SinBeRISE

Singapore-Berkeley Research Initiative for Sustainable Energy

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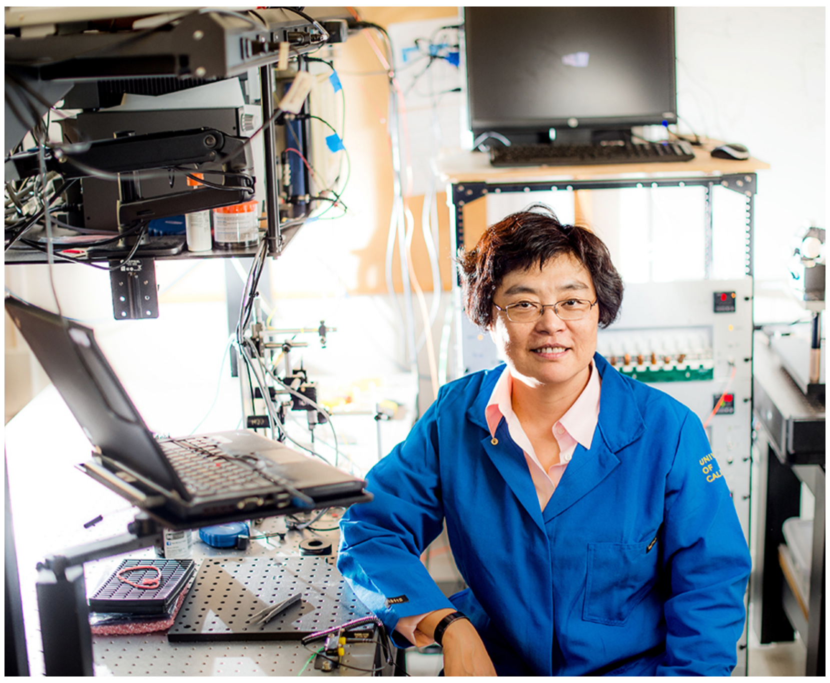
***SinBeRISE* explores novel approaches to harvest solar energy with high conversion efficiencies by advancing material and device technologies readily applicable for low cost manufacturing processes.**

Foreword



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The Singapore Berkeley Research Initiative on Sustainable Energy (SinBeRISE) is a programme in the Campus for Research Excellence and Technological Enterprise (CREATE) funded by the National Research Foundation (NRF) of Singapore, started in April 2013. I became the Program Leader of SinBeRISE since April 2015. It is a great pleasure for me to provide you with this SinBeRISE report with summary of accomplishments of very active past 2 years, with plenty of stellar research results, news, press releases, and other achievements. In addition, we are pleased to congratulate SinBeRISE colleagues, being recognized by prestigious domestic and international awards, and promoted to positions with higher ranks and more responsibilities.

SinBeRISE has three major thrusts: photovoltaics (PV), solar-to-fuel conversion, and devices and applications. Although solar power is the world's most abundant source of energy, the difficulty has always been converting solar energy in an efficient and cost-effective manner. In Thrust 1, we are investigating photovoltaic materials, focusing on organic-inorganic halide perovskite materials. In a little over three years, the efficiencies of perovskite-based photovoltaics have risen from a few percents to more than 20%. SinBeRISE is leading the world in serveral fronts with excellent material qualities and producing environmentally friendly (lead-free) perovskite materials for solar cells.

The second thrust focuses on rapid discoveries of catalysts for CO_2 reduction. Currently human existence relies nearly completely on energy derived from fossil fuels, which provide 82% of the world's primary energy use. A sustainable energy future for the world will require a radical change in energy generation. With this in mind SinBeRISE is designing multi-functional, nanoscale, heterostructures capable of efficient light harvesting and CO_2 reduction, providing a sustainable alternative to fossil fuels.

To have a lasting impact on the world, the scientific advances made in solar cell and cataylitic materials and processes need to be scaled up, which is the focus of Thrust 3. This thrust began execution later than the other two as efforts were focused to solve scientific problems first. When we have made good progress on the scientific front, we embarked on Thrust 3 with well-defined deliverables on building integrated PV and PV powered sensors etc.

The SinBeRISE program has engaged in collaborative research projects with industrial and government partners. Dyesol and SinBeRISE are actively working on scaling up of commercially feasible dye-sensitized solar cells and lead free perovskites. While with RDECOM, SinBeRISE is studying the fundamental limits of perovskite solar cells towards scalability. Together with Johnson Mathey, SinBeRISE are investigating materials for perovskite based solar cells. BASF has provided support for the chemical synthesis and characterization equipment of the materials being developed. I look forward to create an even better platform to enhance collaboration among SinBeRISE researchers and industrial collaborators toward a greater success in the years to come.

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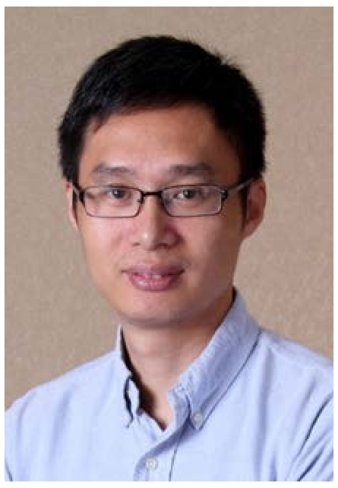

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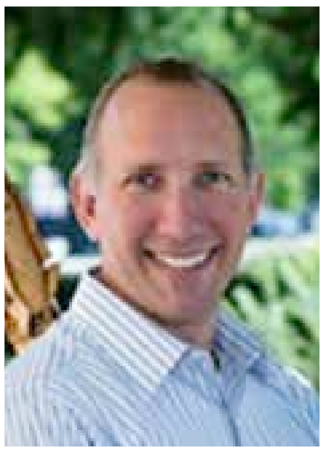

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Thrust 1: Photovoltaics

Overview

Although solar power is the world's most abundant source of energy, the difficulty has always been converting solar energy in an efficient and cost-effective manner. For photovoltaic energy to become competitive with fossil fuels and to capture a significant share of the electricity market, it is necessary to reduce the total cost of solar energy. This can be achieved by either reducing the cost of photovoltaic cells or by increasing their power conversion efficiencies. The photovoltaic market is currently dominated by crystalline Si solar cells with lab scale efficiencies close to 25%. Alternative "third generation" technologies such as organic photovoltaics (OPVs), dye sensitized solar cells (DSCs) and quantum dot solar cells (QDSCs), which are fabricated through solution based processes such as blade coating, screen printing and spraying, promise low cost solar power while allowing the utilization of unconventional substrates.

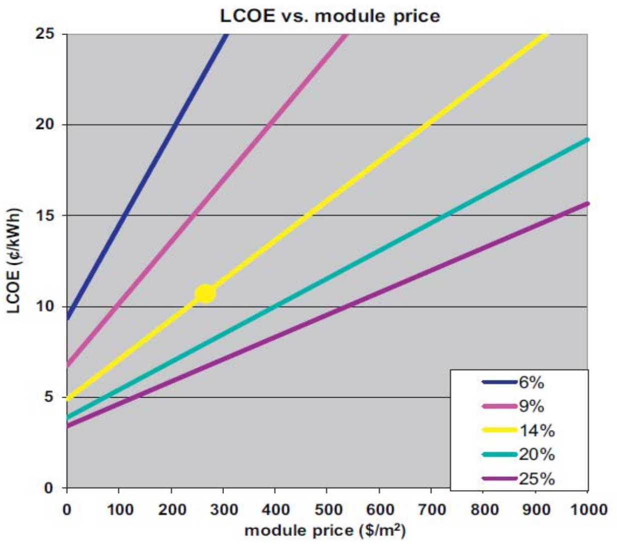


Figure 1: In order to hit specific electricity cost targets (LCOE), it is necessary to not only reduce costs, but to target high efficiencies. (Ex-tracted from Renewable and Sustainable Energy Reviews 15(2011) 4248-4254.

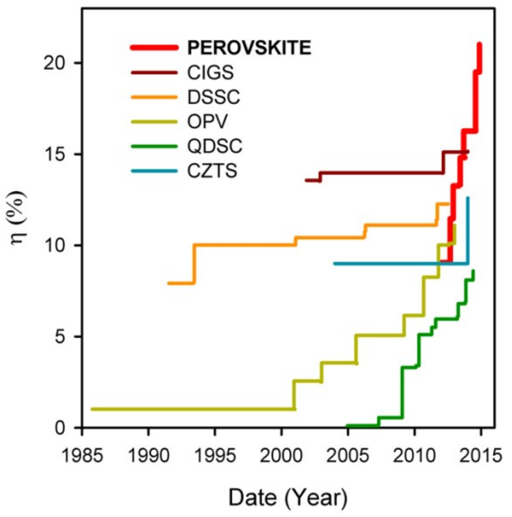


Figure 2: The rapid growth in efficiencies in haide perovskite solar cells have made it the most efficient solar cell technology.

Although the utilization of low temperature processes reduces the energetic costs and the energy payback time, the power conversion efficiencies (PCEs) of these solar cells still lag significantly behind conventional solar cells. The levelized cost of energy (LCOE), (Fig 1), which allows for the comparison of various electricity generation sources, depends critically on the efficiency of the solar cells produced. A more efficient module yields more power per unit area. A significant fraction of a solar cell cost scales proportional to the installation area, including the cost of the glass, inverter costs and installation costs, among others. A more efficient solar cell allows for a reduction in all the costs associated with installation, while requiring much lower numbers of solar panels to be installed. Thus the PCE is a primary driver of cost for solar cells.

Organic–inorganic halide perovskite solar cells have been the most significant development in the field of photovoltaics in the present decade, and are the best bet at satisfying the need for high efficiencies while allowing for low cost solution based manufacturing. Since the first reports of stable solid state solar cells based on the $CH_3NH_3PbI_3$ perovskite in mid-2012, the PCEs of the solar cells have already exceeded 20%, leapfrogging every other solution-processed solar cell technology, (Fig 2). Our work aims the improvement of $CH_3NH_3PbI_3$ efficiency and stability through a deep understanding of the fundamental properties of this material, as well as the development of new perovskite absorbers (lead-free and multidimensional) and device concepts (tandem). In the following, we summary results of four tasks in this Thrust aimed at solar cells with higher efficiency, stability and scalability.

1. Lead iodide solar cells: novel devices

Designing innovative device concepts and fabrication methods is the main strategy to boost the efficiency of $CH_3NH_3PbI_3$ devices. Since the first reports on solid state perovskite solar cells, the role of the Cl in the formation of $CH_3NH_3PbI_3$ has been discussed with sequential deposition technique[1] and single step process[2], resulting in publications in Nanoscale and Chemistry of Materials respectively.

Spincoating $PbCl_2$ + PbI_2 on a mesoporous TiO_2 film followed by the perovskite transformation. The role of Cl in determining the optical, electrical, structural and morphological properties is correlated with the photovoltaic performance. The highest photovoltaic efficiency of 14.15% respectively was achieved with 10 mol% of $PbCl_2$ addition due to an increase of the film conductivity induced by better perovskite morphology. This is linked to an improvement of the hysteresis and reproducibility of the solar cells.

With single step deposition, pin holes free and uniform films could be formed by slowing down the crystallization rate through the addition of excess $CH_3NH_3^+$. Though better film coverage is obtained, the device series resistance increases with excess CH_3NH_3I. Thermogravimetric analysis confirms the presence of residual excess CH_3NH_3I in the final film. When chlorine is added to the $CH_3NH_3^+$ rich system, CH_3NH_3Cl is formed which easily sublimes during annealing at 100°C leading to improved device performance.

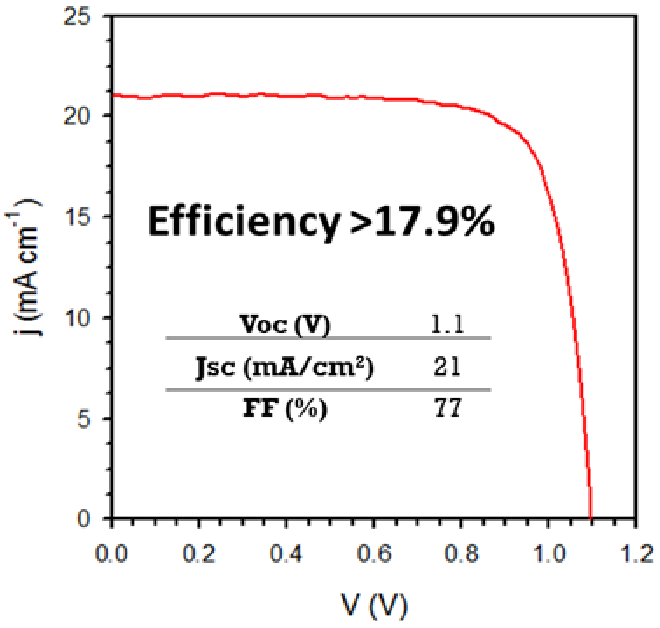


Figure 3 Current-voltage characteristic of the record efficiency perovskite solar cells.

To understand the basic materials and structural limitations, ‘model systems’ can be created with pristine thin films grown from physical vapour deposition and near perfect single crystals from high purity precursors, using methods that also enable precise tuning of the composition and doping levels of the synthesised materials. Nanostructuring often used to compensate for inherent charge transport limitations in thin film solar cells may not be essential in the perovskite systems. Materials synthesis, device fabrication, will be coupled with and materials characterization that will include optical (absorption, PL), electrical (Hall Effect, impedance spectroscopy) and structural (TEM, XRD) characterization. This needs to be further extended with an in depth study of interaction of perovskites with functional interfaces. The TEM studies have been undertaken by PI at Berkeley (Andy Minor). Initial studies of 2-step solution processed material have revealed a variety of microstructures. As shown in Figures 4a and 4b, these devices consist of a porous titania matrix with perovskite interspersed, and a pure perovskite capping layer on top. Studies of the perovskite-titania interface reveal both nanocrystals decorating the titania as well as a lead and iodine-containing phase wetting titania particles in some areas. Additionally, PbI_2, a reaction byproduct, is observed within both the porous matrix and the pure perovskite-capping layer (Fig 4e). Tomographic studies reveal the dispersion of the perovskite in the matrix, as well as the overall porosity of the matrix and its interaction with the bottom electrode (Figs. 4f and 4g).

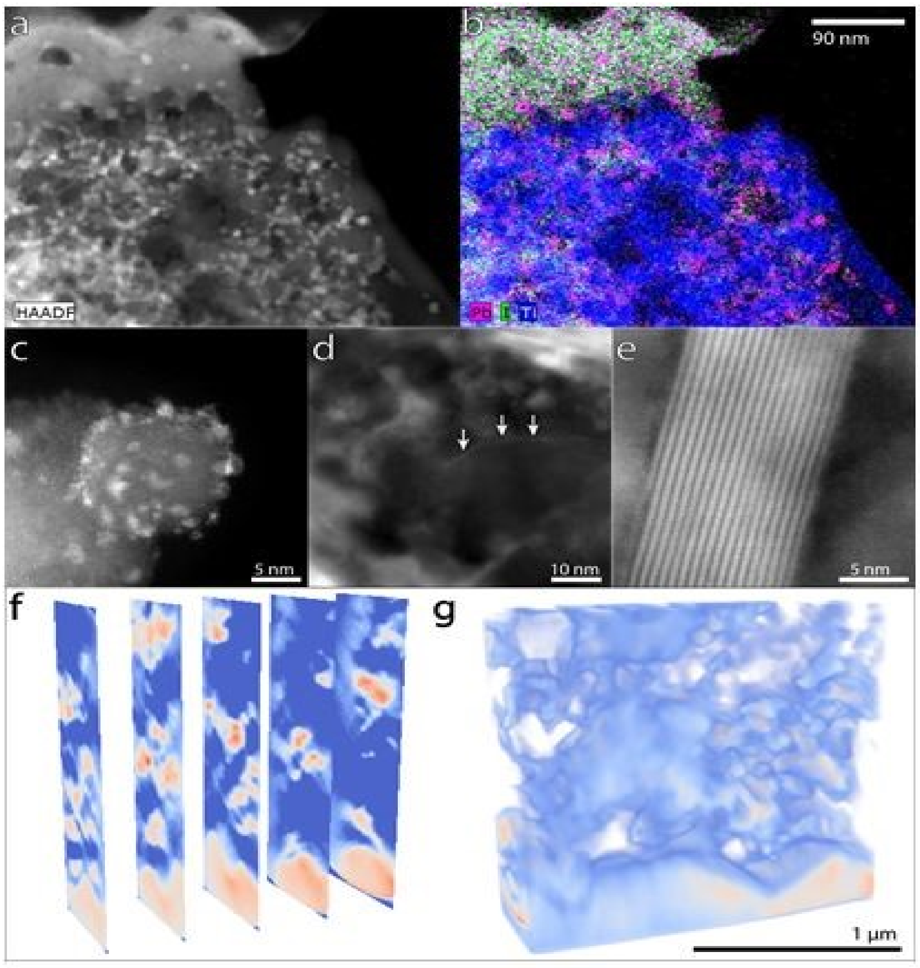


Figure 4: TEM studies of 2-step deposited lead halide photovoltaic completed thus far. a) STEM overview of a lead halide device, with $MAPbI_3$ at the top and $MAPbI_3$ particles decorating the titania matrix underneath.
b) EDS of the same region, indicating that the bright regions are the lead-containing phase. c), d) and f) show various phases present in these complex samples. a) small, non-crystalline particles of $MAPbI_3$ decorate larger titania particles, d) a continuous layer of MAPbI3 coats the titania and f) PbI2 crystals present with the system. f) and g) are orthoslices and a volume rendering of a tomographic reconstruction of the MAPbI3-containing porous titania network atop the conducting electrode.

2. Lead iodide solar cells: stability study

We conducted a study of long term stability at different temperatures (room T and 70ºC) under atmospheres for unsealed lead-iodide perovskite solar cells with thin and thick perovskite layer (capping layer) onto the mesoporous TiO_2. At room T, solar cells in dry atmosphere (desiccator), N_2 atmosphere and ambient atmosphere with thick perovskite capping layer were stable for more than 1000h (degradation of efficiency <5%). In contrast, solar cells at 70ºC dramatically decreased the efficiency (~50% drop) in less than 400% (see figure 5). These results suggest the sensitivity of $CH_3NH_3PbI_3$ to the phase transition from tetragonal to cubic phase (at ~55ºC). Remarkably, to lead these efforts we have developed screen printing methods for both the blocking layer and mesoporous TiO_2 layers, where we have achieved power conversion efficiencies greater than 16%. Most of the reported high power conversion efficiencies for solar cell devices using perovskite absorbers contained a blocking layer prepared by spray pyrolysis or ALD process, and spin coated mp-TiO_2 scaffold layer. However, for the perovskite-based solar cells to be commercially viable, larger scale devices will need to be constructed.

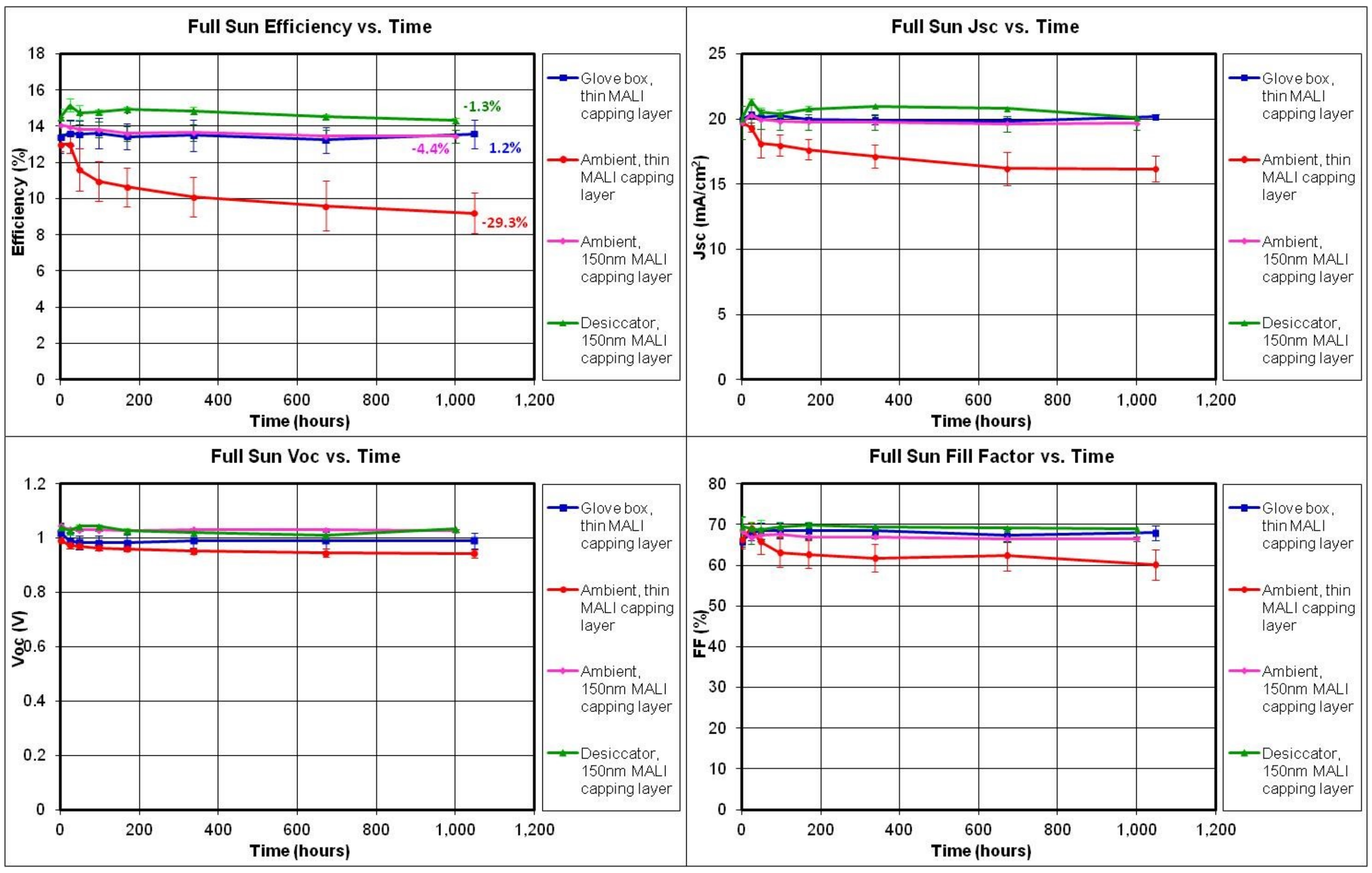


Figure 5 Study of the stability of $CH_3NH_3PbI_3$ cells stored at room T.

