department of Physics, The University of Texas at Arlington, Arlington, Texas, United States; ²Department of Physics, Worcester Polytechnic Institute, Worcester, Massachusetts, United States; ³Department of Mechanical Engineering, Worcester Polytechnic Institute, Worcester, Massachusetts, United States.

Metal oxide semiconductors with moderate band gaps are highly desired for high-efficiency, low-cost, stable, and environmentally-friendly solar cells. CuBiW₂O₈ (CBTO) has been predicted by density functional theory (DFT) to be a promising metal oxide light absorber with band gap of 1.43 eV.¹ However, this semiconductor has not been experimentally synthesized so far, and the optical and transport properties have not been measured. Here, CBTO was successfully synthesized for the first time by solid-state reaction in a Cu-rich environment, and identified by X-ray diffraction. The light absorption spectrum of CBTO was measured, and a light absorption edge of 820 nm (~ 1.5 eV) with absorption coefficient of 104 cm⁻¹ at 700 nm, was observed. Electron mobility in CBTO (~ 200 cm²v⁻¹s⁻¹) was determined by time-resolved THz spectroscopy. This CBTO showed promising performance as a photocathode for photoelectrochemical water reduction. However, the photovoltaic performance of the CBTO solar cell is still limited by granular CBTO film quality and impurities introduced by inter-diffusion between CBTO and other layers in the cell. By modifying the synthesis methods, we believe CBTO with ~ 1.5 eV band gap and promising charge mobility can achieve higher efficiency than Cu₂O, which is the best-performing metal oxide photovoltaic absorber to date.

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ET11.12.20

Structural and Electronic Properties of the Pentanary Compound (Ag_xCu_{1-x})₂ZnSnS₄ Synthesized via Solution Route [Jitendra Kumar](#) and Sarang Ingole; Indian Institute of Technology Kanpur, Kanpur, India.

Silver (Ag) has been incorporated at the copper sub-lattice sites in the quaternary compound Cu₂ZnSnS₄ (CZTS) which is being under intense investigation as an absorber material for the photovoltaic application. Thin films of the resulting pentanary compound (Ag_xCu_{1-x})₂ZnSnS₄ ($0 \leq x \leq 1$) show remarkable changes in their microstructure and electronic properties. With the increasing Ag content, the grain size increased from 0.13 to 2 μ m which could be attributed to the liquid assisted grain growth mechanism. While the observed increase in the optical band gap from 1.5 to 2.0 eV could be attributed to the influence of d -orbitals of Ag atoms on the valence band edge of the CZTS compound. The charge carrier density decreased by two orders of magnitude with only 4 atomic % Ag ($x = 0.04$) incorporated in the films which indicate the strong influence of Ag_{Cu} on the density of Cu_{Zn} and V_{Cu} point defects which are the major acceptors in CZTS. The reduction of these intrinsic point defects is also being reflected in the observed decrease in the Urbach energy from 336 meV (for $x = 0.00$) to 230 meV (for $x = 0.21$). This has been further correlated with the ordering-disordering detected by the near-resonant Raman scattering. These observed changes with increasing Ag content could possibly be used for tailoring the properties of CZTS for the better performance of CZTS based photovoltaics.

ET11.12.21

Band Alignment at the Back Contact of CdTe Devices—What Bands Need to Align? [Adam Phillips](#), Geethika K. Liyanage, Fadhil K. Alfadhili, Randy Ellingson and Michael J. Heben; University of Toledo, Toledo, Ohio, United States.

The deep valence band position of CdTe (~ 5.9 eV) makes it difficult to form an Ohmic back contact in CdTe devices. Back contact formation typically results in significant downward band bending in the CdTe that forms an energetic barrier to hole transport. Historically, the addition of Cu at the back of CdTe results in a doped interface region in which the width of the band bending is limited, effectively reducing the barrier. In addition to limiting hole transport, the band bending in the conduction band attracts electrons to the interface. While the Cu doping reduces the width of the band bending, the achievable doping levels do nothing to repel the electrons from this interface. Addition of semiconducting buffer layers with a conduction band higher than that of CdTe have been incorporated into devices to prevent the electrons from recombining in the back contact and are often referred to as electron reflectors.

Recent numerical modeling of CdTe devices has shown that band alignment of the conduction band at the *front contact* is critically important to device performance.¹ In this case, the a modest 0.1-0.2 eV “spike” at the emitter/CdTe interface results in the best device performance even though, energetically, it would appear to restrict electron flow. Recently, we used numerical modeling to understand how the band alignment at the *back contact* affects device performance. We showed that in an ideal case, one in which the CdTe/semiconductor buffer interface is outside the depletion regions, band alignment of the valence bands plays a significantly larger role than band alignment of the conduction bands, and, in fact, the overall device efficiency is independent of the conduction band offsets at the back of the device. In this presentation, we will discuss these generalized results and how to apply these results to real world applications.

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ET11.12.22

Modeling PV/TPV Devices Based on Exact Analytical Solution of the Generalized Shockley-Queisser Model [Andrei Sergeev](#), Sunny Karnani and Christopher M. Waits; Army Research Laboratory, Adelphi, Maryland, United States.

Currently, interplay of electron and photon processes in the open-circuit regime is understood substantially better than that in the regime with optimal conversion of electromagnetic power. First, the open-circuit regime is well described by classical thermodynamics. Second, there is exact analytical solution for the open-circuit voltage as a function of photon flux characteristics. This analytical solution has been generalized to include other losses due to nonradiative recombination processes in terms of luminescence quantum yield. Therefore, analysis of the open circuit regime is very often employed for optimization of electron and photon processes related to PV conversion. The Shockley-Queisser limit is described by the endoreversible thermodynamics, which includes irreversible processes and entropy generation due to thermal energy transfer from the radiation source to the solar cell. Despite extensive

theoretical research, the analytical expression for the maximal efficiency as a function of photon flux characteristics and electronic properties has not been reported yet.

For advanced modeling of PV/TPV devices with sophisticated photon management we obtained exact solution of the generalized Shockley – Queisser model and developed original modeling tool. Our modelling takes into account spectral absorption/emission characteristics, nonradiative recombination processes, and photon management. For noninteracting electrons and for electrons interacting via Auger processes we obtained exact analytical solution for photovoltaic efficiency, output power, and all other PV characteristics. The obtained solution provides mathematical base of PV conversion and endoreversible thermodynamics controlled by the chemical potential. We derive exact equations for useful energy, emission losses, and total thermal losses (electron-phonon relaxation and nonradiative recombination) per absorbed photon. The developed formalism is very convenient for analysis of analysis of photocarrier kinetics. In particular, we derived the universal relation between the optimal photocarrier collection time and the photoelectron lifetime with respect to all radiative and nonradiative processes. Let us highlight that due to the short photocarrier collection time with respect to the photocarrier lifetime, the photocarrier kinetic and transport processes in the optimal power regime may differ from the processes in the open circuit regime. Our preliminary analysis also shows that in traditional devices without photon management, it is not possible to realize simultaneously both high absorption and fast photocarrier collection, which is required by the optimal collection rate. In PV/TPV devices with enhanced photon trapping and recycling, the thickness of the base may be reduced below the characteristic value, at the characteristic value, at which the diffusion processes do not limit the optimal photocarrier collection.