3. Material development of lead-free and multidimensional halides

SinBeRISE targets the development of new lead-free perovskites for highly efficient photovoltaic applications, based on the understanding and design of their fundamental optoelectronic properties. A candidate for effective Pb-replacement is Sn, forming a +2 oxidation state, which is required to adopt the octahedral coordination in the perovskite structure. However, two main drawbacks have prevented the development of effective Sn-based perovskites for photovoltaic applications: i) the low band gap and high conductivity generally presented for Sn-compounds and ii) the instability of the Sn_2^+ which tends to form Sn_4^+. The instability of the Sn_2^+ can be tackled from a chemical perspective, where the doping of the solutions will stabilize the material avoiding the formation of Sn_4^+. We have recently demonstrated this strategy in $CsSnI_3$ through the addition of SnF_2, which hinders the oxidation of the Sn ions and thus reduces the background carrier concentration3 (Fig 6). Other alternative solution processable perovskites where the Sn element is already in the Sn_4^+ state (eg. Cs_2SnI_6) such that it is stable to further oxidation would also be pursued.

Due to the wide variety of alternatives available as metallic replacement, a first-principle based screening strategy is essential. PIs at Berkeley (Mark Asta, Matt Sherburne) focus on high throughput computational screening that will initially search for candidate materials based on calculated bandgaps and thermodynamic stability. For materials that pass initial screening, further levels of computational modelling will be used to investigate stability, band alignments, and intrinsic defect properties including formation energies and energy levels.

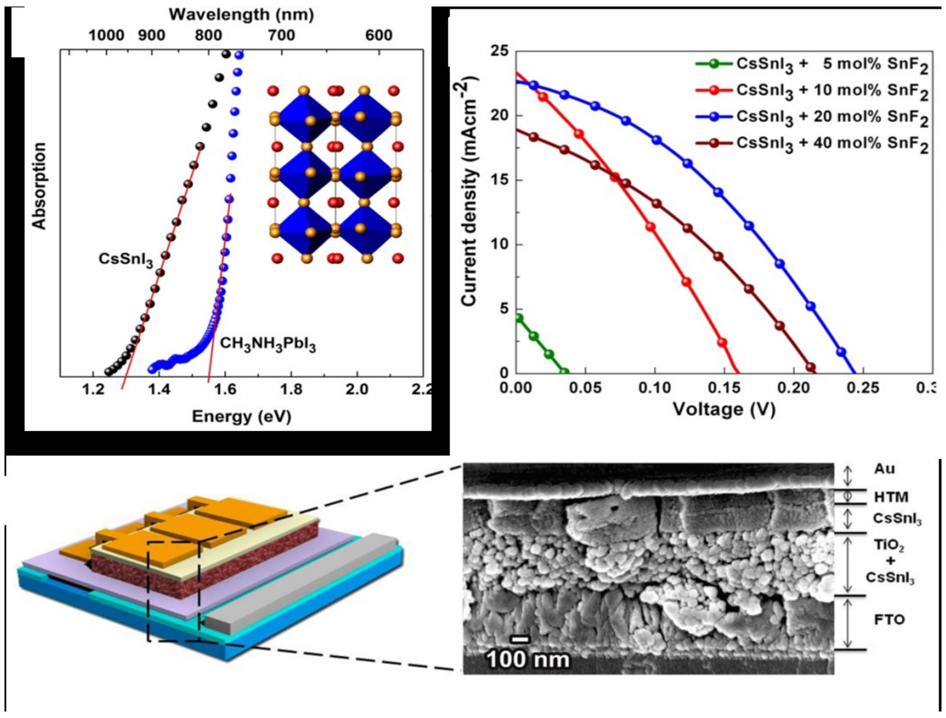


Figure 6: (Top Left): CsSnI$_3$ optical absorption compared to CH3NH3PbI3 (Top right) Only with the addition of SnF$_2$, does CsSnI$_3$ act as a promising photovoltaic material (Bottom) Mesoporous device configuration of the lead-free solar cells

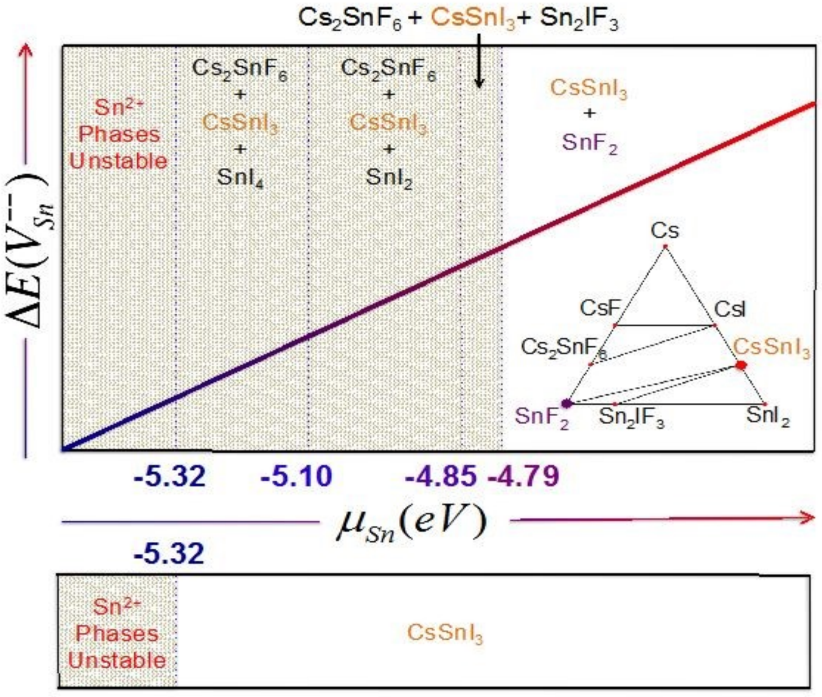
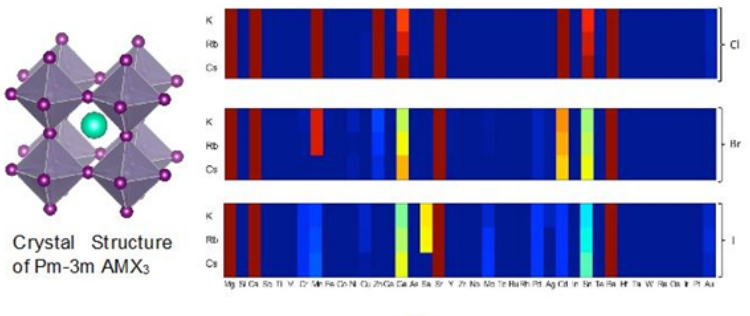


Figure 7: Results of density-functional-theory calculations, showing the effect of phase-equilibria with SnF$_2$ on the range of Sn chemical potential (2+Sn) compatible with stability of the CsSnI$_3$ compound. The range of stability (white regions) is pushed to less-negative values of 2+Sn in the presence of SnF$_2$ (top panel) relative to that found without (lower panel). This has a consequence of raising the value of the Sn vacancy formation energy (plotted schematically in the top panel) and thus lowering the equilibrium vacancy concentration and associated p-type carrier density.

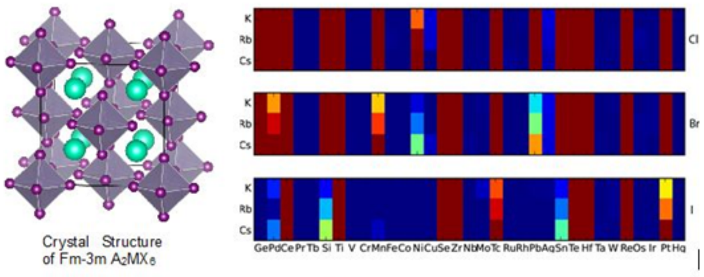
In the first collaborative publication between Berkeley and NTU on the subject of Pb-free perovskites[1], it was demonstrated that the halide perovskite material CsSnI3, which can be processed at low temperature (70 °C), could be used to form solar cells with photocurrents exceeding 22 mA/cm^2 and a spectral response extending to 950 nm. The reduction of background carrier densities, through the addition of SnF$_2$, was found to be critical in ensuring efficient photovoltaic effects. The result was explained computationally by the effect of SnF$_2$ on the chemical potential of Sn, and the thus the Sn vacancy formation energy (Fig. 4); it is predicted that the equilibrium concentration of vacancies, and therefore the charge-compensating hole carriers, decreases dramatically with SnF$_2$ addition. This effect has also been found to play a key role in controlling the performance of CsSnI$_3$ for near-infrared lasing applications [4].

In an effort aimed at identifying other, potentially higher-performing, Pb-free halide perovskite compounds for photovoltaic applications, researchers at Berkeley (Asta and Sherburne) have undertaken high-throughput computational studies, based on electronic density-functional theory (DFT). The goal of the work was to use computations as a framework to rapidly screen for candidate Pb-free halide perovskite and perovskite-derivative compounds with compositions AMX$_3$ and A$_2$MX$_6$, respectively, with the aim of discovering materials with bandgaps comparable to those for CsSnI$_3$ that are thermodynamically stable (see Fig. 7). Results from a recently submitted co-authored paper by NTU and Berkeley researchers[5] revealed Ge as an element suitable for replacing Pb in halide perovskite compounds with bandgap values suitable for light harvesting. Experimentally, three AGeI$_3$ (A=Cs, CH$_3$NH$_3$ or HC(NH$_2$)$_2$) halide perovskite materials were synthesized, shown to be stable up to 150^{o}C, and have bandgaps correlated to the A-site cation size. The experimentally observed trends in bandgap values were consistent with those derived from DFT calculations. The results demonstrated the strong potential of combining computational screening and experimental efforts to develop Pb-free halide perovskite compounds for photovoltaic applications.

Current work in this area is focused in two main directions, both aimed ultimately at the discovery of Pb-free halide perovskite compounds which feature better device performance and enhanced air stability. In the first direction, we are undertaking computational screening studies of A$_2$MX$_6$ compounds (see. Fig. 8(b)), where the M-site Pb-replacement ion (e.g., Ge or Sn) resides in a higher oxidation state (4+) and is anticipated to display increased stability with respect to oxidation.



(a)



(b)

Figure 8: Results from high-throughput screening of bandgap values for perovskite AMX$_3$ (a) and perovskite-derivative A$_2$MX$_6$ (b) are presented for 657 compounds, corresponding to different choices of A and M (y-axis and x-axis in the color plots, respectively), with X=Cl, Br or I. In the color plots, cooler (hotter) colors indicate lower (higher) values of the bandgap. Based on these calculations, combined with analyses of thermodynamic stability, five new compounds have been identified as promising for potential photovoltaic applications.

The second direction for the current computational work is motivated by the experimental findings for $CsSnI_3$, where the intrinsic p-type character of the material led to the need to employ SnF_2 as an additive in the solution processing to control background carrier densities. To avoid the need to identify such additives, and hence to simplify processing, it would be desirable to identify compounds that have self-compensating intrinsic point defects. In the computational work this has led to a new focus on the high-throughput calculation of the so-called branch-point energy, the position of which, relative to the valence band maximum and conduction band minimum, provides an indication of whether the material will be intrinsically n-type (branch-point energy located in or near the bottom of the conduction band), p-type (branch-point energy located in or near the top of the valence band) or feature compensating intrinsic defects (branch-point energy located in the band gap). Preliminary results of band-alignment and branch-point energy calculations are shown in Fig. 9, which correctly identify $CsSnI_3$ as being intrinsically p-type. The assumption that the branch-point energy displays a near-universal value provides the framework for high-throughput computations to screen for intrinsic n-type and p-type behavior, as illustrated in Fig. 9b.

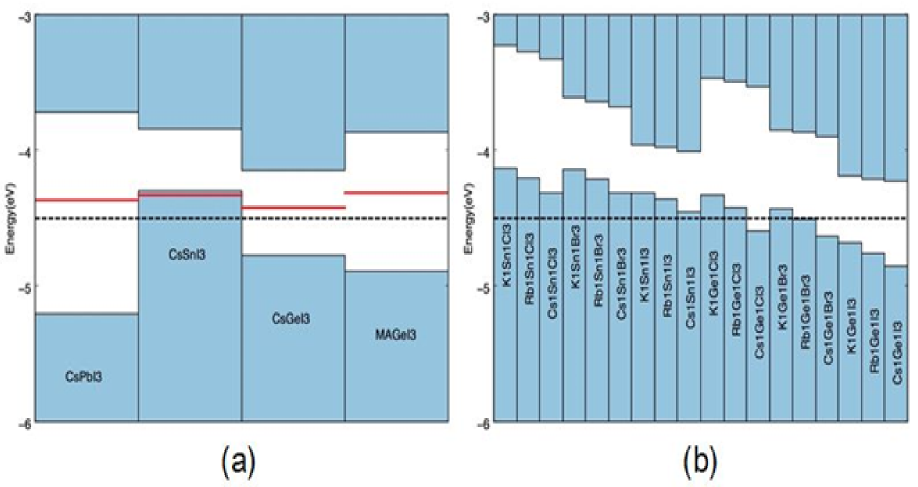


Figure 9: Results of density-functional-theory calculations, showing the effect of phase-equilibria with SnF_2 on the range of Sn chemical potential (Sn) compatible with stability of the $CsSnI_3$ compound. The range of stability (white regions) is pushed to less-negative values of Sn in the presence of SnF_2 (top panel) relative to that found without (lower panel). This has a consequence of raising the value of the Sn vacancy formation energy (plotted schematically in the top panel) and thus lowering the equilibrium vacancy concentration and associated p-type carrier density.

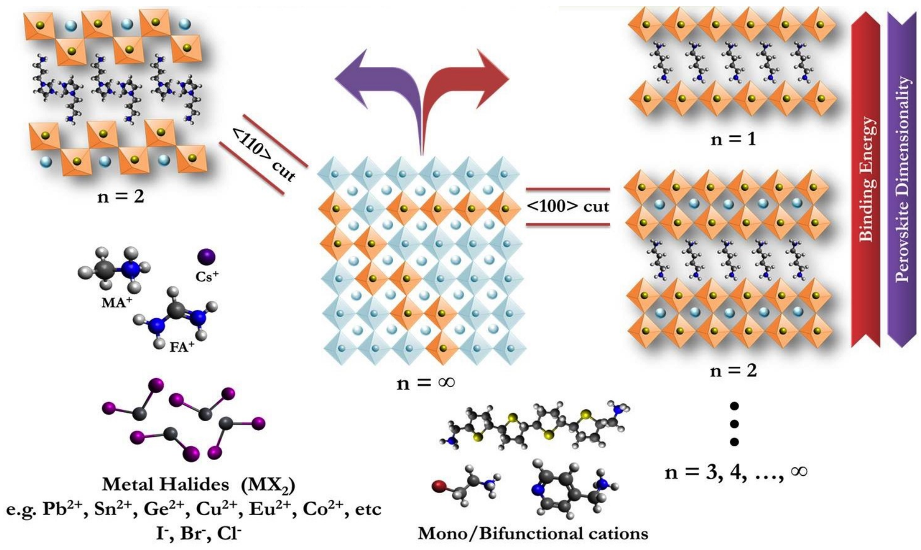


Figure 10 Schematic representation of the multidimensional halide perovskite alternatives

The validation of the predictions from these calculations and the hypothesis that the position of the branch-point energy displays a near-universal value when the bands are referenced to the vacuum level, are the subject of collaborative experimental research between the Berkeley (Wu) and NTU (Mhaisalkar, Mathews and Sum) groups. In particular, the branch-point energy converges with the energy position toward which the Fermi level of the material would be pulled by native defects (i.e., vacancies, interstitials and anti-sites). Therefore, the branch-point energy could be experimentally identified with respect to the conduction and valence bands of the material by artificially generating such native defects and probing the resultant type and density of free charge carriers. This will be achieved by irradiation of the material with high-energy particles (i.e., 3MeV alpha particles and 200keV Ne+ particles). The density and species of native defects will be obtained as a function of the irradiation recipe and doses with Monte Carlo simulation, and their electronic activities will be determined by comparing with free carrier type and density obtained from Hall effect data. By doing so, we seek to establish a nearly universal model that governs the native doping type and concentration, extrinsic dopability, band offset, and defects immunity of lead-free perovskites.

The objectives of this task includes investigations of multidimensional perovskite solar cells, processed by environmentally friendly means as well as to develop a fundamental understanding of the light harvesting, recombination dynamics, and charge transport phenomena in these devices. One of the most crucial elements in the design of newer perovskites is the size/type of the organic cation, which plays a critical role in determining the thickness, separation of the inorganic layers. Increasing the cation size separates the system into layers, forming lower dimensional (eg. 2D) networks. This substitution allows for hydrogen or halogen bonding between the organic cation and inorganic framework to reduce the band gap/ increase stability, while the charge carrier mobility in 2D perovskites can possibly be improved by connecting the inorganic layers by covalent bridges.

Perovskite-structured materials are characterized by very high crystallinity even in solution processed form and long charge carrier diffusion lengths[1], which enable their use for high-efficiency photovoltaics in device architectures with mesoporous structures -either injecting or non-injecting ones- and thin films. The use of $CH_3NH_3PbI_3$ has resulted in power conversion efficiencies above 20%, nevertheless the rich diversity these compounds offer enables the formation of a plethora of 0, 1, 2 and 3-D organic-inorganic structures through substitutions at the A M, and X sites (Figure 10).

Cu_2^+ is a suitable non-toxic, abundant and environmentally friendly option for the perovskite formation. $(CH_3NH_3)_2CuX_4$ (X being a halide compound) are promising candidates. Variation of cations and the halide tuning in order to improve and reduce the space between the different perovskite layers to improving the charge transport will be attempted. $(CH_3NH_3)_2CuCl4$ forms a 2D layered perovskite structure; analogous to that adopted by the high temperature superconductor $La_{2-x}Ba_xCuO_4$. At room temperature $(CH_3NH3)_2CuCl_4$ is shown to adopt a distorted monoclinic structure, which displays a band gap of 2.48 eV. A gradual replacement of Cl for Br (i.e. $(CH3NH_3)_2CuCl_4$-xBrx), leads to less distorted orthorhombic/tetragonal structures with a corresponding reduction in band gap. In addition, a judicious selection of organic component can give careful control of the interlayer spacing and an alternative approach to tailoring the physical properties of these materials. Other alternatives being explored include Bismuth and Antimony based halides or mixed double perovskite based halides.

4. Tandem perovskite cells with Si and GaAs devices

The combination of perovskites with Si, InP and GaAs solar cells in tandem architectures will be pursued to further enhance the efficiency beyond theoretical limit of single junction solar cells. In addition, we will explore integration of perovskites with InP nanopillar solar cells grown on a silicon substrate[6] for a triple junction solar cell. The four configurations explored (Figure 11) will be:

4-terminal mechanically stacked solar cells. In this case we can have two separate solar cells, top cell having the absorber of high energy photons and bottom cell having the absorber of low energy photons. The top cells placed mechanically over the bottom cells and we will have the 4 terminals to get connection. Both solar cells can be fabricated separately, thus avoiding the complexity of integrating two very different fabrication techniques. We can use these two cells either at series connected or parallel connected.

3 terminal tandem solar cells. The top cells should be integrated monolithically over the bottom cells so that top and bottom cell will have one common electrode and whole tandem device will have three terminals for connection. In this case the overall tandem device efficiency would be voltage limited. The advantage of this configuration is that we can use tunable bandgap materials to have minimum voltage loss.

2 terminal tandem solar cells. In this case, two separate cells are integrated monolithically through a recombination layer and we will have only two terminals for connection. The recombination layer is placed between the electron collecting electrode of one cell and the hole collecting electrode of the other cell, so the cells are integrated in series. In this case the overall tandem cell efficiency is current limited and current matching between top and bottom cells is needed. The proper choice of compatible recombination layer is required to achieve good efficiency. A few candidates for the bottom layer such as Silicon, GaAs, InP, CIGS and CZTS solar cells will be investigated.

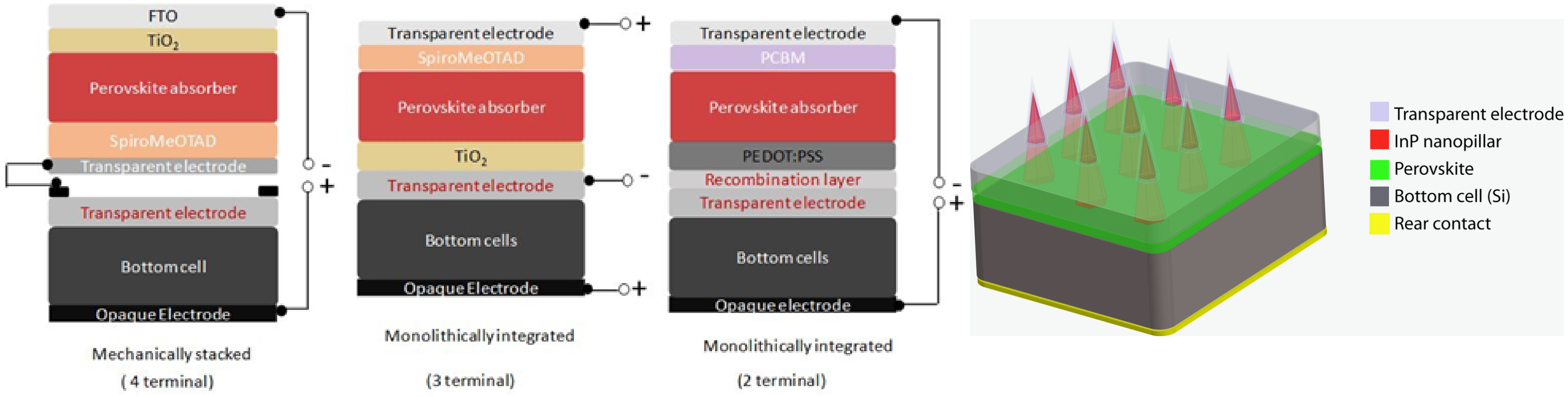


Figure 11. (left) Different architecture of Perovskite tandem cells showing 4, 3 and 2 terminals. Silicon, GaAs, CIGS or CZTS or InP solar cells can be used as the bottom cell. (right) proposed triple-junction solar cells with InP nanopillars grown on silicon.

Conclusions

The high efficiency (17.9%) achieved with the perovskite solar cells, along with the wide range of lead-free and multidimensional alternatives demonstrated, allow us to envision halide perovkite solar cells within high-rise building facades (view glass), where in combination with appropriate optical management layers, they present an attractive yet sustainable energy source relevant to Singapore.

References

1. S. Dharani, H. A. Dewi, R. R. Prabhakar, T. Baikie, C. Shi, D. Yonghua, N. Mathews, P. P. Boix and S. G. Mhaisalkar, Nanoscale, 2014, 6, 13854-13860.

2. N. Yantara, Y. Fang, S. Chen, H. A. Dewi, P. P. Boix, S. G. Mhaisalkar and N. Mathews, Chemistry of Materials, 2015, DOI: 10.1021/cm502710r.

3. M. H. Kumar, S. Dharani, W. L. Leong, P. P. Boix, R. R. Prabhakar, T. Baikie, C. Shi, H. Ding, R. Ramesh, M. Asta, M. Graetzel, S. G. Mhaisalkar and N. Mathews, Advanced Materials, 2014, 26, 7122-7127.

4. G. Xing, M. H. Kumar, W. K. Chong, X. Liu, Y. Cai, H. Ding, M. Asta, M. Graetzel, S. Mhaisalkar, N. Mathews and T. C. Sum, “Near Infrared Lasing from Solution-Processed Lead-Free Perovskites,” Nature Photonics (submitted).

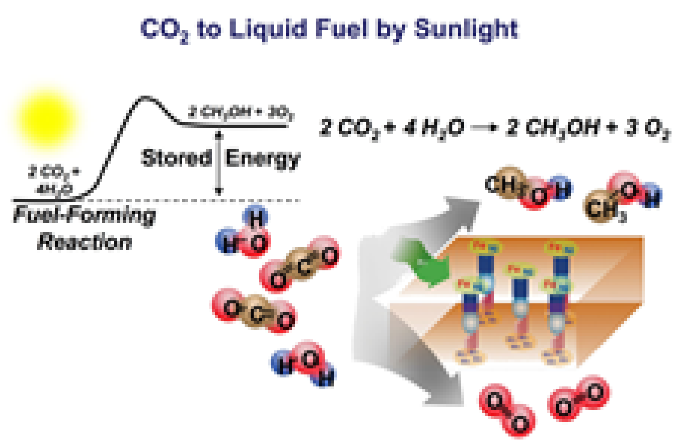
5. T. Krishnamoorthy, H. Ding, C. Yan, W. L. Leong, T. Baikie, Z. Zhang, M. Sherburne, S. Li, M. Asta, N. Matthews, and S. B. Mhaisalkar, “Lead-free Germanium Iodide Perovskite Materials for Photovoltaic Application,” J. Mater. Chem. A (submitted).

6. Wai Son Ko,Thai-Truong D. Tran, Indrasen Bhattacharya, Kar Wei Ng, Hao Sun and Connie Chang-Hasnain, “Illumination Angle Insensitive Single Indium Phosphide Tapered Nanopillar Solar Cell”, Nano Lett., 2015, 15 (8), pp 4961–4967, DOI: 10.1021/acs.nanolett.5b00756, July 1, 2015

Thrust 2: Solar-to-Fuel Conversion

Overview

The present state of human existence relies nearly completely on energy derived from fossil fuels; coal, oil, and natural gas provide 82% of the world's primary energy use. The effects of the carbon dioxide produced by the use of these fuels on the current and future climate of the planet have been well-documented by the Intergovernmental Panel on Climate Change (IPCC). A sustainable energy future for the world will require a radical change in energy generation.[1] In particular, there is a critical need for sustainable fuels, for example in the transportation sector.[2] While biofuels may be able to fill some of this demand, creation of "artificial photosynthesis" approaches with much high solar conversion efficiencies will be essential on a global basis.[3,4]



The goal of Thrust 2 is the production of fuels directly from sunlight.

Solar energy can be used to produce clean fuels efficiently.[5] It is thus important to explore pathways to convert CO_2 into fuels (such as methanol, formic acid and other higher order fuels), using the energy of solar photons to catalyze the chemical reaction. Use of the abundant, renewable solar energy may provide efficient routes to producing fuel without negative impact to the environment.

This thrust focuses on discovering new catalysts, which will be powered by solar energy to convert carbon dioxide to hydrocarbons, providing a sustainable alternative to fossil fuels. The approaches are organized in two main tasks: using a comprehensive synthesis platform (Task 1) in combination with state of the art rapid screening and evaluation techniques (Task 2) to discover new solar fuels catalysts. Cross-cutting activities in predictive electronic structure theory and advanced electron microscopy are used to guide the discovery efforts.

1. Discovery of novel, efficient catalysts

a. Combinatorial Synthesis

Material libraries of catalysts will be generated by continuous composition spread (CCS) pulsed laser deposition (PLD) and molecular beam epitaxy (MBE) techniques. Two PLD systems will be used at NUS Nano science and Technology Institute (NUSNNI) and at the CREATE facility (new equipment to be installed) (Thirumalai Venky Venkatesan). An existing PLD facility at NUSNNI is being used primarily for oxide based catalyst libraries, an example of which is shown in Fig 1. A new PLD system in CREATE will be fully setup by January 2016 with ability to deposit all chalcogens (sulphide and selenides) based inorganic compounds in addition to oxides. A schematic of this system is shown in Fig. 2. In addition, a brand-new custom-designed MBE system is commissioned in CREATE for the generation of a variety of catalysts in thin films form (Loh Kian Ping).

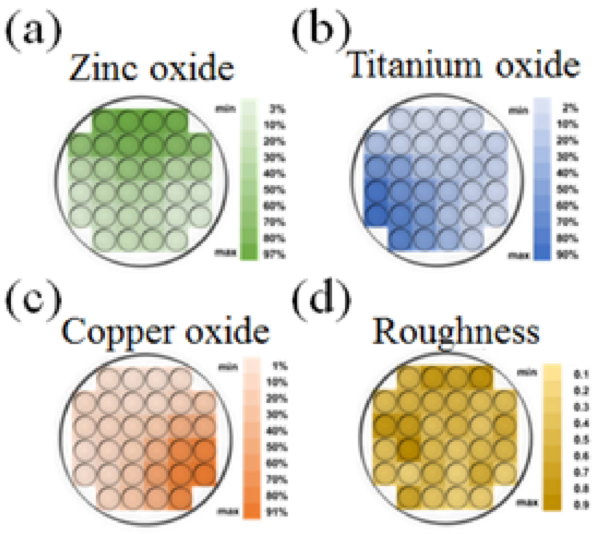


Fig. 1. Example of analysis of a ternary Zn-Ti-Cu catalyst library performed using specially constructed Rutherford backscattering chamber installed on the accelerator beam line at Center for Ion Beam Application (CIBA).

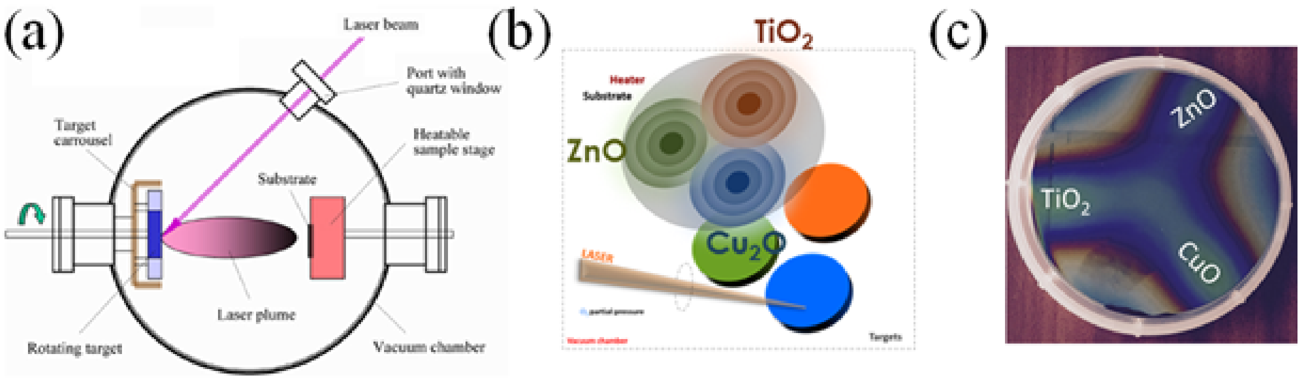


Fig. 2. Pulsed laser deposition is used to deposit catalysts libraries on 4 inch wafers.

b. Novel Catalysts

In the process of solar to fuel production, both CO_{-2} reduction and water oxidation are important. Currently, the efficiencies of these reactions under visible light are still quite low and more active catalysts need to be developed. Profs. Xu Rong, Chen Zhong, Jason ZC Xu, and Han Sen Soo at NTU are engaged in discovery of new catalysts for water oxidation and CO_2 reduction from basic catalyst design principles. The team seek to achieve a significant improvement in energy conversion efficiency from solar energy to chemicals and fuels by developing metal complex, nano-engineered particulate and thin-film semiconductor systems for water reduction, water oxidation and CO_2 reduction reactions. Special emphasis is on the design of well-defined molecular and solid structures and investigation of their key structural factors for understanding of reaction mechanism through comprehensive analytical techniques. Selected highlights from these efforts are shown in Fig. 3. For example, a cobalt phosphonate catalyst that mimics the structure of Mn_4CaO_5 cluster in photosystem II (PSII) has been discovered as an efficient catalyst for water oxidation with promising activities (Fig. 3b).

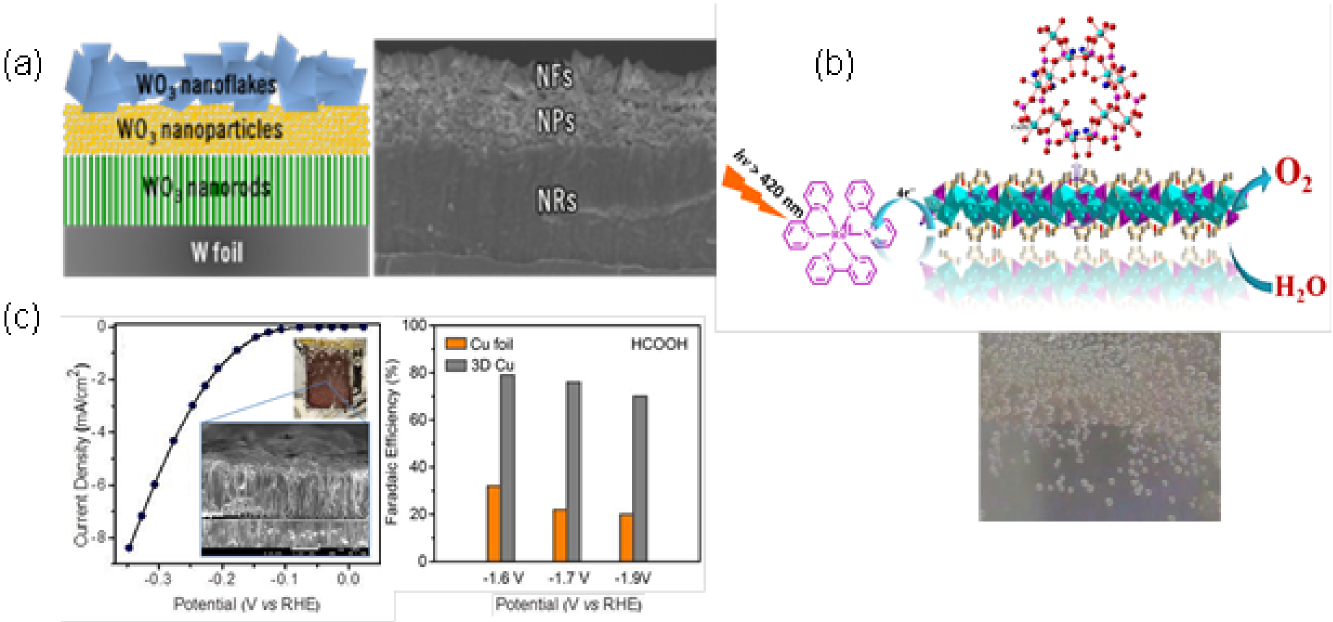


Figure 3: (A) a unique nanorod/nanoparticle/nanoflake triple-layer WO3 as efficient photoanode for visible light water splitting (Nanoscale, 2014, 6, 13457), (B) a new layered cobalt-organo phosphonate crystal mimicking the structure of Mn_4CaO_5 cluster in PSII as an efficient catalyst for water oxidation (Energy Environ. Sci., 2015, 8, 526), and (C) nanostructured 3D Cu electrode for efficient reduction of CO_2 to formate.

2. Rapid screening technique for characterizing the performance of catalysts

a. Mass-spectrometer-based detection

A special mass spectrometer based on selected ion flow tube (SIFT) ionization is being interfaced to electrochemical cells for the rapid, real-time detection of CO_2 reduction products (Jens Martin, Joel Ager, Jason Yeo and Venkatesan). The SIFT ionization eliminates fragmentation found with electron ionization (Fig. 4) and, as a result, this instrument is capable of parts per trillion detection ability for volatile organic compounds. In SinBeRISE, this approach is being adapted for rapid screening of catalysts both for electro and photo-catalysis. Figure 4 shows a schematic of the SYFT mass spectrometer, and Figure 5 shows the special sample stage deigned for rapid screening of catalysts. Figure 6 shows extremely sensitive liquid and gas detection from a CO_2 reduction photo catalysis experiment using a typical catalysts like TiO_2 nanotubes

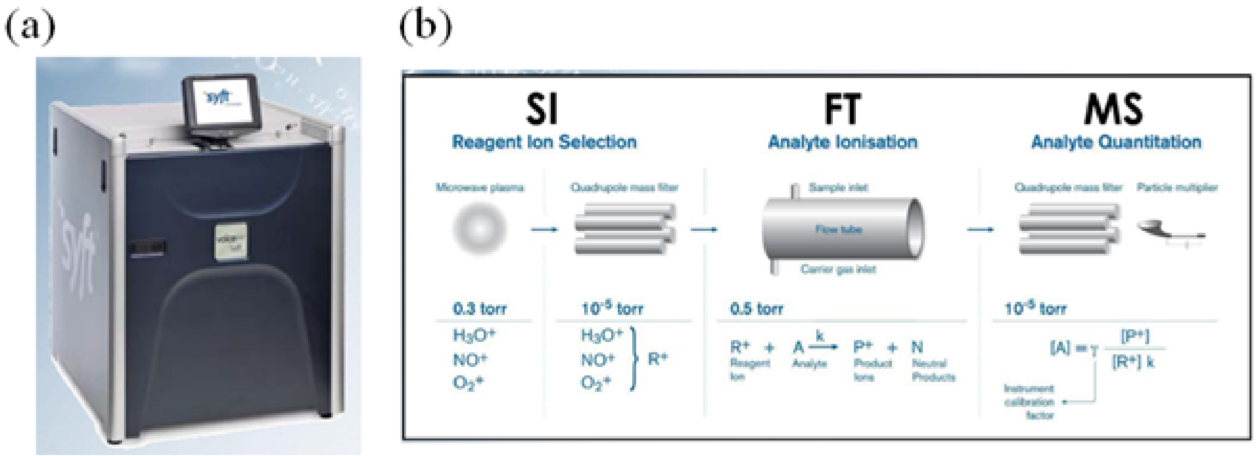


Figure 4: Overview of Selected Ion Flow Tube (SIFT) ionization mass spectrometry.

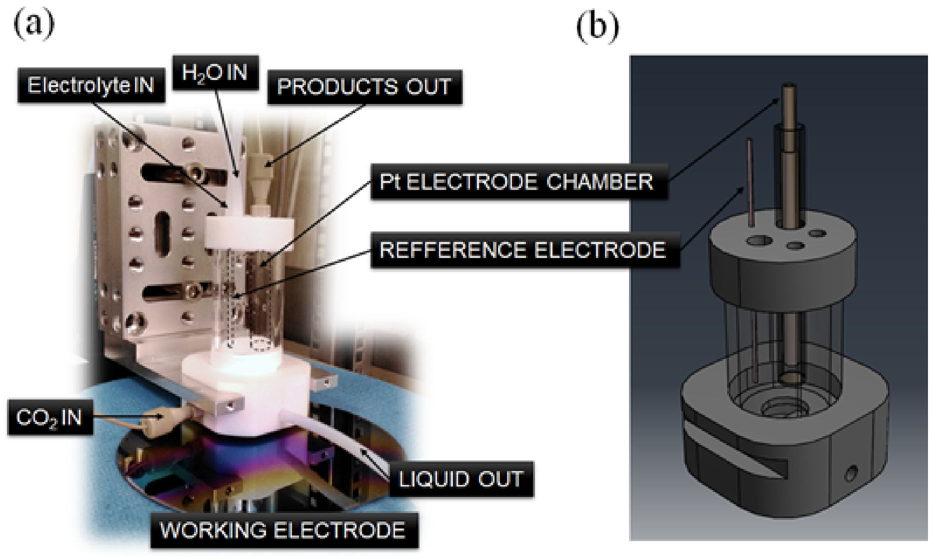


Figure 5 Cell for scanning of catalyst libraries using SIFT detection.

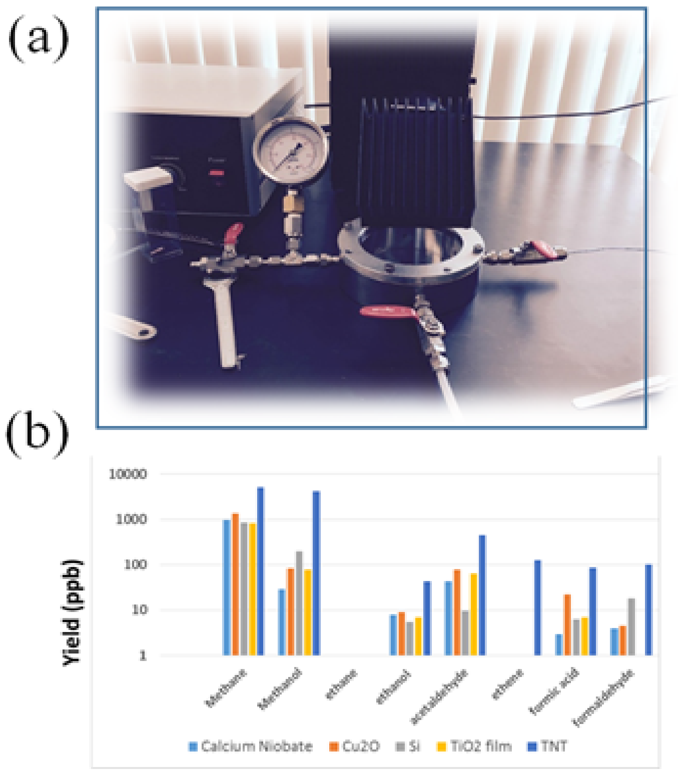


Figure 6 Liquid (methanol, ethanol, acetaldehyde, formic acid, and formaldehyde) and gas (methane) product detection from CO2 reduction on 5 oxide photocatalysts using the SYFT instrument. TNT = TiO2 nanotubes

b. Microfluidic approach to solar fuel conversion

"Traffic control" of chemical reactants, intermediates, electrons and products is critical to affect selective and efficient electrochemical reduction to liquid fuels. While there have been a number of recent demonstrations of solar-driven CO_2 reduction, the production have been either CO or formate, which are not directly usable as chemical fuels.[9–13] Demonstration of an efficient system which separates oxidation and reduction products and yields a pure stream of fuel remains an outstanding challenge.[14]

We will employ a microfluidic testbed as a means to develop selective and efficient CO_2 reduction systems. Prof J.Ager has experimentally demonstrated such an integrated system for water splitting.[15] The design enables control over all relevant length scales: diffusion of protons, reactants, and reaction intermediates. As all functional components in this microfluidic test-bed can be easily exchanged, the performance of various components in the integrated system can be quickly assessed and tailored for optimization (Figure 7). Moreover, it allows local control of temperature, chemical potential (when integrated with PV), and, possibly, chemical separation via biphasic flow in the channels.[16]

SinBeRISE is well-poised to implement microfluidic approaches for solar fuel generation, having world class capabilities in high aspect ratio lithography (Van Kan) and roll to roll nanoprinting (Groves). At present, efforts are under way to fabricate microfluidic devices and demonstrate CO_2 reduction with model catalysts (e.g. Cu). In parallel, we are developing the ability to catalyst patterns and/or libraries in microfluidic format (Venkatesan, Xu Rong, Jason Xu). There is a synergy with the combinatorial synthesis efforts, and we will investigate stamping of patterned microfluidic structure, which will incorporate proton diffusion elements, directly on catalyst libraries. Evaluation of libraries with spatially varying composition by the use of linear channels will provide direct insight into sequential catalysis pathways. We will also investigate functionalization of channel walls with catalysts and/or promoters designed to influence selectivity and activity. The sensitive SIFT detection method will enable fast scanning of libraries and allow sequential catalysis to be evaluated rapidly. Local/sequential control of temperature, chemical potential, and, possibly, chemical separation will also be investigated.

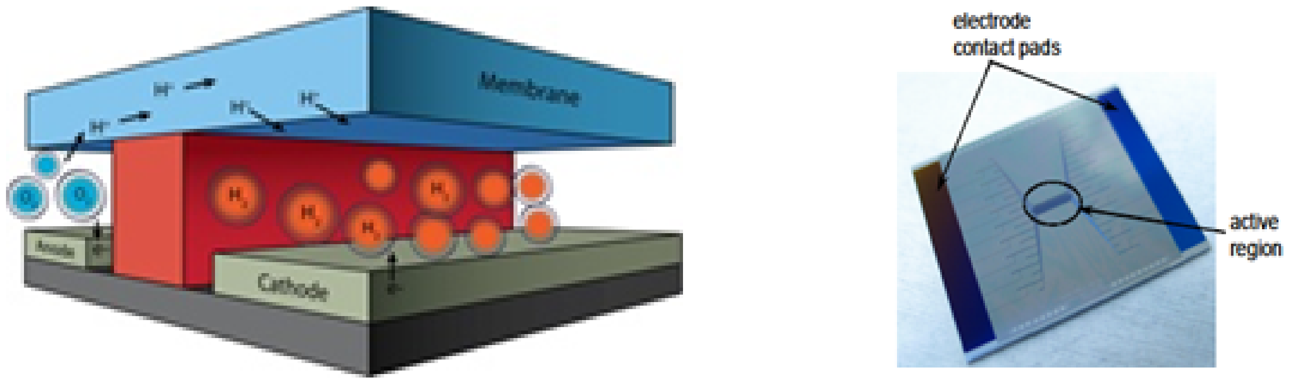


Figure 7 Schematic of microfluidic water splitting device, adapted from ref. 15 In this microfluidic water electrolysis device, the channels in which O_2 and H2 are generated by splitting water are separated by a chemically inert wall (red). The conduction of protons from one channel to the other, which is required for continuous operation, occurs via a Nafion® membrane cap. A photo of a test device is shown on the right.