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ET11.12.23

Solution-Processed Vanadium Oxide as an Efficient Hole Injection Layer for Phosphorescent Organic Light-Emitting Diodes Deepak K. Dubey, Yu C. Lo, Rohit Ashok Kumar Yadav, Sujith Sudheendran Swayamprabha and Jwo-Huei Jou; Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu City, Taiwan.

Organic light-emitting diodes (OLEDs) have attracted significant attention in both industry and academic research because of the increasing demand of flat panel displays for televisions, smartphones and tablets, etc., and solid-state lighting applications. With the development of highly efficient materials, innovative fabrication and out-coupling techniques, the power efficacy of OLEDs can reach as high as, >100 lm/W, meeting the requirements for flat panel display and lighting applications. Nevertheless, most OLEDs with high efficiency are fabricated by thermal evaporation, which is suffering from the high manufacturing cost and difficulties to realize large area devices. To address these issues, all or partly solution-processed OLEDs offer an opportunity to significantly lower the fabrication cost and also enable the application of large area devices and flexible substrates, thanks to its compatibility to roll-to-roll processing. However, relatively low efficiency is often a challenge for solution-processed OLEDs.

To achieve high efficiency, hole injection/transport layers (HIL/HTL) and the charge blocking layers are usually incorporated to maintain charge balance and to confine the excitons in the emitting layer. Most solution processed OLEDs use PEDOT: PSS (polyethylene dioxythiophene : polystyrenesulfonate) as a hole injection material because of its high transparency, high work-function and high conductivity. However, PEDOT: PSS exhibits an acidic and hygroscopic nature, which induces the corrosion of ITO electrodes, resulting in the decrease of device performance lifetime. Therefore, much effort has been devoted to finding a new substitute. In this work, we develop a solution processed vanadium pentoxide (V_2O_5) as an alternative. The proposed approach can be easily processed under the simple conditions of room temperature and a water-free and solution-based process, which distinguish this approach from vacuum thermal evaporation or temperature annealing processes. OLEDs fabricated with V_2O_5 HIL exhibit a current efficiency of 64.3 cd/A, a power efficiency of 57.4 lm/W and an external quantum efficiency of 19.2% at the brightness of 100 cd/m², which are respectively 21, 23 and 31% higher to those fabricated with a conventional PEDOT: PSS HIL. Moreover, by substituting the problematic PEDOT: PSS with the inorganic V_2O_5 , the operating voltage and maximum luminance of the OLEDs is also substantially improved. Our study demonstrates that the presented new approach can serve as a new and simple route for the emerging technologies of low-cost and large-scale organic optoelectronic devices.

ET11.12.24

Solar Photo-Crystallization in the Production of Thin-Film Solar Cells Jesus Capistran Martinez, Laura Guerrero Martínez, Perla Yoloxóchitl García Ayala, Alessandra Beauregard León, M.T. Santhamma Nair and P.Karunakaran Nair; Universidad Nacional Autónoma de México, Temixco, México.

We present an innovative method of crystallization under concentrated sunlight of antimony sulfide thin films in solar cell structure: F-doped SnO_2 (FTO)/CdS/ $Sb_2S_3Se_{3-x}/C$. Here, CdS n-window thin film of 90 nm in thickness, as well as the p-absorbers of $Sb_2S_3Se_{3-x}$ thin films of 300 nm in thickness are produced by chemical deposition at 80 °C. Colloidal graphite paint is applied on the absorber films so as to define cell areas of 0.25 – 1 cm². The absorber films require heating at 250 – 300 °C to transform them to crystalline phase, which till now required heating in a vacuum oven under nitrogen ambient. We report that under clear-sky condition, concentrated sunlight (115 – 215 suns) directed toward the absorber film by a glass lens 8.5 cm in diameter helps achieve this crystallization. The approach has the added advantage that it is a rapid thermal processing technique as well, which minimizes loss of volatile components of the absorber film (S and Se) when heated in conventional way. The absorption of concentrated sunlight at the absorber-electrode interface helps increase the temperature toward the crystallization temperature. The acrylic-based graphite paint also encapsulates the cell, thereby eliminating the need for a vacuum environment to prevent degradation of the cell through oxidation. Solar cell produced this way has open circuit voltage of 0.46 V, short circuit current density of 16 mA/cm² and conversion efficiency of 3 % at this stage. The deposition technique as well as the cell processing described here are low-capital intensive. Hence it offers an accessible alternative in the preparation of this type of solar cells.

ET11.12.25

Functional Prototype Modules of Chemically Deposited Antimony Sulfide Selenide Thin Films Laura Guerrero Martínez, Perla Yoloxóchitl García Ayala, José Diego González Sánchez, Alessandra Beauregard León, M.T. Santhamma Nair and P.Karunakaran Nair; Universidad Nacional Autónoma de México, Temixco, México.

Functional photovoltaic modules of 7 cm² in active area and open circuit voltage 3.3 V and 20 mW power capable of lighting blue-light emitting diode (LED) were prepared by chemical deposition. For this R & D, first a chemically deposited CdS thin film of 100 nm in thickness was prepared on a commercial F-doped tin oxide coated glass (FTO) of sheet resistance 7 Ω. On this, a thin film (300-350 nm) of antimony sulfide selenide was prepared by chemical deposition at 80 °C in two successive depositions lasting 7-8 h from solution containing potassium antimony tartrate, triethanolamine, ammonia (aq), thioacetamide, thiosulfate and selenosulfate. Graphite paint in acrylic base was painted on area 1 cm²; a total of 7 such area painted on each FTO-coated glass cut to 2.5 cm x 7.5 cm. Antimony chalcogenide thin films obtained from chemical deposition are amorphous in nature and they require heating at 270 – 310°C to crystallize them. In this work the heating was done at 300°C during 30 min in nitrogen ambient at 20 Torr. After these, the FTO coating was scribed using silicon carbide point; and the cells were demarked by etching. Colloidal silver paint was applied on the graphite electrode and on the FTO coating along the periphery. Current-voltage characteristics of the cells were measured using solar simulator under standard conditions as well as under the sun (925 W/m²) near mid-day at 24 °C. Average values of the cell parameters are presented: V_{oc} 0.47 V; J_{sc} 18 mA/cm² and conversion efficiency, 3.9%.

ET11.12.26

Spray-Deposited CdS/PbS Solar Cell Nagendra Dhakal¹, Seth Calhoun¹, Robert E. Peale¹, Saiful Khondaker¹ and Isaiah Oladeji²; ¹University of Central Florida, Orlando, Florida, United States; ²Sisom Thin Films LLC, Orlando, Florida, United States.