3. Cross-cutting research

a. Catalyst Library Design

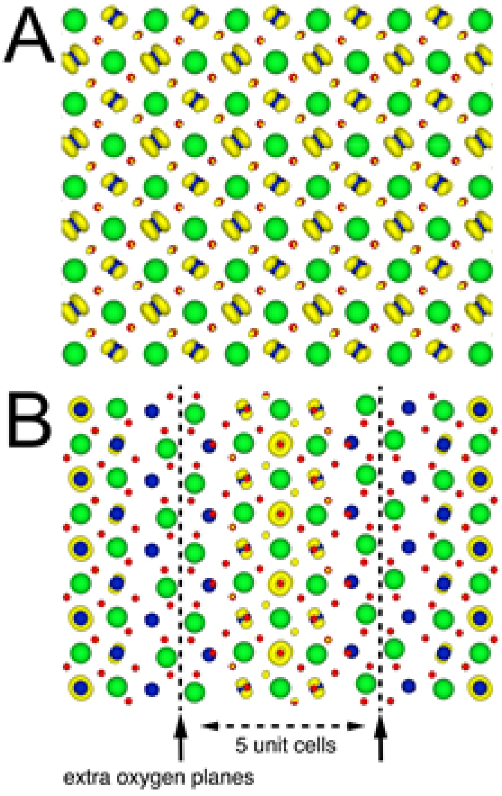


Figure 8: Alternating charge arrangements

Initial research in thrust 2 involved collaborative work between groups at NUS (Venkatesan) and Berkeley (Minor, Asta and Sherburne) focused on the properties of Sr1-xNbO3+ -based materials for water-splitting catalyst applications. The performance of these materials was linked to a high electron carrier density. In the course of this study, electron carriers were found to display novel plasmonic properties, which depended strongly on oxygen content. In conducting Sr0.94NbO3 a conventional plasmon is observed at 1.9 eV, while in insulating-like, oxygen-rich Sr0.94NbO3.4 unconventional plasmons are found at 1.7, 3.0, and 4.0 eV. These latter plasmons were found to originate from collective oscillation of correlated electrons, due to the presence of extra oxygen planes that enhance an unscreened Coulomb repulsion among charges. In Sr0.94NbO3.3 both types of plasmons exist. Our calculations based on coupled harmonic oscillators model and density functional theory were able to closely mimic the experimental data and also suggested the presence of alternating charge arrangements in Sr0.94NbO3.4 (see Fig. 8).[17]

b. Catalyst Characterization

In the past three years, NCEM has carried out materials characterization for a variety of materials for the SinBeRise program, including photovoltaic perovskite materials (T1) and water-splitting catalysts (T2). Complex oxides such as Sr1-xNbO3-d and related materials have shown promise as effective photocatalysts, for example for use in water splitting. Varying the stoichiometry of the Sr1-xNbO3-d not only influences the photocatalytic performance, but also electronic properties, such as electrical resistance and plasmonic behavior. In collaboration with SinBeRISE PIs Venkatesan, Rusydi, and Asta, SinBeRISE PI Minor has identified the source of the anomalous behavior as defects induced by the varied growth conditions. Higher oxygen pressure during growth of these films results in more insulating materials, with more strongly correlated plasmons. TEM studies indicate that this also corresponds to an increase in defects in the films (Figures 9a-c). Furthermore, high resolution studies indicate that these defects correspond to extra oxygen planes in the films (Figure 9d & 1e), which when combined with computational work, directly relates the atomic structure of these materials to the overall functionality.

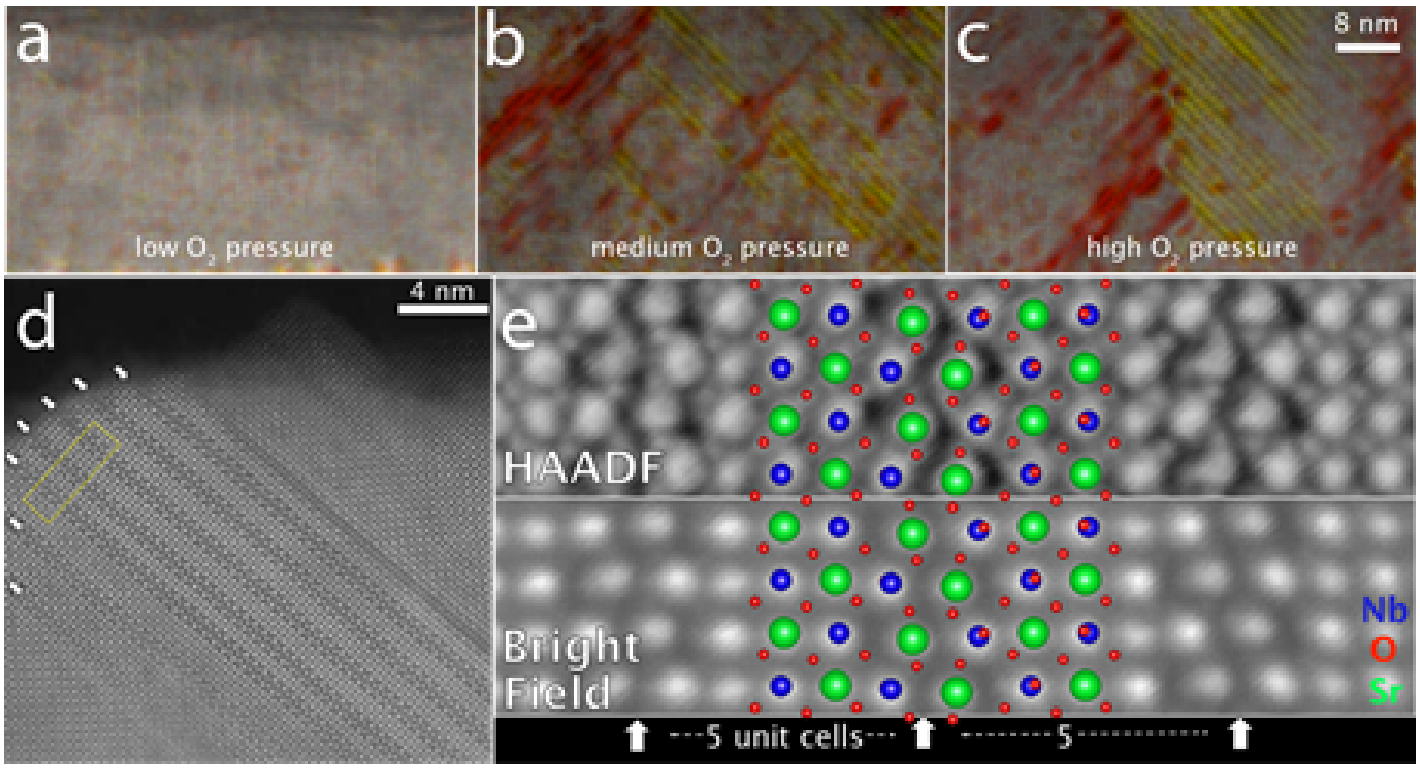


Figure 9: Sr1-xNbO3-d materials characterized by TEM. a-c: Increasing O_2 pressure during film growth yields increasing oxygen defect planes, highlighted yellow and read here. d,e: High resolution studies reveal the atomic structure of the observed defects, which occur at 4-5 unit cell intervals in the low and high pressure material.

References

1. Chu, S.; Majumdar, A. Nature 2012, 488 (7411), 294–303.
2. Newman, J.; Hoertz, P. G.; Bonino, C. A.; Trainham, J. A. J. Electrochem. Soc. 2012, 159 (10), A1722–A1729.
3. Gust, D.; Moore, T. A.; Moore, A. L. Acc. Chem. Res. 2009, 42 (12), 1890–1898.
4. Faunce, T. A.; Lubitz, W.; Rutherford, B.; MacFarlane, D.; Moore, G. F.; Yang, P.; Nocera, D. G.; moore, T.; Gregory, D.; Fukuzumi, S.; Yoon, K. B.; Armstrong, F. A.; Wasielewski, M. R. Energy Environ. Sci. 2013, -.
5. Herron, J. A.; Kim, J.; Upadhye, A. A.; Huber, G. W.; Maravelias, C. T. Energy Environ. Sci. 2015, 8 (1), 126–157.
6. Zhou, T.; Wang, D.; Chun-Kiat Goh, S.; Hong, J.; Han, J.; Mao, J.; Xu, R. Energy Environ. Sci. 2015, 8 (2), 526–534.
7. Qi, H.; Wolfe, J.; Wang, D.; Fan, H. J.; Fichou, D.; Chen, Z. Nanoscale 2014, 6 (22), 13457–13462.
8. Gazi, S.; Hung Ng, W. K.; Ganguly, R.; Putra Moeljadi, A. M.; Hirao, H.; Soo, H. Sen. Chem. Sci. 2015.
9. Jeon, H. S.; Koh, J. H.; Park, S. J.; Jee, M. S.; Ko, D.-H.; Hwang, Y. J.; Min, B. K. J. Mater. Chem. A 2015, 3 (11), 5835–5842.
10. Sugano, Y.; Ono, A.; Kitagawa, R.; Tamura, J.; Yamagiwa, M.; Kudo, Y.; Tsutsumi, E.; Mikoshiba, S. RSC Adv. 2015, 5 (67), 54246–54252.
11. Sekimoto, T.; Shinagawa, S.; Uetake, Y.; Noda, K.; Deguchi, M.; Yotsuhashi, S.; Ohkawa, K. Appl. Phys. Lett. 2015, 106 (7), 073902.
12. Arai, T.; Sato, S.; Morikawa, T. Energy Environ. Sci. 2015, 8 (7), 1998–2002.
13. Schreier, M.; Curvat, L.; Giordano, F.; Steier, L.; Abate, A.; Zakeeruddin, S. M.; Luo, J.; Mayer, M. T.; Grätzel, M. Nat. Commun. 2015, 6, 7326.
14. Rongé, J.; Bosserez, T.; Martel, D.; Nervi, C.; Boarino, L.; Taulelle, F.; Decher, G.; Bordiga, S.; Martens, J. A. Chem. Soc. Rev. 2014, 43, 7963–7981.
15. Modestino, M. A.; Diaz-Botia, C. A.; Haussener, S.; Gomez-Sjoberg, R.; Ager, J. W.; Segalman, R. A. Phys. Chem. Chem. Phys. 2013, 15 (19), 7050–7054.
16. Winterton, J. D.; Myers, D. R.; Lippmann, J. M.; Pisano, A. P.; Doyle, F. M. J. Nanoparticle Res. 2008, 10 (6), 893–905.
17. Asmara, T. C.; Zhao, Y.; Majidi, M. A.; Nelson, C. T.; Scott, M. C.; Cai, Y.; Wan, D.; Schmidt, D.; Yang, M.; Trevisanutto, P. E.; Motapothula, M. R.; Breese, M. B. H.; Sherburne, M.; Asta, M.; Minor, A.; Venkatesan, T.; Rusydi, A. Science(submitted).

Thrust 3: Devices and Applications

Overview

The purpose of this thrust is to demonstrate ideas and achievements proven in small scales in the laboratory in Thrusts 1 and 2, in substantially larger scales for appreciation and acceptance by potential industry partners. Some of the achievements in Thrusts 1 and 2, which are in mm scales, will pose different engineering problems when scale-up is attempted. Hence, a separate thrust is required to tackle engineering issues that do not exist in Thrusts 1 and 2. Though, the devices and systems produced here are also meant for use in the laboratory, they are of substantially large scales (cm scale).

This thrust began execution later than the other two as efforts were focused to solve scientific problems first. When we have made good progress on the scientific front, we embarked on Thrust 3 with well-defined deliverables. Below is a summary of the targets at present.

1. Photovoltaics/Photoelectrochemical Cell (PEC) Tandem Device for Solar Fuel production

Efficient water splitting driven by a single photoelectrode has remained elusive due to stringent electronic and thermodynamic property requirements. A few materials have been identified as potential photoanode materials. Yet, their performance has been limited by low carrier concentration and poor electronic properties that required a high overpotential for water oxidation and low STH efficiency. Efficient water splitting using a photo active anode could be realized by connecting it in series with a solar cell which could provide part of the required overpotential.

Thrust 1 researchers showed that a modified hematite (a-Fe_2O_3) coated on FTO substrate could be used as a semi-transparent anode in tandem with a perovskite solar cell. Pt was used as the cathode. The cell architecture of this small system is shown in Fig 1. Emphasizing the tandem concept, they chose an architecture that required light to pass through the anode and the transmitted light was used to energise the solar cell. Because, some of the incident light was absorbed by the anode, the solar cell was required to have an extended optical absorption of up to ~800 nm to be efficient. Production of a high open circuit voltage by the solar cell is advantageous as this would assist in the anode reaching the required overpotential. Hence, they chose a perovskite solar cell in this application. This concept was shown in a device where the anode was only a few mm in diameter.

In parallel, researchers in Thrust 2 were examining photo- and electro- active catalytic materials for splitting water without the requirement for a solar cell. They found that besides hematite (a-Fe_2O_3), two other materials showed promise namely, W2O3 and BiVO4.

In this task in Thrust 3, we combine these achievements of the other two thrusts, and embark to build a larger system for splitting water to produce H_2 gas. H_2 gas could be used directly as a fuel but it needs to be compressed which will consume energy. Alternatively, H_2 gas could be used as a feedstock in fuel cells or in a Fischer-Tropsch conversion plant, with CO, to produce liquid fuel.

The system built is shown in Figs 2 which comprises a window of several centimeters that allows us to test anodes of large active areas. Although, this system, at present, uses a single solution processed organic-inorganic halide perovskite ($CH_3NH_3PbI_3$) solar cell in tandem with a candidate photoan-ode from among hematite (a-Fe_2O_3), W_2O_3 and $BiVO_4$, the photovoltaic material and the photoanode could be easily inter-changed as the system is very modular. Hence, this will be used as a testbed for different solar cells and photoanodes that could be derived from Thrusts 1 and 2 in future.

The architecture was varied so that two separate light sources could be employed for the anode and the solar cell respectively, thus eliminating the need for transparent electrodes as they are usually a limitation in large area solar cells. The light is incident on both sides of the system and the end elevation in Fig 2 clearly shows the window for illumination.

The hematite electrodes (Fig 3a) examined have 5x5 cm active area. They were hydrothermal synthesized or spray pyrolized. They gave an excellent performance of current density 1 mA/cm2 at 1.4 V vs RHE. $BiVO_4$ electrodes were 7x7 cm (with effective area 45 cm2) (Fig 3b) prepared by a drop casting method. They gave a photocurrent density (@ 2.2 VRHE) around 0.7 mA/cm2 which means maximum total photocurrent obtainable now is around 30 mA. WO_3 photoanodes were made by anodizing a W sheet whose nominal size is 6x7 cm (with effective area 30 cm2) (Fig 3c). The photo-current density (@ 2.2 VRHE) obtained was around 0.75 mA/cm2 which means the total photocurrent we can get now is around 22.5 mA.

We believe we can achieve overall unassisted water splitting with a conversion efficiency of 2.4% with well optimized photoanode and circuits. In addition production of CO from CO_2 by an eletrocatalyst-based method is possible which will make the use of Fischer-Tropsch conversion technique to produce liquid fuels attractive. A desktop micro-FT system is being looked into.

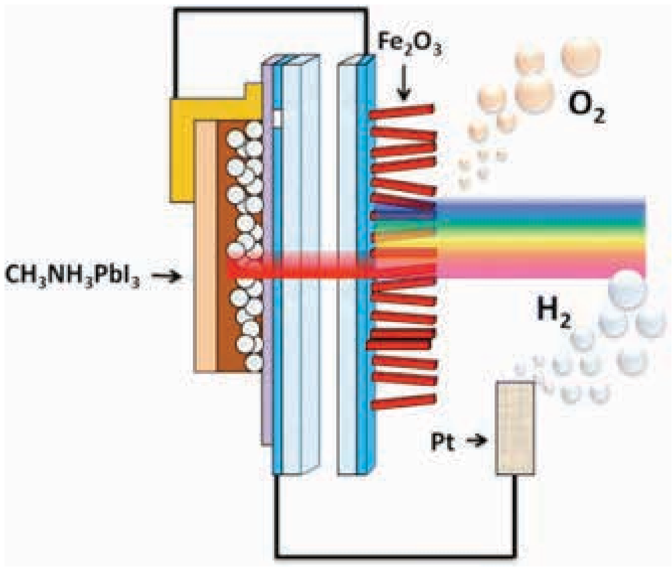


Figure 1. Schematic of the perovskite solar cell - hematite photoanode tandem cell.

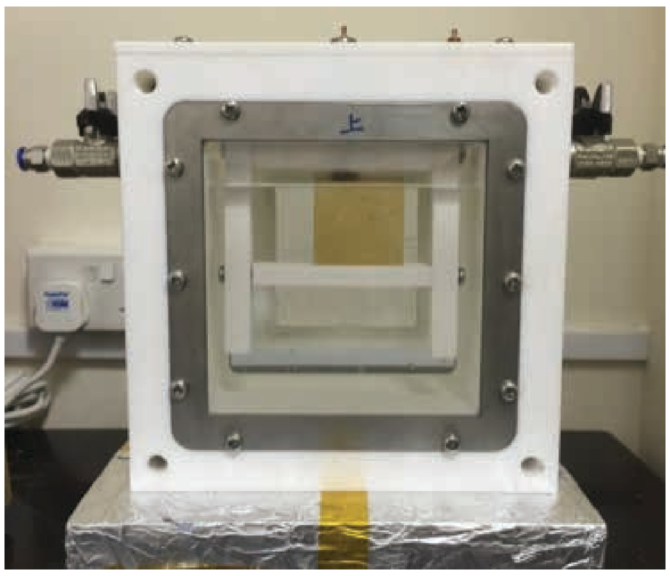


Figure 2: An end elevation of the assembled reactor unit from one illuminating direction. A hematite cathode Is visible.

Figure 3(a): A hematite anode.

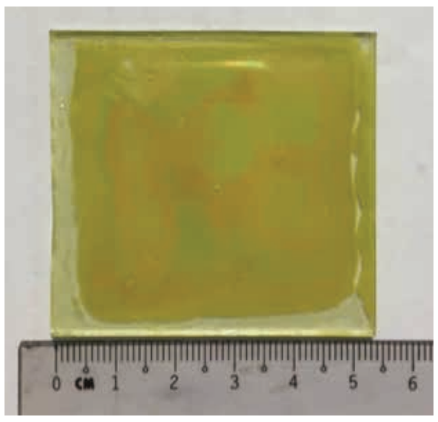


Figure 3(b): A BiVO4 anode.

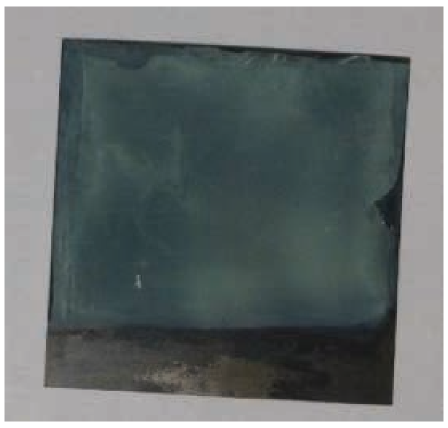


Figure 3(c): A W2O3 anode.

2. Scaling up Synthesis and Processing of PV Materials

The main purpose of this task is to scale up the production of low cost photovoltaics materials in order to produce solar cells with active areas of, at least 25 cm2. This size is comparable to commercial cells and will prove the scalability of the processes used in Thrust 1. We also take the opportunity to improve some steps in the process to obtain better control of quality as we will be purchasing new equipment and commissioning the operations in our CREATE laboratories. The focus in mainly on two PV materials that we have been investigating in Thrust 1, namely, methyl ammonium lead iodide perovskite ($CH_3NH_3PbI_3$) and Cu-chalcopyrite thin films made by solution processes.

For the methyl-ammonium lead iodide perovskite, the outline of the laboratory process being currently used is shown in Fig 4 and compared with the proposed scaled-up process. Note that we aim to replace the spin coating method, frequently used in the current process, with more scalable commercial processes such as spray pyrolysis, and those steps common in the electronics industry such as screen printing. This will increase our capability to produce not only a large area PV films, but also to better control the quality of the films.

The process would also be amenable for non-transparent, metallic conductors which could be alternative substrates to transparent electrodes. However, the architecture of common solar cells need to be changed to eliminate the need for transparent electrodes albeit with some effect on conversion efficiency. Such a loss in large area cells would be mitigated by the improved conductivity of metallic electrodes.

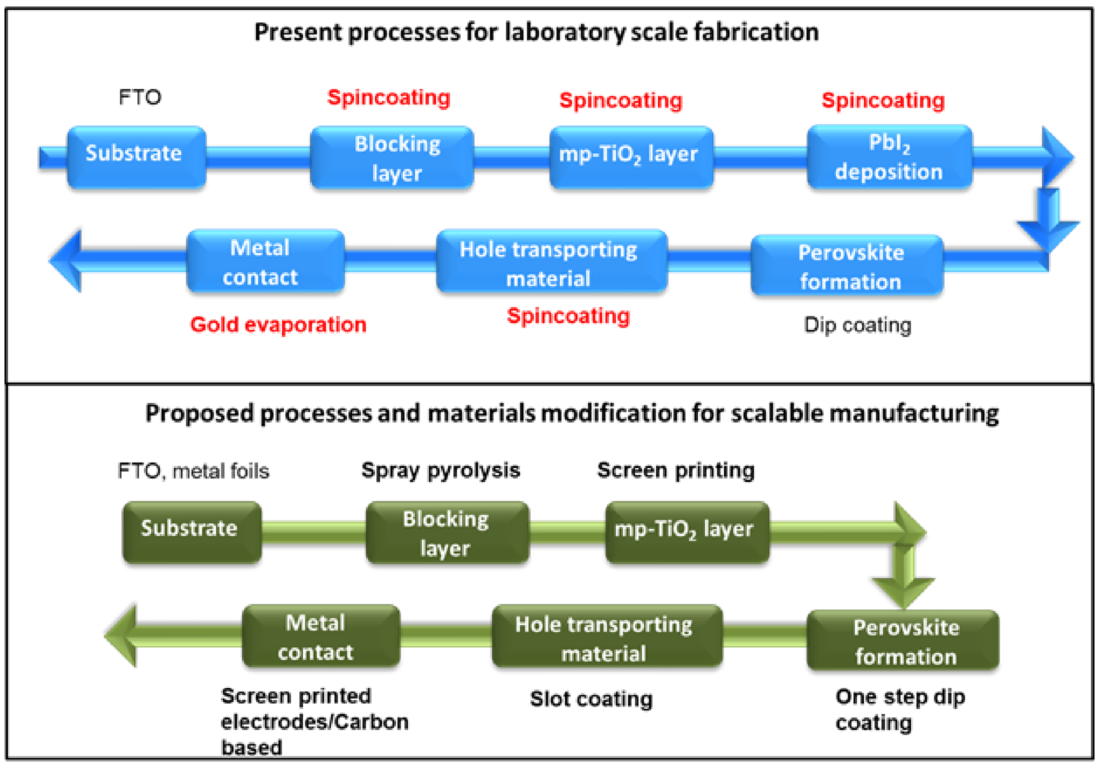


Figure 4: The current perovskite synthesis process and the proposed scaled-up process

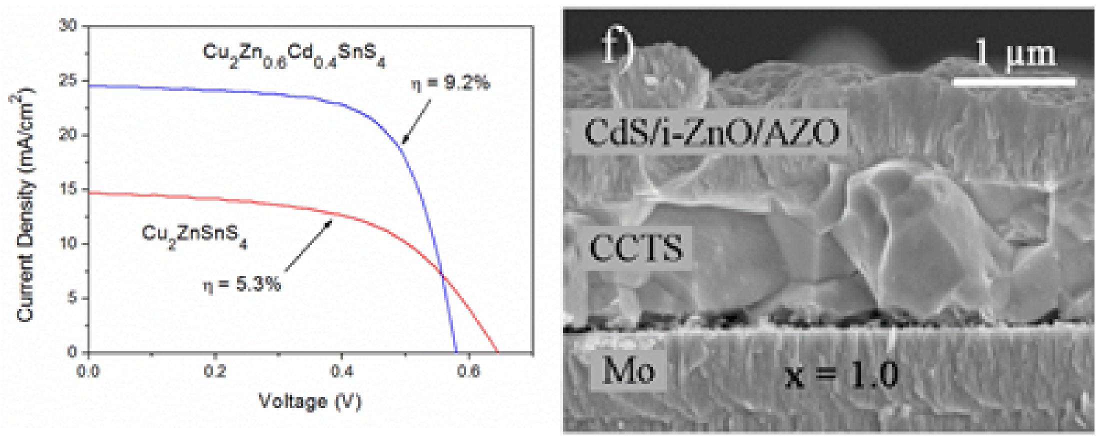


Figure 5: World record CCZTS solar cell (9.2%) with its cross-section device architecture showing large grain (Adv. Energy Materials 2015, DOI: 10.1002/aenm.201500682)

The family of compound materials of copper-indium-gallium-diselenide known as CIGS [including Cu(In,Ga)Se_2, Cu(In,Ga)$(S,Se)_2$, CuIn$(S,Se)_2$, CuZnSn$(S,Se)_2$] have been investigated as absorber materials for thin film solar cells in the past decades because of their high absorption coefficient and suitable bandgap for solar absorption. The state of the art CIGS solar cells are typically fabricated using vacuum based deposition. A part of SinBeRISE Thrust 1 research in the first two years was on the development of solution-processed semiconducting materials for printable CIGS solar cells by spin coating and spray pyrolysis. We have successfully made CIGS solar cells with > 10% efficiency, **which is one of the highest reported for water-based solution processed thin films** (J. Mater. Chem. A, Issue 8, 2015, Pages:4147-4154, DOI: 10.1039/C4TA05783J (inside Front Cover)). We have also identified the key synthesis parameters required to produce single phase wurtzite $CuZnSnS_2$ (CZTS) (J. Am. Chem. Soc. 2014, Volume: 136 Issue: 18 Pages: 6684-6692, DOI: 10.1021/ja501786s). We also recently used Cd doping into $CuZnSnS_2$ to make world-record Cu-sulfide based thin film solar cell with efficiency of > 9% as shown in Fig 5. (Adv. Energy Materials 2015, DOI: 10.1002/aenm.201500682). These solar cells are easy to make, can be scaled for deposition on flexible substrate and shows excellent air stability.

The next target is to scale up these devices to a dimensions of at least 5 x 5 cm2. We are currently optimizing our thin film deposition technique to fabricate such device. Examples of the large area devices are shown in Figure 6. The next step is the modification of post-film deposition annealing, the deposition of transparent conducting film and the design of top electrode for optimum collection efficiency. As this thin film solar cell shows excellent air stability, it will be used in subsequent demonstration in PV-powered sensor and proof-of-concept aesthetic solar cell for building applications.

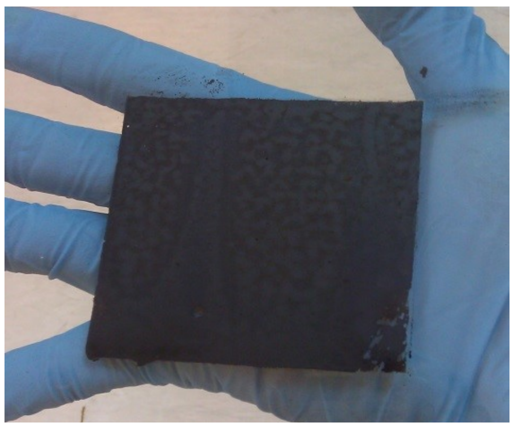


Figure 6: 5 x 5 cm2 Cu-chalcogenide thin film from spray pyrolysis.

3. Integration of NTU PV Cells to Power Sensor Networks

Smart buildings require sensors and transmitters to send a variety of information such as temperature, humidity, noise, human movement etc. to a central computer for suitable action. At the present, such modules are available but they consume a significant amount of energy and are powered by batteries or through mains electricity. A “green” alternative is to power them by photovoltaic (PV) cells energized by internal lighting available within the building. A small storage battery charged by the same PV cells would enable round-the-clock operation and yield a completely autonomous system. This is the aim of this task with special emphasis on using non-traditional PV materials such as perovskites or sulphide complexes which appear promising as cheaper alternatives to commercial PV materials. The concept for a candidate module is shown in Figure 7. It would have a Smart Maximum Power Point Tracker (Smart MPPT) to harvest the maximum amount of power from a series of solar cells. The Battery Charger would convert the small voltages obtained from low intensity light and keep standard Li-ion and Li-Poly batteries charged. The Power Management Unit (PMU) monitors battery health and ensures sufficient power is supplied to the module. The Wireless Sensor Network (WSN) controller operates with commercially available indoor sensors, and a Wireless Sensor Protocol could be used to send signals at specific time intervals through an antenna.

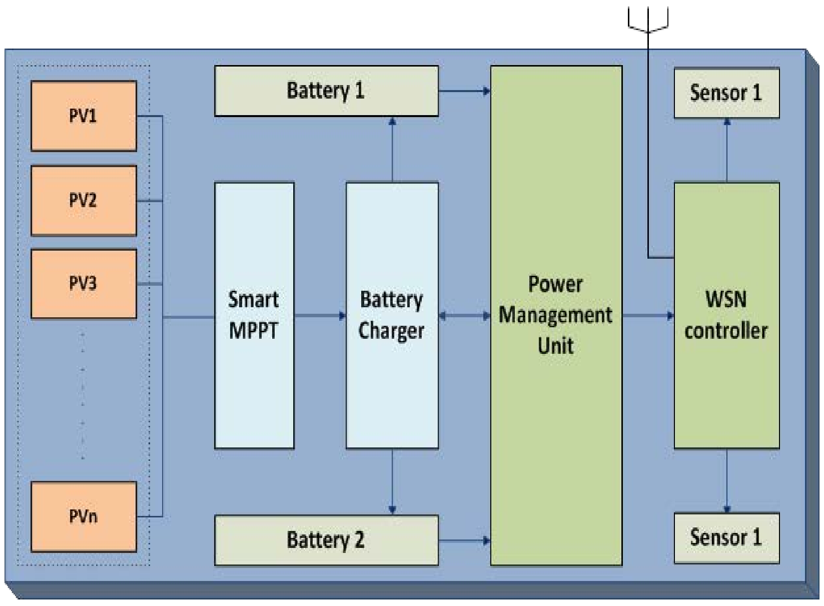


Figure 7 : Concept block diagram of a Wireless Sensor Network Module

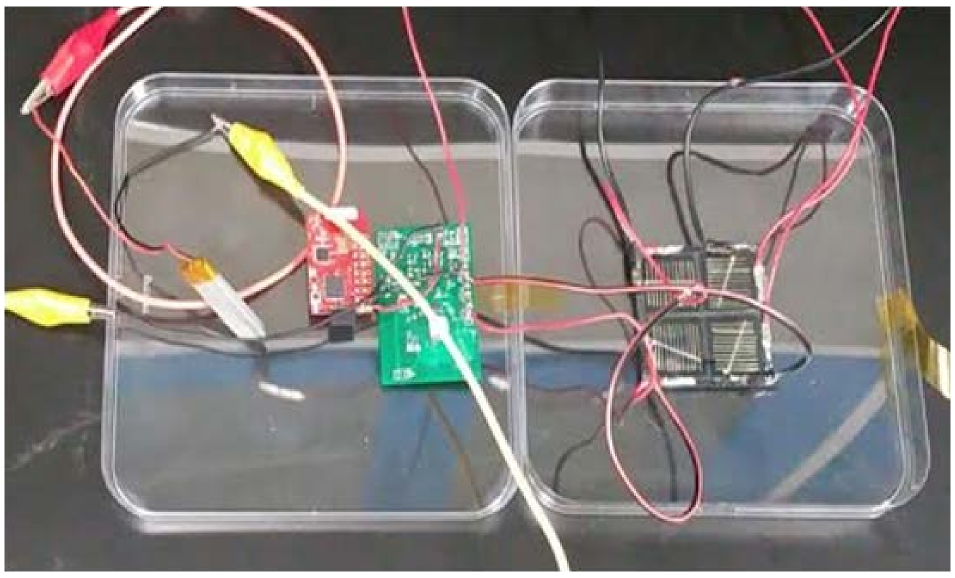


Figure 8: Mockup of a WSN Module with CZTS PV cell

The subdued intensity of internal lighting (100-200 times lower than 1 sun) entails that the power consumption of the module be lowered to mW levels. This is being developed. We intend to integrate our own PV cells, batteries and supercapacitors in this module to prove the viability of our products. Figure 8 shows a mockup of the WSN module with in-house Copper-Zinc-Tin-Sulphide (CZTS) PV cell (batteries not included). A complete re-evaluation of power consumption and aerial footprint is essential.

4. Integration of High Contrast Metastructures (HCM) for Colour Modification and Esthetics of Solar Cells.

The need for efficient solar cells to be good sunlight absorbers has long constrained their appearance to dark colours of deep blue or black, and had thus far rendered surfaces covered by PV panels to a visually unappealing monotonic hue. This has in part deterred the integration of PV by designers and architects for built in environments and other large scale surfaces. The ability to control the perceived colour of PV cells to greatly enhance its esthetic value while having minimal loss in conversion efficiency is tremendously important for future major deployment of PV on high rise buildings in mega metropolis. Currently, many coloured-PV technologies are either semitransparent or absorb only in the non-visible infra-red and ultra-violet wavelengths, incurring losses in energy conversion and reducing the panel efficiency.

Recently, we reported a novel metastructure, called high contrast metastructures (HCM), and show its use to manipulate light in unprecedented ways, including anomalous reflection and tunable colors to produce an effect like the skin of a chameleon (Optica Vol. 2, Issue 3, 2015, Doi: 10.1364/OPTICA.2.000255). One-dimensional HCM is referred to as high contrast gratings (HCG) shown in Fig. 8. The HCGs are very easy to fabricate and scale. We demonstrated many properties with 1D HCGs. A HCM or HCG is a single ultra-thin layer of structures of dielectric material with dimensions substantially less or close to an optical wavelength. Due to the high contrast in refractive indices, the reflection and transmission characteristics can be optimized in ways that could not be done previously, for example >90% in one high order diffraction mode, which can thus split color very efficiently. In addition, it is possible to produce highly enhanced optical intensity in layers between or below the HCM.

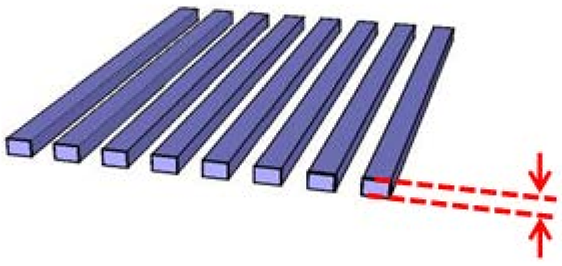


Fig. 9 Schematic of one-dimensional high contrast metastructures, referred to as high contrast gratings (HCG). A HCM or HCG is a single ultra-thin layer (0.1~1 wavelength thick) of structures of dielectric material with dimensions close to an optical wavelength.

In this program, we propose to integrate HCM with photovoltaics so that it can concentrate specific solar spectrum for efficient power conversion, while providing esthetic design. The observed colour of a film by varying the periodicity of the structures during fabrication, reflecting only a specific band of wavelengths and transmitting the rest. Figure 10 provides two examples of such films with diverse colours and patterns on the same substrate. The intention in this task is to incorporate the HCG films with in-house perovskite or chalocopyrite/kesterite solar cells to offer efficient PV panels with colour tunability at low light loss. Figure 11 illustrates a possible schematic for such a coloured PV module.

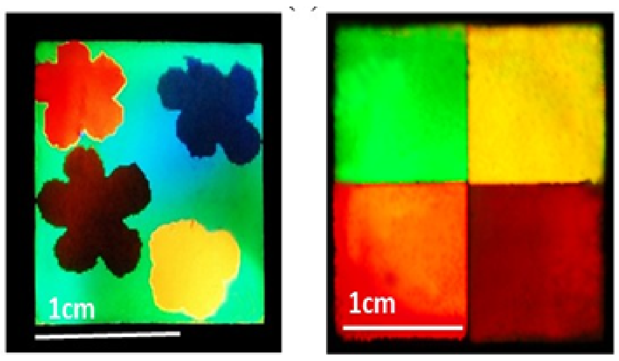


Figure 10: Films of HCG in elastomer displaying different colours on the same substrate by controlling the periodicity of fabricated structures.

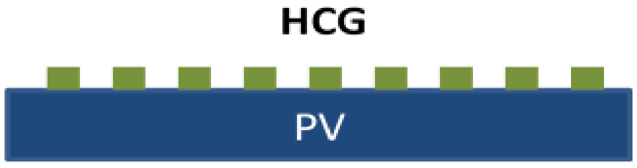
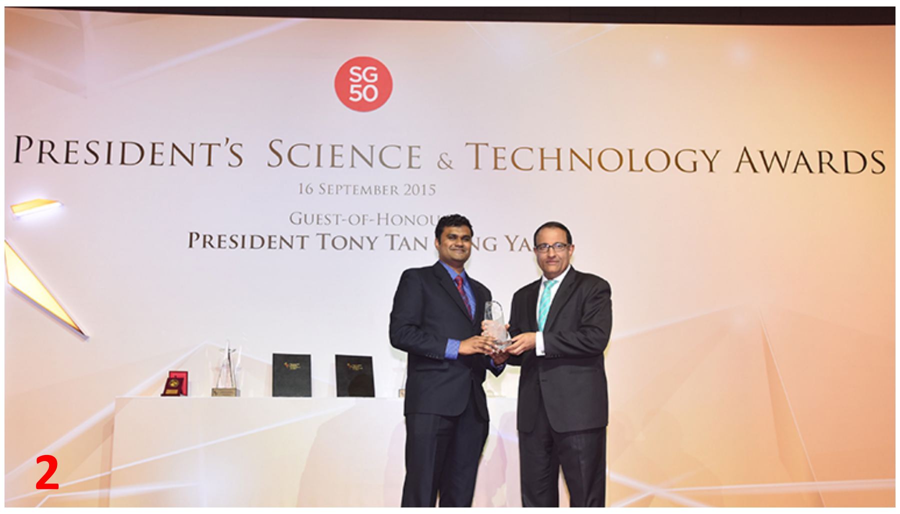
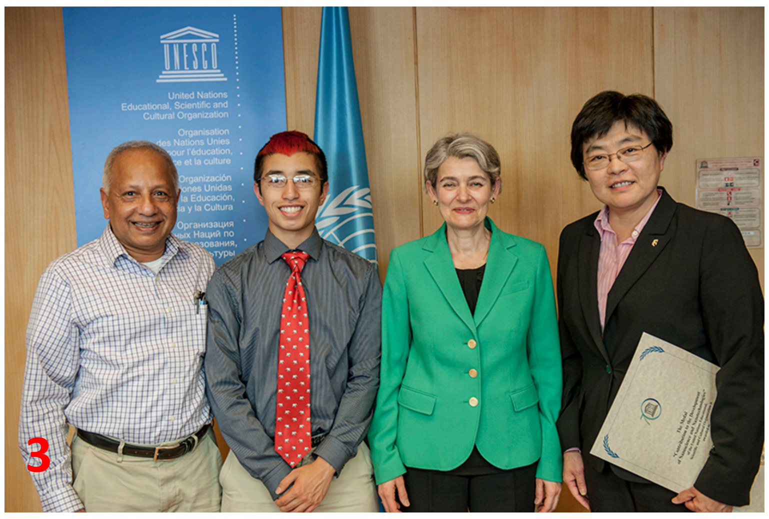
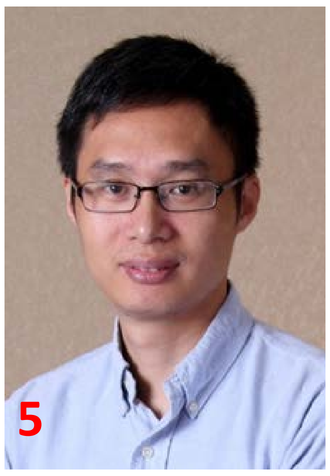


Figure 11: **Schematic of coloured solar modules with HCG fabricated on PV cells**

Awards







1. Professor Junqiao Wu of the Materials Science and Engineering department at the University of California, Berkeley has been awarded the Presidential Early Career Award for Scientists and Engineers (PECASE) 2015.

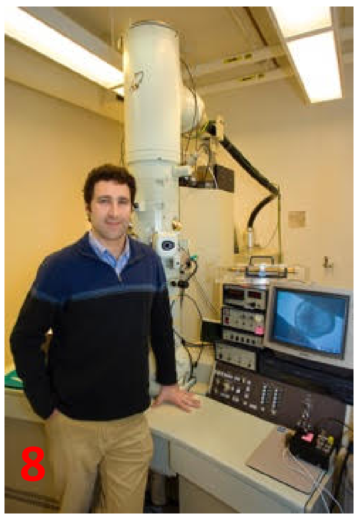
2. Professor Nripan Mathews of School of Materials Science and Engineering at Nanyang Technological University was awarded the Young Scientist Award at the President's Science and Technology Awards ceremony 2015.

3. UNESCO Director-General Irina Bokova presented the UNESCO Medal "For the Development of Nanoscience and Nanotechnologies" to Professor Constance Chang- Hasnain at UNESCO Headquarters on 10 April 2015.

4. Professor Nripan Mathews of School of Materials Science and Engineering and Professor Sum Tze Chien of School of Physical and Mathematical Sciences were awarded the Nanyang Award for Research Excellence,2015.

5. Professor Chen Xiaodong of School Material Science and Engineering of Nanyang Technological University was awarded both the: Small Young Innovator Award, 2015 and The Lubrizol Young Materials Science Investigator Award, 2015.

6 Professors Sum Tze Chien of the School of Physical and Mathematical Sciences at Nanyang Technological University has been awarded Chemical Society of Japan Distinguished Lectureship Award, 2015.



7. Professor Junqiao Wu of the Materials Science and Engineering department at the University of California, Berkeley has been awarded the 2015 Outstanding Alumni Award, Peking University China.

8. Professor Andrew Minor of the Materials Science and Engineering department at University of California, Berkeley has been awarded the Burton Medal 2015 from the Microscopy Society of America.

9. Professor Loh Kian Ping of the Chemistry department at National University of Singapore was awarded the Young Scientist Award at the President's Science and Technology Awards ceremony 2014.

10. Professors Sum Tze Chien of the School of Physical and Mathematical Sciences at Nanyang Technological University has been awarded the 2014 IPS World Scientific Medal and Prize for Outstanding Physics Research.

11. Professor Loh Kian Ping of the Chemistry department at National University of Singapore was awarded the ACS NANO Lectureship,2013.

12. Professor Haimei Zheng of the Materials Science and Engineering department at University of California, Berkeley has been awarded the Lawrence Berkeley National Laboratory Director's Award 2013 for Scientific Achievement for her work on liquid-cell TEM and broad scientific accomplishments.

News and Outreach

THE SUNDAY TIMES, 19 APR 2015, PAGE 43

[science]

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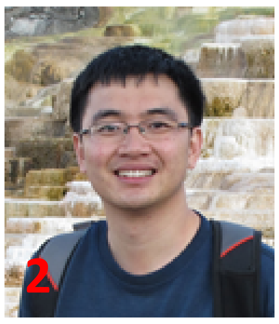
April 19, 2015 thesundaytimes

Man-made crystals – the next wonder material?

Perovskites can be put to many uses and could revolutionise solar power industry

Feng Zengkun

MATERIAL ADVANTAGES



NEWS

1. Assistant Professor Nripan Mathews of the Materials Science and Engineering department and Associate Professors Sum Tze Chien of the Physics department at Nanyang Technological University appeared in an article in The Sunday Times, 19 April 2015. In the article they discussed the new organic – inorganic perovskite that could revolutionize the solar power industry.

2. Former SinBeRISE postdoctoral fellow Dr. Kia Liu, working for Prof Junqiao Wu of the Materials Science and Engineering department at UC Berkeley, has accepted a position as Associate Professor in the School of Materials Science and Engineering at Tsinghua University, Beijing China.

Outreach

3. Prof. Nripan Mathews of the Materials Science and Engineering (MSE) department of Nanyang Technology University visited UC Berkeley and gave the MSE department colloquium. The title of the talk Perovskite Solar Cells: Towards New Materials and New Applications. The goal of this visit was to increase visibility of SinBeRISE research. Prof. Mathews also gave talks at:

- University of California, Davis
- University of California, Los Angeles
- California Institute of Technology
- University of California, Santa Barbara

4. SinBeRISE hosted approximately 30 students from the Asia Nano Forum to the CREATE facility for lab tours and talks about how nanotechnology plays a role in solar energy.

5. Twenty-two students from the Beijing University of Chemical Technology spent the day at SinBeRISE. They heard lectures about solar energy and SinBeRISE research. The students were given lab tours and engaged in a Q&A session about research and applying for graduate school in both the US and Singapore. SinBeRISE has hosted students from Beijing University of Chemical Technology each of the last two years.

6. Showcased our work at Singapore International Energy Week (SIEW) through the panel set up at the entrance of the event. We also engaged some of the ministers (VIP tours) as well as some student (Youth tours) to know more about SinBerBEST and SinBeRISE program.

7. Dr. Matthew Sherburne hosted a visit from Professor Rinlee Butch M. Cervera of the Materials Science and Engineering department at the University of the Philippines, Dilliman, his research group and other visitors from the University of the Philippines to discuss materials science research in renewable energy.

Collaborations/Industry Partners

Dyesol LTD

Dyesol is an Australian company with presence worldwide working on new generation solar cells, including dye-sensitized solar cells and perovskite solar cells. The company develops and distributes material and equipment for device fabrication, as well as functional solar cells. Our collaboration can be summarized within the frame of three projects:

- **Project title: Development of industrially scalable and commercially feasible solutions for solid state dye-sensitized solar cells and variants**

  Description: This project focused on the development of large area solid state solar cells based on perovskites and dye absorbers. The objec-tives included the development of printing methods for the deposition of electron and hole transporting materials.

- **Project title: Lead-free perovskites for photovoltaic applications & scale-up processes**

  Description: This collaboration can be divided in two parts. The first one, lead-free perovskites for photovoltaic applications, focuses on the development of alternative materials for light harvesting. The second part of the collaboration aims the development of processes for large area deposition of perovskites.

- **Project title (proposed): Perovskite-based building integrated photovoltaics: Glass-to-glass façade modules (View Glass)**

  Description: The objective of this proposal is to develop large area solar cells suitable for building integration. In particular, the stability of the materials and the development of semi-transparent electrodes will be studied.