We demonstrate photovoltaic action for a thin-film CdS/PbS heterojunction solar cell fabricated by aqueous spray deposition using earth-abundant elements as a potentially flexible, low-cost solar-cell technology. The structure comprises borofloat glass substrate, fluorine-doped tin oxide as transparent current collector, CdS window layer, and PbS absorber layer. Gold is deposited as ohmic contact to the PbS and light is incident through the substrate. The current-voltage curves in the dark are diode like with threshold voltage ~0.6 V. Under 1 sun illumination with 1.5 air-mass filter, the short circuit current density is ~ 4 microAmp/mm², the open circuit voltage is 0.14 V, the maximum power is ~ 150 nW/mm², and the fill factor is ~30%. The efficiency of these unoptimized first cells is ~0.01%.

ET11.12.27

Green Route Synthesized Copper-Zinc-Tin-Sulphide Nanocrystals for Heterojunction Solar Cells on Silicon Platform Sudarshan Singh¹, Ajit K. Katiyar¹, Arup Ghorai¹, Anupam Midya¹, Dipak K. Goswami¹ and Samit K. Ray^{1,2}; ¹Indian Institute of Technology Kharagpur, Kharagpur, India; ²S. N. Bose National Centre for Basic Sciences, Kolkata, India.

Recently, the kesterite Cu₂ZnSnS₄ (CZTS), comprising earth-abundant and environmental-friendly elements, has been widely considered as the most promising material among the chalcogenide-based semiconductors for thin films photovoltaic (PV) applications. The colloidal CZTS quantum dots and nanocrystals (NCs) are potentially attractive candidates for low-cost PV cells and modules owing to their compatibility with solution processing techniques [1]. A novel, facile and environment-friendly synthesis route, at a relatively low temperature, has been developed to synthesize the CZTS nanocrystals. Natural, edible olive oil containing mainly oleic acid has been utilized as a solvent, which also acts as a capping agent to control the growth of nanocrystals. The CZTS NCs inks were prepared using different sized NCs obtained at various centrifugation speeds and studied in detail by means of their structural and optical characterizations. For the device demonstration, the quaternary nanocrystals ink prepared with different sized NCs have been integrated on n-silicon substrates by spin coating to fabricate the CZTS NCs/Si heterojunctions. The photovoltaic characteristics of the fabricated p-CZTS/n-Si heterojunctions using the synthesized colloidal quaternary NCs are demonstrated in detail. The study reveals that the CZTS nanocrystals having smaller diameter exhibits higher power conversion efficiency in comparison to the nanocrystals having the larger diameter. An improved minority carrier lifetime has been observed in open circuit voltage decay measurement for the CZTS/Si heterojunctions fabricated with smaller sized nanocrystals. Optical reflectance measurements show that the enhanced light scattering in smaller nanocrystals plays an important role in improved power conversion efficiency. The one-step environmental friendly procedure for the production of CZTS NCs along with the demonstration of CZTS/Si photovoltaic cells implying the potential of earth-abundant and non-toxic CZTS in the nanostructured form integrated with the existing Si solar cell technology.

References:

[1] H. Zhou, W. C. Hsu, H. S. Duan, B. Bob, W. Yang, T. B. Song, C. J. Hsu and Y. Yang, "CZTS nanocrystals: a promising approach for next generation thin film photovoltaics", *Energy Environ. Sci.*, vol.6, pp. 2822–38, 2013.

ET11.12.28

Large-Area Flexible Perovskite Solar Cells with Outstanding Mechanical Durability Gunhee Lee¹, Min-cheol Kim¹, Yong Whan Choi¹, Namyoungh Ahn¹, Daeshik Kang², Hyun Suk Jung² and Mansoo Choi¹; ¹Seoul National University, Seoul, Korea (the Republic of); ²Sungkyunkwan University, Suwon, Korea (the Republic of); ³Ajou university, Suwon, Korea (the Republic of).

With the development of wearable electronic devices, the importance of portable power sources has been highlighted. Recently, perovskite solar cells have become promising candidates for portable power sources due to their high power density, lightweight features and low temperature processing. However, there still exist problems in terms of performance and flexibility of large-area device, prior to practical uses of perovskite solar cells as a portable power sources. To improve flexibility of perovskite solar cells, many studies have previously been conducted to replace the brittle transparent conducting oxide (TCO) like indium tin oxide (ITO), but there was no deep understanding about the mechanical properties of perovskite materials themselves. In this work, we experimentally investigated their own mechanical properties and flexibility from cyclic bending test of perovskite-coated film, in which the applied stress is controlled depending on different thickness of the substrate and bending radius. By finding crack-free region of perovskite films, we successfully demonstrated flexible perovskite solar cells with high efficiency (17.03%) and the unprecedented flexibility, sustaining its initial power conversion efficiency (PCE) after 10,000 cycles of bending at 0.5 mm bending radius. Finally, we fabricated large-area flexible perovskite solar cells without TCO, leading to the best PCE of 13.6% (cell size, 1.2 cm²). The large-area device showed outstanding flexibility as well.

SESSION ET11.13: Low Cost High Efficiency Solar Cells
Session Chairs: Erik Garnett and Seth Hubbard
Thursday Morning, November 29, 2018
Hynes, Level 3, Room 304

8:30 AM *ET11.13.01

Bringing III-V Photovoltaics Down to Earth with Dynamic-Hydride Vapor Phase Epitaxy Aaron Ptak, John Simon, Kevin L. Schulte, Kelsey A. Horowitz and Timothy Remo; National Renewable Energy Laboratory, Golden, Colorado, United States.

III-V semiconductors are the gold standard of photovoltaic materials. They have the highest demonstrated conversion efficiencies, and they can be very light, thin, and flexible. III-V devices are also straightforwardly extendable to multijunction structures for even higher efficiencies. What III-Vs are not, however, is cheap. Much of the cost of III-V deposition comes from the expensive precursors used in the incumbent metalorganic vapor phase epitaxy (MOVPE) process, the inefficiency with which they're used, and the low-throughput of traditional batch-style growth reactors. This leads to costly devices that are only prevalent in somewhat niche markets, including space power.

Here, we describe our recent development of dynamic hydride vapor phase epitaxy (D-HVPE), an extension of the standard HVPE process that has been known for decades, but unlike traditional HVPE allows for the deposition of relatively complex heterostructures and devices. HVPE uses much less expensive elemental source material, lower hydride overpressures, and lends itself to high-throughput, in-line deposition. These features project to make III-V deposition costs by D-HVPE much lower than is possible today.

The challenge is to use this low-cost growth platform to create III-V devices that rival the excellent performance of MOVPE-grown solar cells. There is little point in cheap III-V devices if they don't maintain the conversion efficiency advantage that makes them so attractive in emerging markets such as electric vehicles, device charging, and other space-constrained applications. Fortunately, D-HVPE produces bulk material and interface quality that is nearly identical to MOVPE-grown material. We will give a general overview of the D-HVPE development of single-junction GaAs and GaInP devices, tunnel-junction interconnects, and the world's first HVPE-grown multijunction solar cells. We will also describe the next steps for this technology as we attempt to bring photovoltaics that are largely constrained to space applications down to Earth.

9:00 AM ET11.13.01

Engineering Light Absorption, Carrier Collection and Recombination in Atomically-Thin Photovoltaics [Joelson Wong](#)^{1,2}, Deep M. Jariwala^{1,2}, Artur Davoyan¹, Giulia Tagliabuc¹, Michael Kelzenberg¹, Joseph S. DuChene¹, Matthias H. Richter¹, Kevin Tat¹, Michelle Sherratt^{3,1}, Alexandra Welch¹, Wei-Hsiang Lin¹ and Harry A. Atwater¹; ¹California Institute of Technology, Pasadena, California, United States; ²Electrical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, United States; ³Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

The class of layered van der Waals (vdW) materials, materials where their weakly-bonded layered structure provides intrinsically passivated surfaces along the basal plane, allows one to mechanically cleave these materials to produce a single monolayer of atoms. Graphene, cleaved from graphite, was the first member discovered in this layered two-dimensional (2D) family. The group of layered vdW materials now span nearly every material class imaginable, from insulators and semiconductors to superconductors and topological insulators. Furthermore, because of their weak out-of-plane van der Waals interaction, they can be mechanically stacked to form a high-quality heterostructure between the most disparate materials, allowing one to design arbitrary heterostructures with a vast array of unexplored properties and applications.

An interesting member of this 2D family for photovoltaic applications is the semiconducting transition-metal dichalcogenides (TMDCs), compounds of the form MX_2 , where M is a transition metal and X is a chalcogen (e.g. sulfur, selenium, or tellurium). TMDCs have some of the highest absorption coefficients of photovoltaic materials, and in their monolayer form, can be passivated in a way to reach nearly perfect radiative efficiency. Moreover, they offer a wide range of bandgaps ($\sim 1.1 - 2.0$ eV), which can be tuned through quantum confinement effects and chemical alloying. Combined with their inherent stability and use of earth-abundant metals, vdW heterostructures of TMDCs are therefore attractive candidates for photovoltaic applications.

A conventional photovoltaic device that has high efficiency must maximize three figures of merit: optical absorption, subsequent carrier collection, and high photovoltage. Through proper nanophotonic engineering and device design, we show that atomically-thin vdW materials can achieve these three figures of merit and therefore act as efficient photovoltaic materials.

First, we experimentally show that in ultrathin (<10 nm) transition metal dichalcogenides (TMDCs), it's possible to achieve near-unity ($>90\%$) broadband absorption in the visible spectrum. We therefore utilize this optical geometry along with an optimized carrier collection scheme (IQE $> 70\%$) to create a device with record photocurrent density (EQE $> 50\%$) in these materials. Second, we modified the recombination dynamics in these materials through the use of carrier selective contacts, leading to record values of open circuit voltage ($V_{oc} > 700$ mV). Lastly, we present an outlook for large-area integration and schemes to further enhance the efficiency in these atomically-thin devices.

9:15 AM ET11.13.02

Microscopy Reveals the Role of Boundaries in Single-Crystalline-Like GaAs Solar Cells Grown on Flexible Metal Substrates [Jonathan Poplawsky](#)¹, Pavel Dutta², Wei Guo¹, Harvey Guthrey³, Monika Rathi², Devendra Khatiwada², Carlos Favela², Sicong Sun², Chuanze Zhang², Bo Yu² and Venkat Selvamani²; ¹Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; ²University of Houston, Houston, Texas, United States; ³National Renewable Energy Laboratory, Golden, Colorado, United States.

Photovoltaic (PV) devices based on single-crystalline GaAs semiconductors hold the world record for the highest efficiency for a homojunction solar cell. However, the substrates used for these materials are expensive making GaAs based solar cells cost-prohibitive for mainstream terrestrial use, which limits the device applications. A unique method to grow GaAs devices has been developed using roll-to-roll processing on a flexible metal substrate. In addition to decreasing costs, this method allows for GaAs devices to be flexible, which is of interest when considering transportability. In addition to solar cells, GaAs devices made using this process can be used for many other applications. The power conversion efficiencies (PCE) of the flexible GaAs solar cells were measured to be approximately 10%. Although a 10% PCE is about three times less than the world record GaAs solar cell, this is a good preliminary device using roll-to-roll processing. To better understand the efficiency limits, films and devices with different doping concentrations were tested using a suite of microscopy techniques including electron backscatter diffraction (EBSD), electron beam induced current (EBIC), atom probe tomography (APT), and cathodoluminescence (CL). The films showed a unique property in that the mobility increases with increasing dopant concentration, which has been better understood after the microscopy experiments. The EBSD results show that the GaAs films are highly oriented in the [001] direction, however, there is evidence of slight orientation deviations ($<1^\circ$) between ~ 1 μm sized features. The degree of orientation deviation and the presence of twin boundaries between grains has been shown to increase with dopant concentration. Correlative EBSD and EBIC cross-sectional measurements show a decreased EBIC signal in the grain boundary (GB) regions. Higher rotational angles (still $<1^\circ$) have been correlated to a lower EBIC signal, which is indicative of recombination centers that are detrimental to the device performance. CL measurements corroborate the EBIC results showing defect emission in the GB regions. APT has shown C accumulation in the GB regions, which is potentially responsible for recombination in these regions. Overall, the results suggest that the low angle GBs ($<1^\circ$) do not benefit the device and may be detrimental in their current state. Post-deposition heat treatments (HT), such as the CdCl_2 HT for CdTe based solar cells, have been shown to significantly improve other solar cell technologies by passivating or activating GBs. The microscopy results suggest that a GB passivating treatment needs to be developed for these flexible GaAs solar cells to significantly increase their efficiency. A process that removes carbon from the GBs may be a good starting point for improving these devices. This research was supported by ORNL's Center for Nanophase Materials Sciences (CNMS), which is a U.S. DOE Office of Science User Facility.

9:30 AM ET11.13.03

Epitaxy-Free GaAs Nanowire Photovoltaics [Phillip Jahelka](#), Wen-Hui Cheng, Rebecca Glauddell and Harry A. Atwater; California Institute of Technology, Pasadena, California, United States.