RDECOM (US Army)

RDECOM (U.S. Army Research, Development and Engineering Command) creates, integrates and delivers technology-enabled solutions to the US Army. The institution has international collaborations with indus-trial and academic partners, with special interest in new generation solutions. Our collaboration in the field of perovskite solar cells covers the development of high-power devices, as well as the design of scalable and stable solar cells. The two common projects are:

- **Project title: Perovskite solar cells: investigations of fundamental limitations. Towards scalability**

  Description: This project aims the fabrication of 1W photovoltaic device based on perovskite absorber. This objective requires the scale-up of the laboratory-scale solar cells (such as: total active area: 100 cm2 for 10% efficiency solar cell under AM1.5G illumination). The planed work comprises the identification of the main scale-up problems and the design of suitable device architectures.

- **Project title (proposed): Hole-conductor-free carbon based perovskite solar cells with enhanced ambient stability**

  Description: This proposal targets the development of polymer-free perovskite solar cells. The use of mesoporous carbon as hole transport-ing material and hole contact will be analyzed from the fundamental point of view. New devices architectures and the correspondent fabrica-tion processes will be designed and implemented. Special attention will be paid to the long-term stability of the solar cells.

Johnson Matthey

Johnson Matthey is a British multinational specialist in chemicals and sustainable technologies. The company develops and manufactures a wide range of high technology products, namely emission control catalyst, precious metal chemicals and catalyst, catalysts and catalyzed components for use in fuel cells and battery materials.

- **Project title: Investigating the materials for perovskite based solar cells**

  Description: The objective of this project is to test the JM-supplied materials for the perovskite based solar cell application, as well check the feasibility towards the commercialization.

BASF

This German multinational is the largest chemical producer in the world. BASF supplies products to a wide variety of areas, such as biotechnological and chemical industries.

- Project title: Chemical synthesis and characterization

  Amount of support: 3x rotary evaporator, 1x Suntest CPS, 6x Hot Plates, 1x Sonicator, 1x Automatic diamond cutter for TEM/FESEM sample preparation, 1x UV lamp for TLC, 100 different chemicals. Estimated value: 120,000 SGD (BASF’s contribution, equipment and chemicals)

  Description: The company has provided equipment and materials for synthesis and characteriza-tion. These will be used for the development of large area perovskite solar cells.

Labs & Facilities

The primary SinBeRISE research facilities are housed at the CREATE campus with additional labs housed at the three participating universities and the Lawrence Berkeley National Laboratory. These facilities allow the researchers the ability to grow and characterize new materials systems for solar energy applications.

Processing Laboratory

(CREATE Research Wing #04-01)

The chemical labs at SinBeRISE premises will host all key equipment necessary for synthesizing and evaluating a wide variety of functional electronic materials key for the realization of solar cells and photoelectrochemical processes. Besides facilities necessary for synthesis of oxide and chalcogenide nanomaterials, extensive organic synthesis facilities is set to allow the preparation of novel multidimensional halide perovskite precursors, hole transport layers and conjugated polyelectrolytes. Key equipment assembled include:

Multifunctional glovebox system with integrated thermal evaporator, spincoater and solar simulator: For preparation of novel multifunctional perovskites, formation of functional films through spin coating as well as fabrication and testing of photovoltaic devices in completely inert atmospheres to understand key aspects that affect their optoelectronic behavior.

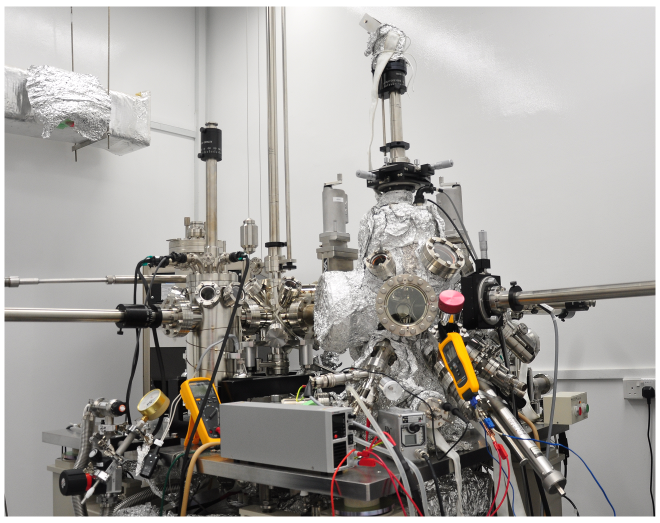
Complete photoelectrochemical characterization systems: Clear and accurate analysis of photoreaction products are enabled by custom-made photocatalytic reactor systems which incorporate an in-line gas chromatography system.

Advanced device characterization: Electrical and optical small amplitude perturbation techniques for the dynamic performance characterization of photovoltaic devices and photoelectrodes.

Scaleup line for printed perovskite solar cells: In order to demonstrate large scale halide perovskite solar cells, multiple large area screen printers and slot-die coaters to enable serial printing of every single layer of the solar cell in ambient conditions

Low Temperature Scanning Tunneling Microscope (STM)

(CREATE Tower #B-03)

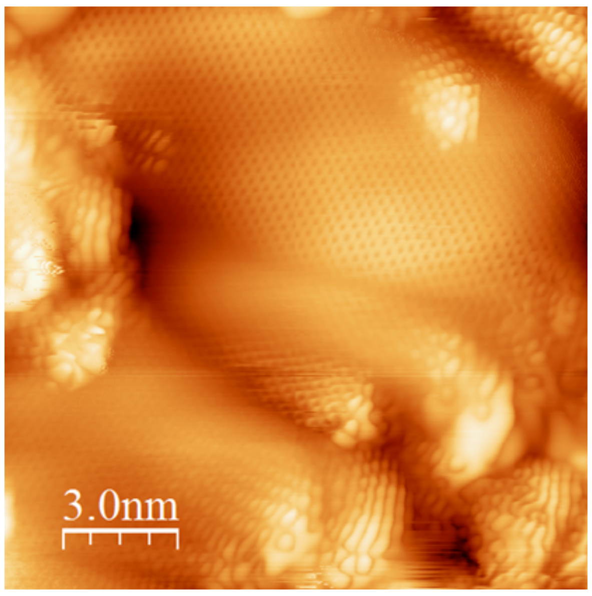


The SinBeRISE characterization lab specializes on comprehensive measurements of electronic properties of the novel materials, which are developed and produced within the SinBeRISE project. In particular, the characterization lab investigates novel two-dimensional (2D)-materials and thin films grown in the SinBeRISE molecular beam epitaxy (MBE) and pulsed laser deposition (PLD) laboratory by employing vari-able temperature electronic transport and scanning probe microscopy techniques.

Electrical transport properties

For the specific technical applications of thin films and 2D-materials, for example as transparent electrodes in photovoltaic cells, comprehensive measurements of the electronic properties are required. While a simple room temperature conductance measurement may suffice to produce a figure of merit, this does not provide a detailed understanding of the transport mechanism and the role of atomic scale defects and material interfaces. To derive compre-hensive information temperature and gate dependent conductance measurements of thin film devices are required.

The SinBeRISE characterization lab offers (soon) two variable temperature set-ups with state-of-the-art electronic measurement equipment. The test-setups offer a wide temperature range from 0.5K – 400K and allow multiple samples to be measured simultaneously.



CVD-Graphene with molecule

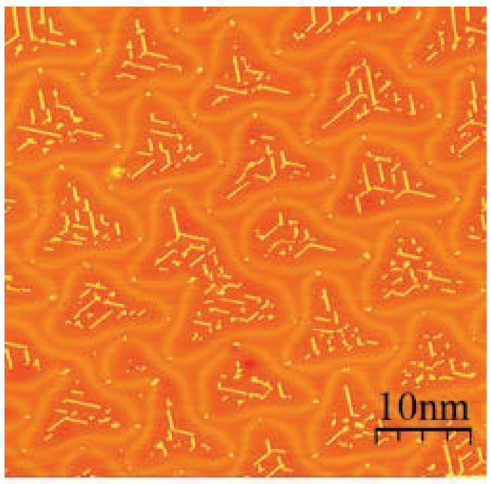
Scanning Probe Microscopy

The role of atomic defects is fundamental to the functionality of semi-conductors. The type and functionality of defects in novel materials systems such as two-dimensional semi-conduct-ing transition-metal dichalcogeneides (TMDCs) produced by SinBeRISE MBE is not sufficiently known and calls for investigation on the atomic scale.

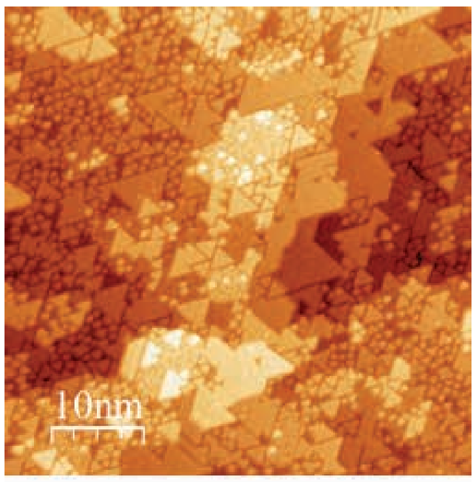
The SinBeRISE characterization lab provides two low temperature scanning probe systems with unique capabilities to investigate the electronic properties on true atomic level. One system is a dedicated scanning tunneling microscope (STM) for atomic scale imaging and spectroscopy. The second system, a scanning single electron transistor microscope (scanning SET) allows the imaging of individual localized electronic states in encapsulated devices.

The 3He-UHV STM (Unisoku) offers ultra-low vibrational environment for tunneling spectroscopy on single atoms. An acoustically shielded lab-space, air-cushioned vibration isolation and low temperature ensure a vibrational level in the pico-meter regime. A separate in-situ growth-chamber and sample-transfer mechanism ensure ultra-clean surfaces. Novel multi- contact sample holders allow for investigation of multi-terminal devices.

The unique advantages of the scanning SET system are that it allows the investigation of individual electrons (localized states) in 2D-materials, which are encapsulated by a protection layer. This enables the investigation of systems, which are closer to actual devices compared to the STM-system



Selenium 1D-nanowires



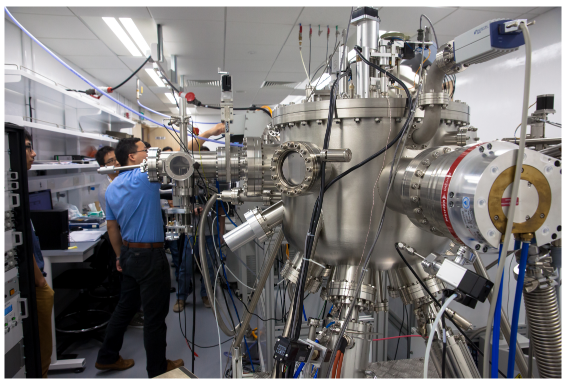
2D-NbSe$_{22}$ nano-islands

Molecular Beam Epitaxy (MBE)

(CREATE Tower #B-07)

At the CREATE facility two Molecular Beam Epitaxy (MBE) systems have been commissioned for the growth of 2-D materials with high optical conductivity. The materials systems that are currently being expolored are the chalcogenides, which are sulfides, selenides and tellurides. Specifically the compounds MoS2, WSe2, and MoSe3 have been grown and are being studied for possible application in photovoltaic cells.

The team is exploring the interfacing of these 2-D materials with photovoltaic materials to enhance the performance of thin film solar cells. The glove box is for the deposition of perovskite solar cell material by thermal evaporation and the processing of films



Joint Center for Artificial Photosynthesis (JCAP)

(Lawrence Berkeley National Laboratory)

World class experimental and theory capabilities are available to SinBeRISE via its interactions with UC Berkeley and with Lawrence Berkeley National Laboratory (LBNL). Notably, LBNL is a major partner in the DOE-funded Joint Center for Artificial Photosynthesis (JCAP), which is the USA's largest dedicated solar fuels program.

JCAP has complete facilities for inorganic synthesis employing both chemical routes and thin film deposition. The facilities of LBNL's Molecular Foundry can also be employed for nanofabrication and characterization including world-leading transmission electron microscopy at the National Center for Electron Microsopy (NCEM). Surface science char-acterization capabilities are extensive and include a number of in-situ x-ray spectroscopy techniques performed at LBNL's Advanced Light Source (ALS) and at the Stanford Synchrotron Lightsource (SSRL). JCAP has deep expertise in ab-initio calculations of electronic structure and interface properties and in the continuum modeling and evaluation of complete solar fuel generating systems.

National Center for Electron Microscopy (NCEM)

(Lawrence Berkeley National Laboratory)

The National Center for Electron Microscopy (NCEM) in the Molecular Foundry is a Department of Energy (DOE) sponsored nanoscience user facility. NCEM has 8 dedicated Transmission Electron Microscopes and one FIB that cover a wide range of state-of-the-art or unique capabilities, including instruments that are specialized for high resolution, analytical, soft materials, and in situ experiments. Among the 8 TEMs there are two double-corrected aberration-corrected microscopes, including TEAM 0.5 which is a double-Cs corrected FEI Titan STEM/TEM and TEAM I that was the world's first Cs and Cc corrected electron microscope. In addition to world-leading instrumentation, the NCEM staff provides expertise in high-resolution imaging, instrumentation, analytical spectroscopy, data analysis, and image simulation and in-situ characterization of a wide variety of materials.

Energy Research Institute @NTU (ERI@N)

(Nanyang Technological University)

Seeks to be a leading research institute for innovative energy solutions and a center of excellence for advanced research, development, and demonstration of innovative energy solutions with global impact. The Solar Cell fabrication facilities are housed in a Class 100k clean room with a floor area of 400 sq m and include large area processing tools such as screen printers, automatic sprayer as well as chemical vapor deposition (CVD) / sputtering and complete device fabrication tools. Solar cell characterization tools include solar simulators, IPCE, as well as various electrochemical characterization tools.

National University of Singapore Nanoscience and Nanotechnology Institute (NUSNNI)

(National University of Singapore)

The National University of Singapore Nanoscience and Nanotechnology Institute (NUSNNI) houses state of the art equipment in all its respective laboratories and affiliated research institutes and thus enable its researcher staff and students to carry out cutting edge research activities. The facilities accessible by SinBeRISE researchers include the Singapore Synchrotron Light Source (SSLS).

The facilities at NUSNNI include the ability to characterize the photovoltaic characterization, photoluminescence lab, lithography lab, Optical characterization lab, spintronic & transport measurement lab, and the ability to characterize the electrical properties under large magnetic field and large temperature range 1.9 – 400 K.

Computational and Software Resources

(University of California, Berkeley)

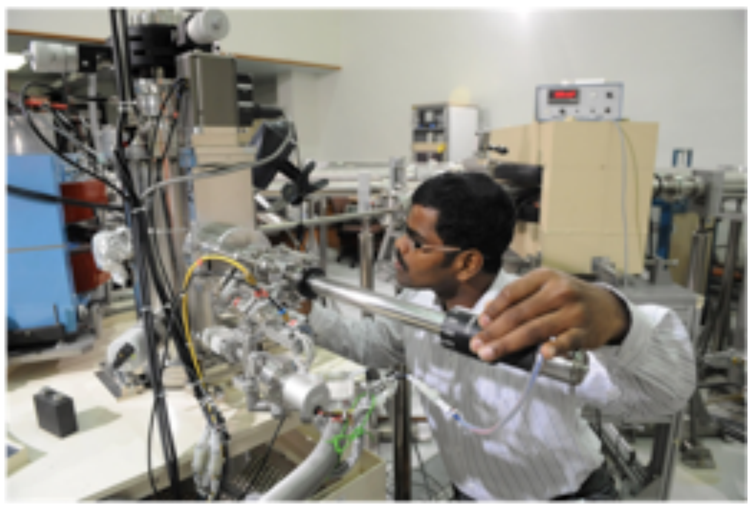
Professor Asta’s computational group develops and integrates software tools to support the application of high-throughput computing, which is being used to enable discovery and design of new photovoltaic materials in Thrust 1. These tools run on a suite of computing clusters maintained by his group at UC Berkeley.

Computational resources available for SinBeRISE research at Berkeley include roughly 600 computing cores in these clusters were purchased with non-federal funds pro-vided by UC Berkeley, and are available to support SinBeRISE research. These local computing resources are augmented by computer time on national supercomputers available through the XSEDE (Extreme Science and Engineering Discovery Environ-ment, www.xsede.org) program, which makes available supercomputing resources to support open research intended for publication.

The computing resources described above are used in SinBeRISE research primarily to support high-throughput and large-scale calculations based on electronic density-functional theory (DFT). For these calculations we make use primarily of the VASP (Vienna ab-initio Simulation Package), a highly developed commercial code for performing DFT calculations for solids, liquids and molecules. To enable high-throughput computations, being performed to guide materials discovery efforts within Thrust 1, the DFT VASP software is being applied in combination with a unique set of open-source software tools developed through the Materials Project effort (www.materialsproject.org) at the Lawrence Berkeley National Laboratory.

Center for Ion Beam Applications (CIBA)

(National University of Singapore, Department of Physics)



The Centre for Ion Beam Applications (CIBA) is a multi-disciplinary research centre, the goals of which are to develop new technologies based on fast protons and ions, and simultaneously to undertake research into novel applications where proton or ion based technologies provide a unique cutting edge advantage. Because of the advanta-geous physical properties of protons, proton technologies have the potential to super-sede the ubiquitous electron based technologies (e.g. electron microscopy, electron lithography - ebeam writing, electron spectroscopy etc.).

CIBA has the ability to produce nano and micro scale structures, which are used to screen catalytic materials.

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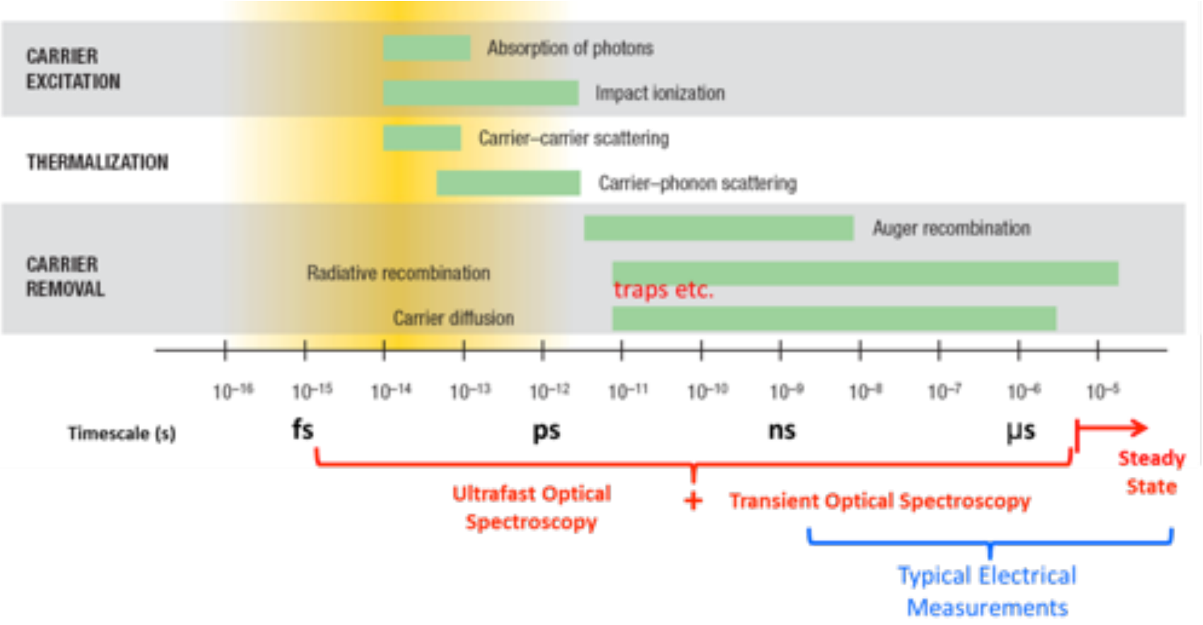
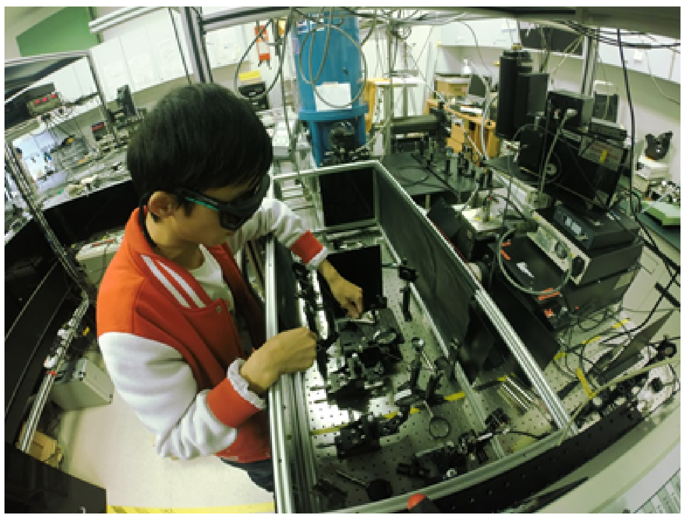


Transient Photoluminescence



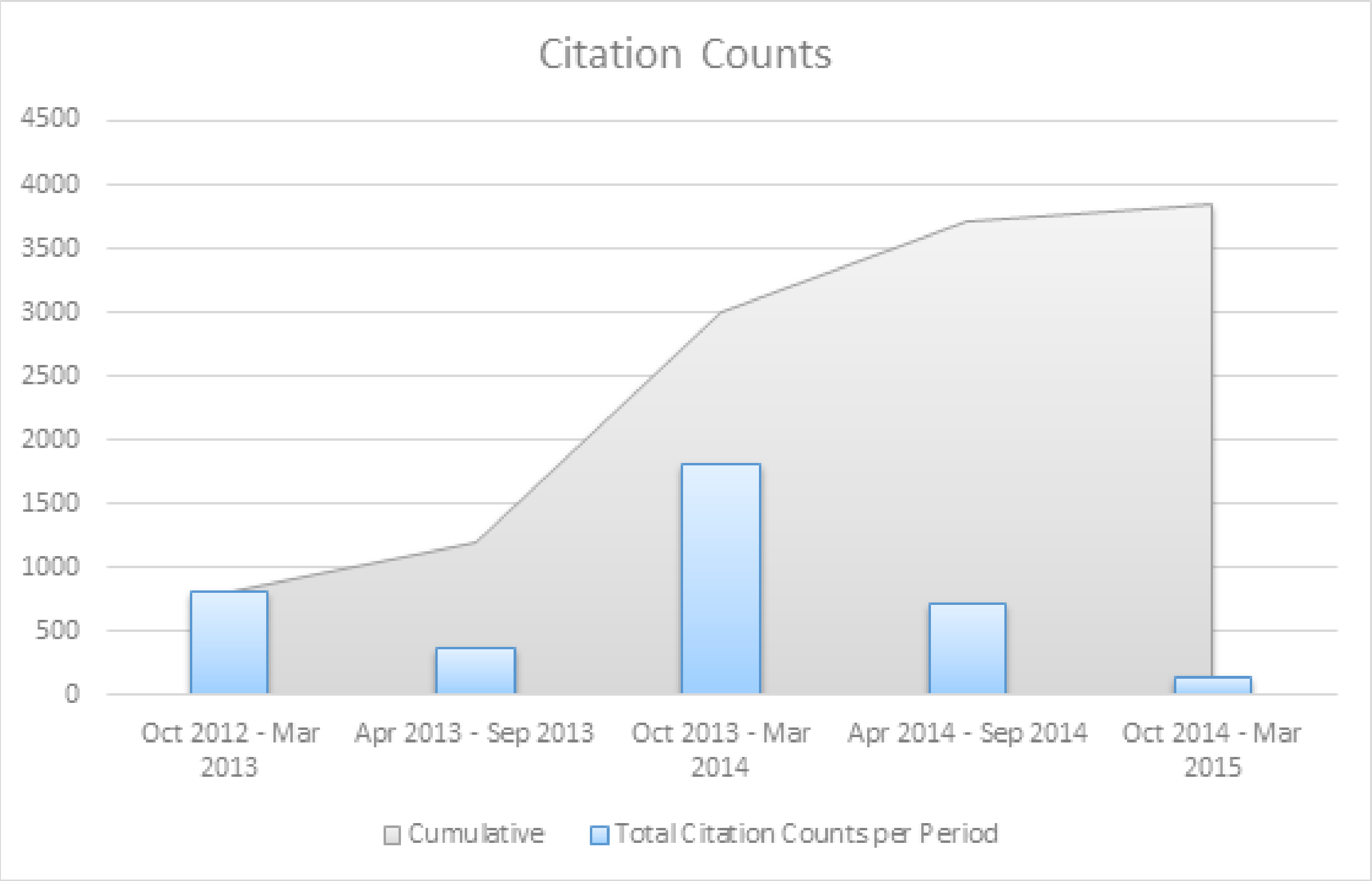
In time-resolved photoluminescence experiments, the spectral and temporal evolution of emissive species in a photo-excited material system can be measured. The emission, or photoluminescence, of the excited material comprises of a range of wavelengths that is spectrally resolved by a monochromator, and passed into a coupled streak camera system to resolve the time-dependent photoluminescence.