We report on an unconventional, epitaxy-free GaAs photovoltaic cell process, designed to enable scalable manufacturing of III-V solar cells. Scalability places constraints on both the overall cost per Watt at the cell level, and the fraction of that cost related to capital equipment expense (capex), which must be minimized for large-scale production. Thin-film III-V compound semiconductors are promising for next generation photovoltaics because of their ideal bandgaps, high radiative efficiencies and mature development. However, almost all previously proposed III-V photovoltaics utilize epitaxial growth to define the cell and the high capital equipment and supply costs of epitaxy currently preclude the economic viability of these cells. In order to leverage the mature development of III-V devices without incurring the capex penalty of epitaxial growth, we have developed epitaxy-free processes for synthesis of

GaAs solar cells where III-V nanostructure arrays are etched using liquid-phase anisotropic etching, and mechanically exfoliated from a bulk III-V crystal, enabling many cells to be generated from a bulk crystal source material. Electron and hole selective contacts and passivation materials are then grown using low-temperature, non-epitaxial techniques.

Because low cost, epitaxy-free designs do not permit use of standard epitaxially-grown III-V heterojunctions and window layers, we first developed a coupled optoelectronic model to understand the design space of the proposed solar cell using nontraditional heterojunction carrier-selective contacts. Using this model, we determined the optimal design to be a radial junction and discovered the absolute necessity of wide-bandgap carrier selective contacts due to the high density of photogenerated carriers throughout the nanowire. Simulations indicate the potential for an optimized GaAs nanowire solar cell using SnO₂ and CuSCN heterojunction contacts to operate as a single junction cell with 32% efficiency with $V_{oc} = 1.13$ V and $J_{sc} = 32.3$ mA/cm².

We have also performed proof-of-principle experiments for each fabrication step of our epitaxy-free cell processes. For GaAs cells, we have developed a metal-free wet chemical etch for defining nanostructures, and have also exfoliated them from a host wafer in a polymer handle. In addition, we have demonstrated very high quality passivation of planar 100 GaAs, with external radiative efficiencies implying a planar V_{oc} of 970 mV, near the theoretical limit of bulk GaAs.

We have also taken first steps to extend this approach to synthesis of epitaxy-free InP solar cells. Highlights to date for InP include developing a plasma etching recipe for defining InP nanowires and successful exfoliation and fabrication of complete nanowire cells from their substrates by embedding them in a polymer handle. In addition, a nanowire-on-wafer InP/TiO₂ heterojunction cell exhibits a 70% increase in photocurrent over its planar counterpart.

9:45 AM ET11.13.04

Interfacial Misfit Growth of GaSb on GaAs by MOCVD for Multijunction Photovoltaics Stephen Polly, Emily Kessler, George Nelson and Seth Hubbard; Rochester Institute of Technology, Rochester, New York, United States.

The long-standing leader in multijunction photovoltaic technology consists of a three junctions made from of InGaP, (In)GaAs, and Ge all grown lattice matched to germanium. While convenient due to the relative ease of growth, the bandgaps of these materials are not ideally matched based on the detailed balance for absorption from the solar spectrum which can be improved through the use of a wider band gap bottom cell. One method of realizing a higher band gap material based on the III/V material design space is through thick metamorphic grading from the Ge lattice constant to 1 eV InGaAs, which must be grown inverted to limit the effects of the inevitable higher threading dislocation density created by this method. In this work, an alternate method is used relying on the large lattice mismatch between GaAs and GaSb (7.8%) to induce an interfacial misfit array, locking 90° dislocations in a thin layer which do not propagate in the growth direction. This method allows for direct heteroepitaxy of GaSb and related direct bandgap materials on GaAs and InGaP heritage device structures without the need for a thick grading buffer, enabling a wider range of more cost effective inverted multijunction photovoltaic devices. Solar cells were grown and fabricated investigating the growth of GaSb single junction solar cells on GaAs substrates using the IMF technique as a function of growth conditions including metalorganic precursor type. Device results including 1-sun light-IV, quantum efficiency, and minority carrier lifetime will be discussed and compared against GaSb homoepitaxial devices, as well as the integration and performance of multijunction devices using this method.

10:00 AM BREAK

SESSION ET11.14: Thin Films III
Session Chairs: Sarah Kurtz and Roger Welsler
Thursday Morning, November 29, 2018
Hynes, Level 3, Room 304

10:30 AM *ET11.14.01

Demonstrating the Hot Carrier Solar Cell—The Ultimate Thin Photovoltaic Device Nicholas Ekins-Daukes¹, James Dimmock², Paul Stavrinou³, Huiyun Liu⁴, Mattias Kauer² and Jiang Wu⁴; ¹School of Photovoltaic & Renewable Energy Engineering, University of New South Wales, Sydney, New South Wales, Australia; ²Sharp Laboratory Europe, Oxford, United Kingdom; ³University of Oxford, Oxford, United Kingdom; ⁴University College London, London, United Kingdom.

The hot carrier solar cell has the potential for high efficiency and has recently been demonstrated experimentally in using both semiconductor and metallic absorbers. The latter is particularly interesting from the viewpoint of thin solar cells since a metal layer of only a few tens of nanometers can almost completely absorb broadband sunlight. Experimental hot carrier IV data has been measured from a chromium absorber deposited onto a GaAs based tunnel diode. Importantly the data confirm that the photo current arises from a hot carrier population as opposed to internal photoemission; the distinction being important since only a hot carrier device can attain high power conversion efficiency. The prospects for the technology as a realistic PV device will be discussed together with alternative applications such as photon energy resolving photodetection.

11:00 AM ET11.14.02

High Efficiency Infrared PbS Colloidal Quantum Dot Solar Cells with 50% EQE at 1.55 μm Haibin Wang¹, Shoichiro Nakao¹, Takaya Kubo¹, Hidenori Saito², Shinichi Magaino², Katsuhiko Takagi², Tetsuya Hasegawa¹, Jotaro Nakazaki¹ and Hiroshi Segawa¹; ¹The University of Tokyo, Tokyo, Japan; ²Kanagawa Institute of Industrial Science and Technology, Kawasaki, Japan.

Colloidal quantum dots (CQDs) have attracted much attention as light absorbers and carrier transporters for next-generation solar cells because mainly of QD-size dependent bandgap tunability, solution process compatibility and so on. Among various types of CQD solar cells, hetero-junction CQD solar cells constructed by combining PbS CQDs and ZnO have been widely studied, and the record high efficiency of 12% was reported [1]. Fundamental studies on CQD solar cells based on a new concept such as multiple exciton generation, hot-carrier concept, and multi-junction concept are also carried out to overcome the single junction efficiency limit (~30% under one-sun illumination). In fact, III-V semiconductors based multi-junction solar cells only have achieved a power conversion efficiency well over the single-junction limit. However, the solar cells rely heavily on high cost solar cell technology, which makes it difficult for the solar cells to be susceptible of wider application. While the size-dependent bandgap tunability and solution process compatibility unique to CQDs are suitable properties to construct low-cost multi-junction solar cells.

Here we constructed PbS colloidal quantum dot/ZnO nanowire solar cells, with the aim of developing solution-processed bottom subcells for multi-

junction solar cells. Spatially-separated carrier pathways formed by ZnO nanowires together with highly infrared-transparent conductive oxide (Ta-doped SnO₂; TTO) electrodes were successfully used to enhance the spectral sensitivity in the infrared region [2, 3]. The EQE for the first exciton peak (1.55 μm) obtained on the solar cells with FTO (F-doped SnO₂) was 30%, which is higher than ever reported on CQD solar cells. The TTO-solar cells reached an even higher EQE of 50% at 1.55 μm due mainly to high infrared-transparency of the TTO electrode. This EQE value is, to the best of our knowledge, the highest value ever reported on the solution-processed solar cells. The results that we have obtained indicate that the solution-processed PbS CQD/ZnO NW solar cells are one of the promising candidates for the bottom subcells to construct flexible, low-cost multi-junction solar cells.

1. J. Xu, O. Voznyy, M. Liu, A. R. Kirmani, G. Walters *et al.*, *Nature Nanotech.*, **13**, (2018) 456.
2. H. Wang, T. Kubo, J. Nakazaki, T. Kinoshita, and H. Segawa, *J. Phys. Chem. Lett.*, **4** (2013) 2455.
3. H. Wang, T. Kubo, J. Nakazaki, and H. Segawa, *ACS Energy Lett.*, **4** (2017) 2110.

11:15 AM ET11.14.03

Enhanced Charge Carrier Transport Assisted by a Piezoelectric Effect in a Flexible Quantum Dot Solar Cell Yuljae Cho, Paul Giraud, John Hong, Sangyeon Pak and SeungNam Cha; University of Oxford, Oxford, United Kingdom.

Colloidal quantum dots are promising materials for flexible solar cells because they have a large absorption coefficient ranging from visible to infrared wavelengths, a band gap that can be tuned across the solar spectrum, and compatibility with solution processing. However, the performance of flexible solar cells can be degraded by the loss of charge carriers due to recombination pathways that exist at a junction interface as well as the strained interface of the semiconducting layers. Therefore, fundamental strategies for actively controlling the junction properties are required to boost charge extraction and reduce the recombination of photo-generated charges. In this regard, the modulation of charge carrier transport using the piezoelectric effect is one of the effective ways to resolve the inherent material and structural defects. Towards this end, we have employed a porous piezoelectric poly(vinylidene fluoride-trifluoroethylene), P(VDF-TrFE), polymer layer between a zinc oxide (ZnO) ETL and a PbS QD heterojunction in a flexible QDSC. Through the active control of strain/stress of the flexible form factors, the inserted porous P(VDF-TrFE) layer generates a piezoelectric potential which modulates the junction properties and consequently changes the behavior of the charge carriers. As a result of the modulated electric field at the junction, the photo-generated charges are effectively extracted along with reduced radiative recombination, which results in a 38% increase in the current density and a concomitant increase of 37% in the power conversion efficiency of the flexible QDSC.

11:30 AM ET11.14.04

Development of Copper-Free, Low Barrier Back Contact to Cadmium Telluride Thin-Film Solar Cells Fadhil K. Alfadhili, Geethika K. Liyanage, Jacob M. Gibbs, Adam B. Phillips and Michael J. Heben; Wright Center for Photovoltaics Innovation and Commercialization, Department of Physics and Astronomy, University of Toledo, Toledo, Ohio, United States.

The cadmium telluride (CdTe) thin film solar cells have attained over 20% efficiency with low-cost fabrication. However, the high efficiency CdTe devices has been achieved by increasing the photo-generated current by changing the traditional window layer (CdS) of CdTe to a wider bandgap material with better band alignment. The open circuit voltage (V_{oc}) remains below the theoretical limit due a barrier at the back of the device due to the deep valence band edge of CdTe (-5.7 eV). V_{oc} can be increased by adding a buffer layer between CdTe and the back electrode due to a decrease in band bending and reducing carrier recombination at the back surface. Previous modelling work shows that adding a Tellurium (Te) layer at the back contact of CdTe reduces band bending, which leads to higher performance CdTe thin film solar cells. Recently, we developed a way to form a Te layer at the back surface of CdTe by interacting the surface of CdTe sample with methylammonium iodide (CH₃NH₃I, MAI) solution followed by a mild thermal treatment. The MAI treatment is more effective than evaporated Te at the back of CdTe due to reducing the interface defect states between CdTe and the Te buffer layer. This leads to increasing the efficiency up to 10% compared to standard Cu/Au back contact. To further reduce the carrier recombination at the back surface, we need to increase the barrier for minority carrier (electrons) and reduce the barrier for majority carrier (holes) at the back surface. This can be achieved by adding a higher bandgap layer to act as an electron reflector (ER). Here, we demonstrate the use of Zinc Telluride (ZnTe) as an electron reflector at the back surface of CdTe devices with a Te layer between CdTe/ZnTe and ZnTe/metal interfaces to break down the large Schottky barrier at the CdTe/metal interface into four smaller ones. We show that this is an effective method to reduce the carrier recombination at the back surface despite not using Cu. The V_{oc} of Cu-free devices with Te/ZnTe/Au back contact are notably higher than the CdTe device fabricated with standard Cu/Au back contact.

SESSION ET11.15: Organic Photovoltaics III
Session Chairs: Thomas Unold and Jia Zhu
Thursday Afternoon, November 29, 2018
Hynes, Level 3, Room 304

1:30 PM *ET11.15.01

A Novel Approach to Multi-Junctions—The Heterojunction Bipolar Transistor Solar Cell Elisa Antolín, Pablo García-Linares, Marius Zehender and Antonio Martí; Instituto de Energía Solar, Universidad Politécnica de Madrid, Madrid, Spain.

Conventional multi-junction solar cells achieve unparalleled efficiencies at the price of a complex structure, high fabrication cost and low spectral tolerance. Recently a new device has been proposed called three-terminal heterojunction bipolar transistor solar cell (HBTSC) which has the same efficiency limit of a double-junction solar cell but consists of a much simpler structure with no tunnel-junctions or isolating layers¹. Being a three-terminal device, it enables higher spectral tolerance than series-connected multi-junction cells through the engineering of module interconnection. The HBTSC comprises only three main active layers. These layers may be called emitter, base and collector since they resemble the structure of an npn (or pnp) transistor. However, the operation of this device is antagonistic to the operation of a transistor. In the HBTSC the emitter and base terminals form the top sub-cell and the base and collector terminals form the bottom sub-cell. For the device to achieve a high efficiency it is necessary that the voltage of the top sub-cell exceeds the voltage of the bottom sub-cell even though they share the base layer. In this talk we will present the theoretical model of the device and will show how that situation can be realized if the emitter injection efficiency approaches zero. One of the most interesting aspects of the HBTSC model is that biasing one sub-cell can improve the conversion efficiency of the other sub-cell. We will analyze the impact of the base layer design on the HBTSC operation and its effect on how the sub-cell efficiencies are interrelated. We have produced proof-of-concept HBTSC prototypes based on epitaxial AlGaAs/GaAs structures. We will show experimental proof that the two sub-cells can be operated at their respective maximum power points, with the voltage of the top sub-cell exceeding the voltage of the bottom sub-cell. The operation of five HBTSC assembled in a prototype module with two-terminal output will also be demonstrated.