Transient Absorption Spectroscopy

Transient absorption spectroscopy, also known as pump-probe spectroscopy, uses two ultrashort pulses: the first being a pump pulse which is used to first excite and perturb the material system; and the second is a weaker, delayed probe pulse which monitors the excited state of the material system after a time delay between the pump and probe pulses. Utilising two pulses has an added benefit: it allows the probing of dark states, or non-radia-tive states, which are common electron or hole loss channels.

With such temporal resolution, we are able to study photo-induced charge transfer processes of pristine materials or heterojunctions down to the femtosecond regime. For example, by pumping the perovskite active material across the bandgap, we can study electron and hole transfer or separation, and subsequent relaxation processes. This allows us to characterise and estimate the efficiency of charge acceptors to improve and push for even higher solar power conversion efficiencies, and to leverage on its light emissive capabilities.

Publications



Submitted

G. Xing, M. H. Kumar, W. K. Chong, X. Liu, Y. Cai, H. Ding, M. Asta, M. Graetzel, S. Mhaisalkar, N. Mathews and T. C. Sum, “Near Infrared Lasing from Solution-Processed Lead-Free Perovskites,” Nature Photonics (submitted).

T. C. Asmara, Y. Zhao, M. A. Majidi, C. T. Nelson, M. C. Scott, Y. Cai, D. Wan, D. Schmidt, M. Yang, P. E. Trevisanutto, M. R. Motapothula, M. B. H. Breese, M. Sherburne, M. Asta, A. Minor, T. Venkatesan, and A. Rusydi, “Tunable and strongly-correlated plasmons in wide band-gap oxides,” Science (submitted).

In Review

Wen Fan, Xi Zhu, Feng Ke, Yabin Chen, Kaichen Dong, Jie Ji, Bin Chen, Sefaattin Tongay, Joel W. Ager, Kai Liu, Haibin Su, and Junqiao Wu, Vibrational spectrum renormalization in two-dimensional heterostructures by enforced interlayer coupling, Phys. Rev. B, (in review).

Accepted (In Press)

T. Krishnamoorthy, H. Ding, C. Yan, W. L. Leong, T. Baikie, Z. Zhang, M. Sherburne, S. Li, M. Asta, N. Matthews, and S. B. Mhaisalkar, “Lead-free Germanium Iodide Perovskite Materials for Photovoltaic Application,” J. Mater. Chem. A (accepted).

1 October 2014 – 31 March 2015

Gurudayal, Dharani Sabba, Hemant Kumar Mulmudi, Lydia H. Wong, James Barber, Michael Grätzel, and Nripan Mathews, “Perovskite-Hematite Tandem Cells for Efficient Overall Solar Driven Water Splitting,” Nano Letters, vol. 15, pp 3833-3839, 2015.

J. Suh, T.-E. Park, D.-Y. Lin, D. Fu, J. Park, H. J. Jung, et al., "Doping against the Native Propensity of MoS2: Degenerate Hole Doping by Cation Substitution," Nano Letters, vol. 14, pp. 6976-6982, 2014.

J. Y. Chen, Hong Bin: Miao, Jianwei: Wang, Hsin-Yi: Liu, Bin, "Thermodynamically Driven One-Dimensional Evolution of Anatase TiO2 Nanorods: One-Step Hydrothermal Synthesis for Emerging Intrinsic Superiority of Dimensionality," Journal of the American Chemical Society, vol. 136, pp. 15310-15318, 2014.

R. W. Chen, Hsin-Yi: Miao, Jianwei: Yang, Hongbin: Liu, Bin, "A flexible high-performance oxygen evolution electrode with three-dimensional NiCo2O4 core-shell nanowires," Nano Energy, vol. 11, pp. 333-340, 2015.

J. Y. Hong, Shengming: Pan, Yunxiang: Han, Jianyu: Zhou, Tianhua: Xu, Rong, "Porous carbon nitride nanosheets for enhanced photocatalytic activities," Nanoscale, vol. 6, pp. 14984-14990, 2014.

M. A. T. Hossain, Zhang: Keat, Lee Kian: Xianglin, Li: Prabhakar, Rajiv R.: Batabyal, Sudip K.: Mhaisalkar, Subodh G.: Wong, Lydia H., "Synthesis of Cu(In,Ga)(S,Se)2 thin films using an aqueous spray-pyrolysis approach, and their solar cell efficiency of 10.5%," Journal of Materials Chemistry A, vol. 3, pp. 4147-4154, 2015.

X. L. Lang, Wan Ru: Zhao, Jincai: Chen, Xiaodong, "Synergistic photocatalytic aerobic oxidation of sulfides and amines on TiO2 under visible-light irradiation," Chemical Science, vol. 6, pp. 1075-1082, 2015.

X. H. Liu, Son Tung: Zhang, Qing: de la Mata, Maria: Magen, César: Arbiol, Jordi: Sum, Tze Chien: Xiong, Qihua, "Whispering Gallery Mode Lasing from Hexagonal Shaped Layered Lead Iodide Crystals," ACS Nano, vol. 9, pp. 687-695, 2015.

J. T. Luo, S. David: Steier, Ludmilla: Schreier, Marcel: Mayer, Matthew T.: Fan, Hong Jin: Grätzel, Michael, "Solution Transformation of Cu2O into CuInS2 for Solar Water Splitting," Nano Letters, vol. 15, pp. 1395-1402, 2015.

R. R. H. L. Prabhakar, Nguyen: Kumar, Mulmudi Hemant: Boix, Pablo P.: Juan, Sun: John, Rohit Abraham: Batabyal, Sudip K.: Wong, Lydia Helena, "Facile Water-based Spray Pyrolysis of Earth-Abundant Cu2FeSnS4 Thin Films as an Efficient Counter Electrode in Dye-Sensitized Solar Cells," ACS Applied Materials & Interfaces, vol. 6, pp. 17661-17667, 2014.

H.-Y. H. Wang, Ying-Ya: Chen, Rong: Chan, Ting-Shan: Chen, Hao Ming: Liu, Bin, "Ni3+-Induced Formation of Active NiOOH on the Spinel Ni–Co Oxide Surface for Efficient Oxygen Evolution Reaction," Advanced Energy Materials, vol. 5, pp. n/a-n/a, 2015.

X. L. Wang, Zhen: Xu, Wenjing: Kulkarni, Sneha A.: Batabyal, Sudip K.: Zhang, Sam: Cao, Anyuan: Wong, Lydia Helena, "TiO2 nanotube arrays based flexible perovskite solar cells with transparent carbon nanotube electrode," Nano Energy, vol. 11, pp. 728-735, 2015.

X. L. Wang, Chihao: Bisht, Ankit: Liu, Xinfeng: Sum, Tze Chien: Chen, Xiaodong: Li, Shuzhou, "Engineering Interfacial Photo-Induced Charge Transfer Based on Nanobamboo Array Architecture for Efficient Solar-to-Chemical Energy Conversion," Advanced Materials, vol. 27, pp. 2207-2214, 2015.

R. W. Wu, Dan Ping: Han, Jianyu: Liu, Hai: Zhou, Kun: Huang, Yizhong: Xu, Rong: Wei, Jun: Chen, Xiaodong: Chen, Zhong, "A general approach towards multi-faceted hollow oxide composites using zeolitic imidazolate frameworks," Nanoscale, vol. 7, pp. 965-974, 2015.

R. W. Wu, Dan Ping: Kumar, Vipin: Zhou, Kun: Law, Adrian W. K.: Lee, Pooi See: Lou, Jun: Chen, Zhong, "MOFs-derived copper sulfides embedded within porous carbon octahedra for electrochemical capacitor applications," Chemical Communications, vol. 51, pp. 3109-3112, 2015.

F.-X. H. Xiao, Sung-Fu: Tao, Hua Bing: Miao, Jianwei: Yang, Hong Bin: Liu, Bin, "Spatially branched hierarchical ZnO nanorod-TiO2 nanotube array heterostructures for versatile photocatalytic and photoelectrocatalytic applications: towards intimate integration of 1D-1D hybrid nanostructures," Nanoscale, vol. 6, pp. 14950-14961, 2014.

F.-X. M. Xiao, Jianwei: Tao, Hua Bing: Hung, Sung-Fu: Wang, Hsin-Yi: Yang, Hong Bin: Chen, Jiazang: Chen, Rong: Liu, Bin, "One-Dimensional Hybrid Nanostructures for Heterogeneous Photocatalysis and Photoelectrocatalysis," Small, vol. 11, pp. 2115-2131, 2015.

G. W. Xing, Bo: Chen, Shi: Chua, Julianto: Yantara, Natalia: Mhaisalkar, Subodh: Mathews, Nripan: Sum, Tze Chien, "Interfacial Electron Transfer Barrier at Compact TiO2/CH3NH3PbI3 Heterojunction," Small, pp. n/a-n/a, 2015.

J. C. Yin, Daniele: Krishna, Anurag: Chen, Shi: Mathews, Nripan: Grimsdale, Andrew C.: Soci, Cesare, "Interfacial Charge Transfer Anisotropy in Polycrystalline Lead Iodide Perovskite Films," The Journal of Physical Chemistry Letters, vol. 6, pp. 1396-1402, 2015.

Q. H. Zhang, Son Tung: Liu, Xinfeng: Sum, Tze Chien: Xiong, Qihua, "Room-Temperature Near-Infrared High-Q Perovskite Whispering-Gallery Planar Nanolasers," Nano Letters, vol. 14, pp. 5995-6001, 2014.

W. Z. Zhang, Tianhua: Zheng, Jianwei: Hong, Jindui: Pan, Yunxiang: Xu, Rong, "Water-Soluble MoS3 Nanoparticles for Photocatalytic H2 Evolution," ChemSusChem, vol. 8, pp. 1464-1471, 2015.

T. W. Zhou, Danping: Chun-Kiat Goh, Simon: Hong, Jindui: Han, Jianyu: Mao, Jianggao: Xu, Rong, "Bio-inspired organic cobalt(ii) phosphonates toward water oxidation," Energy & Environmental Science, vol. 8, pp. 526-534, 2015.

A. R. Srivastava, Helene; Saha, Surajit; Pal, Banabir; Kalon, Gopinadhan; Mathew, Sinu; Motapothula, Mallikarjuna; Dykas, Michal; Yang, Ping; Okunishi, Eiji; Sarma, D. D.; Venkatesan, T., "Selective growth of single phase VO2(A, B, and M) polymorph thin films," APL Materials, vol. 3, p. 026101, 2015.

Y. N. Shengyuan, A. Sreekumaran; Ramakrishna, Seeram, "Morphology of the Electrospun TiO2 on the Photovoltaic Properties of CdS Quantum Dot-Sensitized Solar Cells," Journal of Nanoscience and Nanotechnology, vol. 15, pp. 721-725, 2015.

X. G. Yin, Yanjun; Xue, Zhaosheng; Xu, Peng; He, Meng; Liu, Bin, "Performance enhancement of perovskite-sensitized mesoscopic solar cells using Nb-doped TiO2 compact layer," Nano Research, vol. 8, pp. 1997-2003, 2015.

1 April 2014 – 30 September 2014

S. Chen, T. W. Goh, D. Sabba, J. Chua, N. Mathews, C. H. A. Huan, et al., "Energy level alignment at the methylammonium lead iodide/ copper phthalocyanine interface," Apl Materials, vol. 2, 2014.

W. K. Chong, G. C. Xing, Y. Liu, E. L. Gui, Q. Zhang, Q. H. Xiong, et al., "Direct measurement of coherent phonon dynamics in solution-processed stibnite thin films," Physical Review B, vol. 90, 2014.

S. Dharani, H. A. Dewi, R. R. Prabhakar, T. Baikie, C. Shi, D. Yonghua, et al., "Incorporation of Cl into sequentially deposited lead halide perovskite films for highly efficient mesoporous solar cells," Nanoscale, vol. 6, pp. 13854-13860, 2014.

K. Fu, S. S. Lim, Y. Fang, P. P. Boix, N. Mathews, T. C. Sum, et al., "Modulating CH3NH3PbI3 Perovskite Crystallization Behavior Through Precursor Concentration," Nano, vol. 09, p. 1440003, 2014.

S. T. Ha, X. Liu, Q. Zhang, D. Giovanni, T. C. Sum, and Q. Xiong, "Synthesis of Organic–Inorganic Lead Halide Perovskite Nanoplatelets: Towards High-Performance Perovskite Solar Cells and Optoelectronic Devices," Advanced Optical Materials, vol. 2, pp. 838-844, 2014.

J. C. W. Ho, T. Zhang, K. K. Lee, S. K. Batabyal, A. I. Y. Tok, and L. H. Wong, "Spray Pyrolysis of CuIn(S,Se)2 Solar Cells with 5.9% Efficiency: A Method to Prevent Mo Oxidation in Ambient Atmosphere," ACS Applied Materials & Interfaces, vol. 6, pp. 6638-6643, 2014.

J. Hong, W. Zhang, Y. Wang, T. Zhou, and R. Xu, "Photocatalytic Reduction of Carbon Dioxide over Self-Assembled Carbon Nitride and Layered Double Hydroxide: The Role of Carbon Dioxide Enrichment," ChemCatChem, vol. 6, pp. 2315-2321, 2014.

T. M. Koh, S. Dharani, H. Li, R. R. Prabhakar, N. Mathews, A. C. Grimsdale, et al., "Cobalt Dopant with Deep Redox Potential for Organometal Halide Hybrid Solar Cells," ChemSusChem, vol. 7, pp. 1909-1914, 2014.

M. H. Kumar, S. Dharani, W. L. Leong, P. P. Boix, R. R. Prabhakar, T. Baikie, et al., "Lead-Free Halide Perovskite Solar Cells with High Photocurrents Realized Through Vacancy Modulation," Advanced Materials, vol. 26, pp. 7122-7127, 2014.

Z. Li, S. A. Kulkarni, P. P. Boix, E. Shi, A. Cao, K. Fu, et al., "Laminated Carbon Nanotube Networks for Metal Electrode-Free Efficient Perovskite Solar Cells," ACS Nano, vol. 8, pp. 6797-6804, 2014.

X. Liu, B. Wu, Q. Zhang, J. N. Yip, G. Yu, Q. Xiong, et al., "Elucidating the Localized Plasmonic Enhancement Effects from a Single Ag Nanowire in Organic Solar Cells," ACS Nano, vol. 8, pp. 10101-10110, 2014.

J. Luo, J.-H. Im, M. T. Mayer, M. Schreier, M. K. Nazeeruddin, N.-G. Park, et al., "Water photolysis at 12.3% efficiency via perovskite photovoltaics and Earth-abundant catalysts," Science, vol. 345, pp. 1593-1596, 2014.

S. K. Muduli, S. Wang, S. Chen, C. F. Ng, C. H. A. Huan, T. C. Sum, et al., "Mesoporous cerium oxide nanospheres for the visible-light driven photocatalytic degradation of dyes," Beilstein Journal of Nanotechnology, vol. 5, pp. 517-523, 2014.

Y.-x. Pan, H. Zhuang, J. Hong, Z. Fang, H. Liu, B. Liu, et al., "Cadmium Sulfide Quantum Dots Supported on Gallium and Indium Oxide for Visible-Light-Driven Hydrogen Evolution from Water," ChemSusChem, vol. 7, pp. 2537-2544, 2014.

H. Qi, J. Wolfe, D. Wang, H. J. Fan, D. Fichou, and Z. Chen, "Triple-layered nanostructured WO3 photoanodes with enhanced photocurrent generation and superior stability for photoelectrochemical solar energy conversion," Nanoscale, vol. 6, pp. 13457-13462, 2014/09/18 2014.

S. Shukla, N. H. Loc, P. P. Boix, T. M. Koh, R. R. Prabhakar, H. K. Mulmudi, et al., "Iron Pyrite Thin Film Counter Electrodes for Dye-Sensitized Solar Cells: High Efficiency for Iodine and Cobalt Redox Electrolyte Cells," ACS Nano, vol. 8, pp. 10597-10605, 2014.

A. Solanki, B. Wu, T. Salim, E. K. L. Yeow, Y. M. Lam, and T. C. Sum, "Performance Improvements in Polymer Nanofiber/Fullerene Solar Cells with External Electric Field Treatment," Journal of Physical Chemistry C, vol. 118, pp. 11285-11291, 2014.

T. C. Sum and N. Mathews, "Advancements in perovskite solar cells: photophysics behind the photovoltaics," Energy & Environmental Science, vol. 7, pp. 2518-2534, 2014.

J. M. R. Tan, Y. H. Lee, S. Pedireddy, T. Baikie, X. Y. Ling, and L. H. Wong, "Understanding the Synthetic Pathway of a Single-Phase Quarternary Semiconductor Using Surface-Enhanced Raman Scattering: A Case of Wurtzite Cu2ZnSnS4 Nanoparticles," Journal of the American Chemical Society, vol. 136, pp. 6684-6692, 2014.

H. B. Tao, H. B. Yang, J. Chen, J. Miao, and B. Liu, "Biomolecule-assisted synthesis of carbon nitride and sulfur-doped carbon nitride heterojunction nanosheets: An efficient heterojunction photocatalyst for photoelectrochemical applications," Beilstein Journal of Nanotechnology, vol. 5, pp. 770-777, 2014.

T. T. Trang Pham, T. M. Koh, K. Nonomura, Y. M. Lam, N. Mathews, and S. Mhaisalkar, "Reducing Mass-Transport Limitations in Cobalt-Electrolyte-Based Dye-Sensitized Solar Cells by Photoanode Modification," ChemPhysChem, vol. 15, pp. 1216-1221, 2014.

C. Wei, L. Yu, C. Cui, J. Lin, C. Wei, N. Mathews, et al., "Ultrathin MnO2 nanoflakes as efficient catalysts for oxygen reduction reaction," Chemical Communications, vol. 50, pp. 7885-7888, 2014.

F. X. Xiao, J. Miao, H. Y. Wang, H. Yang, J. Chen, and B. Liu, "Electrochemical construction of hierarchically ordered CdSe-sensitized TiO2 nanotube arrays: towards versatile photoelectrochemical water splitting and photoredox applications," Nanoscale, vol. 6, pp. 6727-37, 2014.

F.-X. Xiao, S.-F. Hung, J. Miao, H.-Y. Wang, H. Yang, and B. Liu, "Metal-Cluster-Decorated TiO2 Nanotube Arrays: A Composite Heterostructure toward Versatile Photocatalytic and Photoelectrochemical Applications," Small, pp. n/a-n/a, 2014.

G. Xing, N. Mathews, S. S. Lim, N. Yantara, X. Liu, D. Sabba, et al., "Low-temperature solution-processed wavelength-tunable perovskites for lasing," Nature Materials, vol. 13, pp. 476-480, 2014.

H. B. Yang, J. Miao, S.-F. Hung, F. Huo, H. M. Chen, and B. Liu, "Stable Quantum Dot Photoelectrolysis Cell for Unassisted Visible Light Solar Water Splitting," ACS Nano, vol. 8, pp. 10403-10413, September 30, 2014.

X. Zeng, K. F. Tai, T. Zhang, C. W. J. Ho, X. Chen, A. Huan, et al., "Cu2ZnSn(S,Se)(4) kesterite solar cell with 5.1% efficiency using spray pyrolysis of aqueous precursor solution followed by selenization," Solar Energy Materials and Solar Cells, vol. 124, pp. 55-60, 2014.

M. I. R. Dar, F. Javier; Xue, Zhaosheng; Liu, Bin; Ahmad, Shahzada; Shivashankar, Srinivasrao A.; Nazeeruddin, Mohammad Khaja; Grätzel, Michael, "Photoanode Based on (001)-Oriented Anatase Nanoplatelets for Organic–Inorganic Lead Iodide Perovskite Solar Cell," Chemistry of Materials, vol. 26, pp. 4675-4678, 2014.

Z. L. Huang, Z. Q.; Yang, M.; Zeng, S. W.; Annadi, A.; Lü, W. M.; Tan, X. L.; Chen, P. F.; Sun, L.; Renshaw Wang, X.; Zhao, Y. L.; Li, C. J.; Zhou, J.; Han, K.; Wu, W. B.; Feng, Y. P.; Coey, J. M. D.; Venkatesan, T.; Ariando,, "Biaxial strain-induced transport property changes in atomically tailored SrTiO3- based systems," Physical Review B, vol. 90, p. 125156, 2014.

F. J. Li, James Robert; Wang, Xingzhu; Fan, Li; Koh, Zhen Yu; Yu, Hao; Yan, Lei; Wang, Qing, "Influence of Ionic Liquid on Recombination and Regeneration Kinetics in Dye-Sensitized Solar Cells," The Journal of Physical Chemistry C, vol. 118, pp. 17153-17159, 2014.