Finally, we will describe possible architectures to implement the HBTSC concept with low-cost technologies. These proposals will include a design comprising a perovskite absorber and another one based on the use of nanowires.

1. Martí, A. & Luque, A. Three-terminal heterojunction bipolar transistor solar cell for high-efficiency photovoltaic conversion. *Nat Commun* **6**, 6902 (2015).

2:00 PM ET11.15.02

Enhancing the Performance of Polymer Bulk Heterojunction Solar Cells by Large Sized Gold Nanoparticles via Near- And Far-Field Plasmonic Coupling Min Seok Lee, Dong Hyun Kim, Justin Jesuraj Periyanyagam, Hassan Hafeez and Seung Yoon Ryu; Korea University, Sejong city, Korea (the Republic of).

Nobel metal nanoparticles are well-known to unveil plasmonic coupling with molecular excitons to enhance the performances of opto-electronic devices especially light emitting diodes and solar cells. The higher momentum associated with metal surface plasmons can alter the lifetime of molecular excitons, thereby the efficiency increased in respective devices. However, this kind of coupling is stronger within the near- field of surface plasmons and is highly dependent on distance between metal surface to exciton and also on the size of metal nanoparticles.

In this scenario, we have investigated the effect of incorporating large size gold nanoparticles (AuNPs) in polymer bulk heterojunction (BHJ) solar cells. In addition, we exclusively studied the near- (Localized surface plasmonic resonance; LSPR) and far-field (scattering) interaction of AuNPs plasmons with BHJ excitons through theoretical and experimental tools. To clearly understand the efficiency improvement tactics, we have fabricated three BHJ solar cells containing three different donor active materials with [6,6]-phenyl-C_{61,71}-butyric acid methyl ester (PC_{61,71}BM). AuNPs have been incorporated in BHJ solar cells through the poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) solution as hole injection layer (HIL). To understand size dependent behaviors, AuNPs with sizes 71, 80, 87, 103 nm were inserted in PEDOT:PSS and employed as HIL for the two polymer solar cells containing PBDDTT-C: PC₆₁BM and PTB7: PC₇₁BM as BHJ systems. Interestingly, smaller size AuNPs (equal or less than 80 nm) very active in establishing near-field interaction with excitons, whereas bigger size (> 80 nm) particles were found to produce superior far-field scattering. By monitoring the lifetime of the excitons through time resolved photoluminescence found to be beneficial to identify the near- and far-field coupling. In other words, the AuNPs (< 87 nm) showing lifetime lesser than the reference were considered to demonstrate near-field (LSPR) effect and AuNPs (> 87 nm) revealed longer lifetimes indicating far-field (scattering) effect. At 87 nm, AuNPs yielded a fair combination of near-field coupling along with far-field scattering resulting in enhanced absorption and dissociation of photons in BHJ. Therefore, 87 nm found to be an optimum (maximum) size for AuNP to attain superior efficiency in BHJ solar cells through the cultivation of near- and far-field interactions. Further, full-wave simulation (COMSOL) investigations were employed to reveal the plasmonic interaction and electric field distribution of AuNPs respectively. These findings are coincided with the experimental results of BHJ solar cell performances.

2:15 PM ET11.15.03

Side Chain Engineering of Polymer Donors and Non-Fullerene Small Molecule Acceptors for Organic Photovoltaics Micaela Matta, Tobin J. Marks and George Schatz; Chemistry, Northwestern University, Evanston, Illinois, United States.

Organic bulk-heterojunction (BHJ) solar cells made of polymeric donors and small molecule non-fullerene acceptors (NFA) have been the subject of interest due to their record-high efficiencies.[1] Tremendous effort is being directed at the development of novel donor and acceptor building blocks, and the optimization of energetics and morphology of donor/acceptor systems.

In order to make these highly conjugated materials soluble and thus processable at low cost, the presence of side alkyl chains is fundamental. However, their role in determining key morphological and structural properties in both donors and acceptors has been often overlooked by the organic photovoltaics (OPV) community.

Our work investigates how the length of alkyl side chains influences the properties of some of the best performing donors and NFAs available to date. The polymer donor PBTZF4[2] was characterized using a combination of molecular dynamics (MD) simulations, X-ray scattering and spectroscopic techniques. MD provided a rationalization for the observed trends among a series of PBTZF4-R devices with alkyl chains R of different length, elucidating the subtle equilibrium between the conjugated backbone rigidity and the folding enhancement provided by longer alkyl chain substituents. The results established a relationship between the single polymer chain behavior, its aggregation in solution and the subsequent formation of domains in the BHJ.[3] This study shows how side chain engineering can be used to fine tune the BHJ morphology without significantly changing the HOMO-LUMO levels of polymer backbone.

Moreover, a series of ITIC-derived[4] NFA having alkyl chain substituents of different length[6] was also investigated by means of quantum chemical calculations, MD simulations, X-Ray diffraction and other spectroscopic measurements. It emerges that the alkyl chain length has a dramatic effect on OPV performances. Side chains effectively mediate intermolecular interactions by preventing excessive aggregation and crystallization of the acceptor while allowing efficient π -stacking in the amorphous and semi-crystalline domains.

In summary, this work highlights the importance of side chain engineering as a strategic tool for OPV morphology control, where MD simulations have been instrumental in providing a correlation between molecular-scale properties and device performances.

1. Hou, J. et al. Organic solar cells based on non-fullerene acceptors. *Nat. Mater.* **17**, 119-128 (2018).

2. Timalina, A. et al. New donor polymer with tetrafluorinated blocks for enhanced performance in perylenediimide-based solar cells. *J. Mater. Chem. A* **5**, 5351-5361 (2017).

3. Wang, G. et al. Directing Photovoltaic Blend Microstructure for High-Efficiency Post-Fullerene Solar Cells. *to be submitted* (2018).

4. Aldrich, T. et al. Enhancing Indacenodithiophene Acceptor Crystallinity via Substituent Manipulation Increases Organic Solar Cell Efficiency. *Chem. Mater.* **29**, 10294-10298 (2017).

2:30 PM ET11.15.04

Enhanced Photovoltage and Short Circuit Current Density for the Polymer:Fullerene Solar Cells Using Individual Bis-PC₆₀BM Isomers Xueyan Hou^{1,2}, Jun Yan², Xingyuan Shi², James McGettrick³, Jenny Nelson² and T. John S. Dennis¹; ¹School of Physics and Astronomy, Queen Mary University of London, London, United Kingdom; ²Physics and Centre for Plastic Electronics, Imperial College London, London, United Kingdom; ³SPECIFIC, Swansea University, Swansea, United Kingdom.

It has been a longstanding goal to enhance the power conversion efficiency (PCE) of polymer donor: molecular acceptor solar cells by tuning the acceptor energy levels to raise the open-circuit voltage (V_{oc}). Previous work showed that replacing the most commonly used fullerene acceptor, [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM), with its bis-adduct raised the V_{oc} of poly(3-hexylthiophene-2,5-diyl) (P3HT):fullerene solar cells by ~100 mV and increased the PCE¹. The increased V_{oc} could be assigned to the higher lying LUMO energy of the bis adduct. However, when combined with other polymers, higher fullerene adducts tend to reduce PCE via losses in short-circuit current density (J_{sc}) and fill factor (FF) due to poor electronic properties².

This is assigned to a combination of (i) energetic disorder, which results from varying frontier orbital levels of the individual isomers in the mixture that is normally produced³, (ii) poor molecular packing leading to lower electron mobility. Recently, we separated all 19 bis-PCBM isomers from the as-produced mixture by peak-recycling HPLC⁴, and identified their structures by a combination of ¹³C NMR, UV-Vis spectroscopy and HPLC retention time analysis⁵. LUMOs of all isomers lie above that of PCBM, with the highest lying about 100 meV higher than that of the mixture and 200 meV above PCBM. The pure isomers should contain much reduced disorder due to the absence of multiple isomers and be capable of crystallising. Therefore, improved electronic properties and solar cell PCE may be expected. In this work, I will present a comprehensive analysis of the solution- and film-based energy levels, solubility and crystallinity of different bis-PCBM isomers. I will present the performance of devices when blended with different polymer donors of different crystallinity together with an analysis of the V_{oc} loss and transport properties. For example, V_{oc} as high as 1.13 V was observed for some isomers along with a net increase in PCE. The pure isomer with a certain molecular structure can help us understand the intrinsic electronic properties of the higher fullerene adducts more clearly without the disorder of an isomer mix. Finally, I will give some suggestions for the synthetic routes to achieve particular higher adduct fullerenes whilst avoiding the disorder due to multiple isomerism.

References

- [1] M. Lenes, et al. *Adv. Mater.* 2008, 20, 2116-2119.
- [2] M. Faist, et al. *Adv. Energy Mater.* 2013, 3, 744-752.
- [3] J. Frost, et al. *Adv. Mater.* 2010, 22, 4881-4884.
- [4] W. Shi, et al. *Chem. Commun.* 2017, 53, 975-978.
- [5] T. Liu, et al. *J. Phys. Chem. A.* 2018, 122, 4138-4152.

2:45 PM ET11.15.05

Extended Life Photovoltaic Backsheets Using Novel Polymer Materials and the Co-Extrusion Process [Peter Perez](#)¹, Ananya Ghosh¹, Jayant Kumar^{2,3} and Ramaswamy Nagarajan¹; ¹Department of Plastics Engineering, University of Massachusetts Lowell, Lowell, Massachusetts, United States; ²Department of Physics, University of Massachusetts Lowell, Lowell, Massachusetts, United States; ³Center for Advanced Materials, University of Massachusetts Lowell, Lowell, Massachusetts, United States.

The premature failure of photovoltaic backsheets often limits the life span of entire solar modules. These failures are typically due to yellowing, cracking, bubbling, and eventual delamination of the backsheet while in the field. Current backsheets are comprised of various polymeric layers including fluoropolymers, polyethylene terephthalate (PET), polyolefins, and adhesives used to bond these materials together. Tomark-Worthen has developed a backsheet product produced through an alternative process to the traditional lamination process, which uses adhesives and solvents in the production of multi-layer backsheets. Instead, they use coextrusion technology to produce their novel multilayer polymeric backsheet. Their current product, PhotoMark®Reflections™, is a 5-layer film that does not contain PET or fluoropolymers, but rather a proprietary polyamide-ionomer alloy coupled with polyolefin and amide layers. The primary purpose of this research was to compare the performance of Tomark-Worthen's coextruded backsheet films with the current industry standard films and determine modes of failure. Infrared spectroscopy (FTIR) and Scanning Electron Microscopy (SEM) were used in order to: assess the severity of degradation and determine the mechanism degradation after extensive exposure to damp heat and ultraviolet (UV) radiation. Spectroscopy and microscopy results indicate high stability of PhotoMark®Reflections™ after exposure to these severe accelerated weathering conditions. Since the layers of the backsheet are adhered in the coextrusion process as opposed to the traditional use of adhesives, the interlayer bond strength of various backsheet samples was tested via ASTM D903-98. The results obtained from ASTM D903-98 show that Tomark-Worthen's PhotoMark®Reflections™ coextruded films have an interlayer adhesion strength 6.5 times greater than that of the current industry standard. Additionally, several backsheet samples were exposed to harsh hydrolysis conditions in a Highly Accelerated Stress Test (HAST) common to the solar industry. Current industry standard and competitive films experienced dramatic degradation and loss in tensile properties as a result of the HAST, while Tomark-Worthen's PhotoMark®Reflections™ showed minimal degradation.

3:00 PM BREAK

SESSION ET11.16: Rump Session: Wavelength Selective Photonic Structures Applications to Solar Cells
Session Chairs: Nicholas Ekins-Daukes and Kyle Montgomery
Friday Morning, November 30, 2018
Hynes, Level 3, Room 304

8:30 AM INTRODUCTION TO PHOTON MANAGEMENT IN MULTI-JUNCTION SOLAR CELLS BY KYLE MONTGOMERY, AIR FORCE RESEARCH LABORATORY

8:40 AM ET11.16.01

Presentation I [Nicholas Ekins-Daukes](#); University of New South Wales, Sydney, New South Wales, Australia.

Abstract not available.

8:50 AM ET11.16.02

Presentation II [Seth Hubbard](#); Rochester Institute of Technology, Rochester, New York, United States.

Abstract not available.

9:00 AM ET11.16.03

Presentation III [Rao Tatavarti](#); Technology, MicroLink Devices, Inc., Niles, Illinois, United States.

Abstract not available.

9:10 AM ET11.16.04

Presentation IV [Roger E. Welsler](#); Magnolia Solar, Woburn, Massachusetts, United States.

Abstract not available.

9:20 AM ET11.16.05

Presentation V Jeremy N. Munday; University of Maryland, College Park, Maryland, United States.

Abstract not available.

9:30 AM ET11.16.06

Presentation VI Andrew Johnson; IQE, Inc., Cardiff, United Kingdom.

Abstract not available.

9:40 AM ET11.16.07

Presentation VII Stephen Bremner; University of New South Wales, Sydney, New South Wales, Australia.

Abstract not available.

9:50 AM WRAP-UP DISCUSSION BY NED EKINS-DAUKES, UNIVERSITY OF NEW SOUTH WALES