L. Z. Li, Peining; Peng, Shengjie; Srinivasan, Madhavi; Yan, Qingyu; Nair, A. Sreekumaran; Liu, Bin; Samakrishna, Seeram, "Controlled Growth of CuS on Electrospun Carbon Nanofibers as an Efficient Counter Electrode for Quantum Dot-Sensitized Solar Cells," The Journal of Physical Chemistry C, vol. 118, pp. 16526-16535, 2014.

S. A. J. S. C. J. L. S. M. M. B. H. B. T. Venkatesan, "Nanoscale lithography of LaAlO 3 /SrTiO 3 wires using silicon stencil masks," Nanotechnology, vol. 25, p. 445301, 2014.
1 October 2013 – 31 March 2014

P. P. Boix, K. Nonomura, N. Mathews, and S. G. Mhaisalkar, "Current progress and future perspectives for organic/inorganic perovskite solar cells," Materials Today, vol. 17, pp. 16-23, 2014.

S. Dharani, H. K. Mulmudi, N. Yantara, T. Pham Thi Thu, N. G. Park, M. Graetzel, et al., "High efficiency electrospun TiO2 nanofiber based hybrid organic-inorganic perovskite solar cell," Nanoscale, vol. 6, pp. 1675-1679, 2014 2014.

H. Ge, L. Hai, R. R. Prabhakar, L. Y. Ming, and T. Sritharan, "Evolution of nanoplate morphology, structure and chemistry during synthesis of pyrite by a hot injection method," Rsc Advances, vol. 4, pp. 16489-16496, 2014.

C. K. S. Goh, Y. Wang, J. Hong, and R. Xu, "Carbon Nanospheres-A Dark Support for Effective Loading of Pt Catalyst and Protection of Dye Sensitizer in Photocatalytic Hydrogen Evolution," Science of Advanced Materials, vol. 5, pp. 1658-1666, 2013.

J. Hong, Y. Wang, Y. Wang, W. Zhang, and R. Xu, "Noble-Metal-Free NiS/C3N4 for Efficient Photocatalytic Hydrogen Evolution from Water," Chemsuschem, vol. 6, pp. 2263-2268, 2013.

T. M. Koh, K. Fu, Y. Fang, S. Chen, T. C. Sum, N. Mathews, et al., "Formamidinium-Containing Metal-Halide: An Alternative Material for Near-IR Absorption Perovskite Solar Cells," The Journal of Physical Chemistry C, 2013.

T. Krishnamoorthy, F. Kunwu, P. P. Boix, H. Li, T. M. Koh, W. L. Leong, et al., "A swivel-cruciform thiophene based hole-transporting material for efficient perovskite solar cells," Journal of Materials Chemistry A, vol. 2, pp. 6305-6309, 2014.

S. A. Kulkarni, T. Baikie, P. P. Boix, N. Yantara, N. Mathews, and S. Mhaisalkar, "Band-gap tuning of lead halide perovskites using a sequential deposition process," Journal of Materials Chemistry A, vol. 2, pp. 9221-9225, 2014.

M. H. Kumar, N. Yantara, S. Dharani, M. Graetzel, S. Mhaisalkar, P. P. Boix, et al., "Flexible, low-temperature, solution processed ZnO-based perovskite solid state solar cells," Chemical Communications, vol. 49, pp. 11089-11091, 2013.

J. Y. Lek, G. Xing, T. C. Sum, and Y. M. Lam, "Electron Transport Limitation in P3HT:CdSe Nanorods Hybrid Solar Cells," ACS Applied Materials & Interfaces, vol. 6, pp. 894-902, 2013.

Y. Li, W. Wang, W. R. Leow, B. Zhu, F. Meng, L. Zheng, et al., "Optoelectronics of Organic Nanofibers Formed by Co-assembly of Porphyrin and Perylenediimide," Small, pp. n/a-n/a, 2014.

B. Liu, L.-M. Liu, X.-F. Lang, H.-Y. Wang, X. W. Lou, and E. S. Aydil, "Doping high-surface-area mesoporous TiO2 microspheres with carbonate for visible light hydrogen production," Energy & Environmental Science, 2014.

X. Liu, Q. Zhang, J. N. Yip, Q. Xiong, and T. C. Sum, "Wavelength Tunable Single Nanowire Lasers Based on Surface Plasmon Polariton Enhanced Burstein–Moss Effect," Nano Letters, vol. 13, pp. 5336-5343, 2013.

Y. Liu, K. T. Chua, T. C. Sum, and C. K. Gan, "First-principles study of the lattice dynamics of Sb2S3," Phys Chem Chem Phys, vol. 16, pp. 345-50, 2014.

[Y. Liu, W. Zhang, S. Li, C. Cui, J. Wu, H. Chen, et al., "Designable Yolk–Shell Nanoparticle@MOF Petalous Heterostructures," Chemistry of Materials, vol. 26, pp. 1119-1125, 2013.

J. Lu, K. Zhang, X. F. Liu, H. Zhang, T. C. Sum, A. H. Castro Neto, et al., "Order-disorder transition in a two-dimensional boron-carbon-nitride alloy," Nat Commun, vol. 4, p. 2681, 2013.

F. Meng, Y.-M. Hervault, Q. Shao, B. Hu, L. Norel, S. Rigaut, et al., "Orthogonally modulated molecular transport junctions for resettable electronic logic gates," Nature Communications, vol. 5, 2014.

Z. Niu, L. Liu, L. Zhang, Q. Shao, W. Zhou, X. Chen, et al., "A Universal Strategy to Prepare Functional Porous Graphene Hybrid Architectures," Advanced Materials, vol. 26, pp. 3681-3687, 2014.

S. Sun, T. Salim, N. Mathews, M. Duchamp, C. Boothroyd, G. Xing, et al., "The origin of high efficiency in low-temperature solution-processable bilayer organometal halide hybrid solar cells," Energy & Environmental Science, vol. 7, pp. 399-407, 2014.

D. Wang, P. Kanhere, M. Li, Q. Tay, Y. Tang, Y. Huang, et al., "Improving Photocatalytic H2 Evolution of TiO2 via Formation of {001}–{010} Quasi-Heterojunctions," The Journal of Physical Chemistry C, vol. 117, pp. 22894-22902, 2013.

X. Wang, C. Liow, D. Qi, B. Zhu, W. R. Leow, H. Wang, et al., "Programmable Photo-Electrochemical Hydrogen Evolution Based on Multi-Segmented CdS-Au Nanorod Arrays," Advanced Materials, vol. 26, pp. 3506-3512, 2014.

J. I. Wong, N. Mishra, G. Xing, M. Li, S. Chakrabortty, T. C. Sum, et al., "Dual Wavelength Electroluminescence from CdSe/CdS Tetrapods," ACS Nano, vol. 8, pp. 2873-2879, 2014.

J. Wu, X. Zan, S. Li, Y. Liu, C. Cui, B. Zou, et al., "In situ synthesis of large-area single sub-10 nm nanoparticle arrays by polymer pen lithography," Nanoscale, vol. 6, pp. 749-752, 2014.

F.-X. Xiao, J. Miao, and B. Liu, "Self-assembly of aligned rutile@anatase TiO2 nanorod@CdS quantum dots ternary core-shell heterostructure: cascade electron transfer by interfacial design," Materials Horizons, vol. 1, pp. 259-263, 2014.

F.-X. Xiao, J. Miao, and B. Liu, "Layer-by-Layer Self-Assembly of CdS Quantum Dots/Graphene Nanosheets Hybrid Films for Photoelectrochemical and Photocatalytic Applications," Journal of the American Chemical Society, vol. 136, pp. 1559-1569, 2014.

G. Xing, N. Mathews, S. Sun, S. S. Lim, Y. M. Lam, M. Graetzel, et al., "Long-Range Balanced Electron- and Hole-Transport Lengths in Organic-Inorganic CH3NH3PbI3," Science, vol. 342, pp. 344-347, Oct 18 2013.

G. Yu, X. Liu, G. Xing, S. Chen, C. F. Ng, X. Wu, et al., "Spatially-Resolved Ultrafast Optical Spectroscopy of Polymer-Grafted Residues on CVD Graphene," The Journal of Physical Chemistry C, vol. 118, pp. 708-713, 2014/01/09 2013.

W. Zhang, G. Lu, C. Cui, Y. Liu, S. Li, W. Yan, et al., "A Family of Metal-Organic Frameworks Exhibiting Size-Selective Catalysis with Encapsulated Noble-Metal Nanoparticles," Advanced Materials, pp. n/a-n/a, 2014.

W. Zhang, G. Lu, S. Li, Y. Liu, H. Xu, C. Cui, et al., "Controlled incorporation of nanoparticles in metal-organic framework hybrid thin films," Chemical Communications, vol. 50, pp. 4296-4298, 2014.

J. Zhao, J. I. Wong, J. Gao, G. Li, G. Xing, H. Zhang, et al., "Larger [small pi]-extended anti-/syn-aroylenediimidazole polyaromatic compounds: synthesis, physical properties, self-assembly, and quasi-linear conjugation effect," RSC Advances, vol. 4, pp. 17822-17831, 2014.

W. C. L. Liu, Yeru; Jennings, James Robert; Huang, Hui; Wang, Qing, "Low-cost and flexible poly(3,4-ethylenedioxythiophene) based counter electrodes for efficient energy conversion in dye-sensitized solar cells," Journal of Materials Chemistry A, vol. 2, pp. 10938-10944, 2014.

S. A. Mathew, Anil; Chan, Taw Kuei; Asmara, Teguh Citra; Zhan, Da; Wang, Xiao Renshaw; Azimi, Sara; Shen, Zexiang; Rusydi, Andrivo; Ariando,; Breese, Mark B. H.; Venkatesan, T., "Tuning the Interface Conductivity of LaAlO3/SrTiO3 Using Ion Beams: Implications for Patterning," ACS Nano, vol. 7, pp. 10572-10581, 2013.

S. W. M. Tong, Nimai; Su, Chen Liang; Nalla, Venkatram; Wu, Wenya; Ji, Wei; Zhang, Jie; Chan, Yinthai; Loh, Kian Ping, "High-Performance Hybrid Solar Cell Made from CdSe/CdTe Nanocrystals Supported on Reduced Graphene Oxide and PCDTBT," Advanced Functional Materials, vol. 24, pp. 1904-1910, 2014.

Z. J. Xue, Changyun; Wang, Long; Liu, Wei; Liu, Bin, "Fabrication of Flexible Plastic Solid-State Dye-Sensitized Solar Cells Using Low Temperature Techniques," The Journal of Physical Chemistry C, vol. 118, pp. 16352-16357, 2014.

S. N. Yang, A. Sreekumaran; Ramakrishna, Seeram, "Conversion efficiency enhancement of CdS quantum dot-sensitized electrospun nanostructured TiO2 solar cells by organic dipole treatment," Materials Letters, vol. 116, pp. 345-348, 2014.

1 April 2013 – 30 September 2013

S.-W. L. Cao, Xin-Feng; Yuan, Yu-Peng; Zhang, Zhen-Yi; Fang, Jun; Loo, Say Chye Joachim; Barber, James; Sum, Tze Chien; Xue, Can, "Artificial photosynthetic hydrogen evolution over g-C3N4 nanosheets coupled with cobaloxime," Physical Chemistry Chemical Physics, vol. 15, pp. 18363-18366, 2013.

X. Q. Cao, Dianpeng; Yin, Shengyan; Bu, Jing; Li, Fengji; Goh, Chin Foo; Zhang, Sam; Chen, Xiaodong, "Ambient Fabrication of Large-Area Graphene Films via a Synchronous Reduction and Assembly Strategy," Advanced Materials, vol. 25, pp. 2957-2962, 2013.

Z. W. Fang, Yabo; Song, Jibin; Sun, Yimin; Zhou, Jiajing; Xu, Rong; Duan, Hongwei, "Immobilizing CdS quantum dots and dendritic Pt nanocrystals on thiolated graphene nanosheets toward highly efficient photocatalytic H2 evolution," Nanoscale, vol. 5, pp. 9830-9838, 2013.

T. M. L. Koh, Hairong; Nonomura, Kazuteru; Mathews, Nripan; Hagfeldt, Anders; Gratzel, Michael; Mhaisalkar, Subodh G.; Grimsdale, Andrew C., "Photovoltage enhancement from cyanobiphenyl liquid crystals and 4-tert-butylpyridine in Co(ii/iii) mediated dye-sensitized solar cells," Chemical Communications, vol. 49, pp. 9101-9103, 2013.

T. M. N. Koh, Kazuteru; Mathews, Nripan; Hagfeldt, Anders; Grätzel, Michael; Mhaisalkar, Subodh G.; Grimsdale, Andrew C., "Influence of 4-tert-Butylpyridine in DSCs with CoII/III Redox Mediator," The Journal of Physical Chemistry C, vol. 117, pp. 15515-15522, 2013.

M. H. M. Kumar, Nripan; Boix, Pablo P.; Nonomura, Kazuteru; Powar, Satvasheel; Ming, Lam Yeng; Graetzel, Michael; Mhaisalkar, Subodh G., "Decoupling light absorption and charge transport properties in near IR-sensitized Fe2O3 regenerative cells," Energy & Environmental Science, vol. 6, pp. 3280-3285, 2013.

D. S. Lee, Jiwon; Zhu, Xi; Lee, Jiyoul; Shin, Hyeon-Jin; Cole, Jacqueline M.; Shin, Taeho; Lee, Jaichan; Lee, Hangil; Su, Haibin, "Quantum confinement-induced tunable exciton states in graphene oxide," Scientific Reports, vol. 3, p. 2250, 2013.

F. J. Li, James Robert; Wang, Qing; Chua, Julianto; Mathews, Nripan; Mhaisalkar, Subodh G.; Moon, Soo-Jin; Zakeeruddin, Shaik M.; Grätzel, Michael, "Determining the Conductivities of the Two Charge Transport Phases in Solid-State Dye-Sensitized Solar Cells by Impedance Spectroscopy," The Journal of Physical Chemistry C, vol. 117, pp. 10980-10989, 2013.

J. Y. Miao, Hong Bin; Khoo, Si Yun; Liu, Bin, "Electrochemical fabrication of ZnO-CdSe core-shell nanorod arrays for efficient photoelectrochemical water splitting," Nanoscale, vol. 5, pp. 11118-11124, 2013.

D. S. Qi, Haibin; Bastjan, M.; Jurchescu, O. D.; Palstra, T. M.; Wee, Andrew T. S.; Rübhausen, M.; Rusydi, A., "Observation of Frenkel and charge transfer excitons in pentacene single crystals using spectroscopic generalized ellipsometry," Applied Physics Letters, vol. 103, p. 113303, 2013.

D. Z. Qi, Liyan; Cao, Xuebo; Jiang, Yueyue; Xu, Hongbo; Zhang, Yanyan; Yang, Bingjie; Sun, Yinghui; Hng, Huey Hoon; Lu, Nan; Chi, Lifeng; Chen, Xiaodong, "Bio-inspired antireflective hetero-nanojunctions with enhanced photoactivity," Nanoscale, vol. 5, pp. 12383-12387, 2013.

D. M. Sabba, Nripan; Chua, Julianto; Pramana, Stevin S.; Mulmudi, Hemant K.; Wang, Qing; Mhaisalkar, Subodh G., "High-surface-area, interconnected, nanofibrillar TiO2 structures as photoanodes in dye-sensitized solar cells," Scripta Materialia, vol. 68, pp. 487-490, 2013.

H. H. Sun, Jiating; Wang, Jiangyan; Zhang, Shuang-Yuan; Liu, Cuicui; Sritharan, Thirumany; Mhaisalkar, Subodh; Han, Ming-Yong; Wang, Dan; Chen, Hongyu, "Investigating the Multiple Roles of Polyvinylpyrrolidone for a General Methodology of Oxide Encapsulation," Journal of the American Chemical Society, vol. 135, pp. 9099-9110, 2013.

Q. L. Tay, Xinfeng; Tang, Yuxin; Jiang, Zhelong; Sum, Tze Chien; Chen, Zhong, "Enhanced Photocatalytic Hydrogen Production with Synergistic Two-Phase Anatase/Brookite TiO2 Nanostructures," The Journal of Physical Chemistry C, vol. 117, pp. 14973-14982, 2013.

B. W. Wu, Xiangyang; Guan, Cao; Fai Tai, Kong; Yeow, Edwin Kok Lee; Jin Fan, Hong; Mathews, Nripan; Sum, Tze Chien, "Uncovering loss mechanisms in silver nanoparticle-blended plasmonic organic solar cells," Nat Commun, vol. 4, 2013.

X. C. Xia, Dongliang; Qi, Xiaoying; Xiong, Qinqin; Zhang, Yongqi; Tu, Jiangping; Zhang, Hua; Fan, Hong Jin, "Controllable Growth of Conducting Polymers Shell for Constructing High-Quality Organic/Inorganic Core/Shell Nanostructures and Their Optical-Electrochemical Properties," Nano Letters, vol. 13, pp. 4562-4568, 2013.

G. M. Xing, Nripan; Sun, Shuangyong; Lim, Swee Sien; Lam, Yeng Ming; Grätzel, Michael; Mhaisalkar, Subodh; Sum, Tze Chien, "Long-Range Balanced Electron- and Hole-Transport Lengths in Organic-Inorganic CH3NH3PbI3," Science, vol. 342, pp. 344-347, 2013.

T. D. Zhou, Yonghua; Borgna, Armando; Hong, Jindui; Wang, Yabo; Han, Jianyu; Zhang, Wei; Xu, Rong, "Post-synthesis modification of a metal-organic framework to construct a bifunctional photocatalyst for hydrogen production," Energy & Environmental Science, vol. 6, pp. 3229-3234, 2013.

G. S. B. Anjusree, Arun; Balakrishnan, Avinash; Vadukumpully, Sajini; Subramanian, K. R. V.; Sivakumar, N.; Ramakrishna, Seeram; Nair, Shantikumar V.; Nair, A. Sreekumaran, "Fabricating fiber, rice and leaf-shaped TiO2 by tuning the chemistry between TiO2 and the polymer during electrospinning," RSC Advances, vol. 3, pp. 16720-16727, 2013.

N. K. J. Elumalai, Tan Mein; Chellappan, Vijila; Jose, Rajan; Palaniswamy, Suresh Kumar; Jayaraman, Sundaramurthy; Raut, Hemant Kumar; Ramakrishna, Seeram, "Electrospun ZnO Nanowire Plantations in the Electron Transport Layer for High-Efficiency Inverted Organic Solar Cells," ACS Applied Materials & Interfaces, vol. 5, pp. 9396-9404, 2013.

N. K. V. Elumalai, Chellappan; Jose, Rajan; Zhi Ming, Kam; Saha, Amitaksha; Ramakrishna, Seeram, "Simultaneous improvements in power conversion efficiency and operational stability of polymer solar cells by interfacial engineering," Physical Chemistry Chemical Physics, vol. 15, pp. 19057-19064, 2013.

F. J. Li, James Robert; Wang, Qing, "Determination of Sensitizer Regeneration Efficiency in Dye-Sensitized Solar Cells," ACS Nano, vol. 7, pp. 8233-8242, 2013.

J. A. Lian, Kelvin; Lin, Ming; Chan, Yinthai, "Formation of Hollow Iron Oxide Tetrapods via a Shape-Preserving Nanoscale Kirkendall Effect," Small, vol. 10, pp. 667-673, 2014.

Y. X. Liao, Yang; Chan, Yinthai, "Semiconductor nanocrystals in sol-gel derived matrices," Physical Chemistry Chemical Physics, vol. 15, pp. 13694-13704, 2013.

Y. J. Liu, James R.; Wang, Qing, "Efficient Dye-Sensitized Solar Cells Using a Tetramethylthiourea Redox Mediator," ChemSusChem, vol. 6, pp. 2124-2131, 2013.

1 October 2012 – 31 March 2013

T. F. Baikie, Yanan; Kadro, Jeannette M.; Schreyer, Martin; Wei, Fengxia; Mhaisalkar, Subodh G.; Graetzel, Michael; White, Tim J., "Synthesis and crystal chemistry of the hybrid perovskite (CH3NH3)PbI3 for solid-state sensitised solar cell applications," Journal of Materials Chemistry A, vol. 1, pp. 5628-5641, 2013.

Y. H. Cai, John C. W.; Batabyal, Sudip K.; Liu, Wei; Sun, Yun; Mhaisalkar, Subodh G.; Wong, Lydia H., "Nanoparticle-Induced Grain Growth of Carbon-Free Solution-Processed CuIn(S,Se)2 Solar Cell with 6% Efficiency," ACS Applied Materials & Interfaces, vol. 5, pp. 1533-1537, 2013.

J. Z. Hong, Wei; Ren, Jia; Xu, Rong, "Photocatalytic reduction of CO2: a brief review on product analysis and systematic methods," Analytical Methods, vol. 5, pp. 1086-1097, 2013.

R.-L. T. Lee, Phong D.; Pramana, Stevin S.; Chiam, Sing Yang; Ren, Yi; Meng, Siyuan; Wong, Lydia H.; Barber, James, "Assembling graphitic-carbon-nitride with cobalt-oxide-phosphate to construct an efficient hybrid photocatalyst for water splitting application," Catalysis Science & Technology, vol. 3, pp. 1694-1698, 2013.

M. X. Li, Guichuan; Xing, Guozhong; Wu, Bo; Wu, Tom; Zhang, Xinhai; Sum, Tze Chien, "Origin of green emission and charge trapping dynamics in ZnO nanowires," Physical Review B, vol. 87, p. 115309, 2013.

M. C. Liu, Rui; Adamo, Giorgio; MacDonald Kevin, F.; Sie Edbert, J.; Sum Tze, Chien; Zheludev Nikolay, I.; Sun, Handong; Fan Hong, Jin, "Tuning the influence of metal nanoparticles on ZnO photoluminescence by atomic-layer-deposited dielectric spacer," Nanophotonics, vol. 2, p. 153, 2013.

X. Z. Liu, Qing; Xiong, Qihua; Sum, Tze Chien, "Tailoring the Lasing Modes in Semiconductor Nanowire Cavities Using Intrinsic Self-Absorption," Nano Letters, vol. 13, pp. 1080-1085, 2013.

H. B. Min Lim, Sudip K.; Pramana, Stevin S.; Wong, L. H.; Magdassi, Shlomo; Mhaisalkar, S. G., "Chemical welding of binary nanoparticles: room temperature sintering of CuSe and In2S3 nanoparticles for solution-processed CuInSxSe1-x solar cells," Chemical Communications, vol. 49, pp. 5351-5353, 2013.

M. T. Nguyen, Phong D.; Pramana, Stevin S.; Lee, Rui Lin; Batabyal, Sudip K.; Mathews, Nripan; Wong, Lydia H.; Graetzel, Michael, "In situ photo-assisted deposition of MoS2 electrocatalyst onto zinc cadmium sulphide nanoparticle surfaces to construct an efficient photocatalyst for hydrogen generation," Nanoscale, vol. 5, pp. 1479-1482, 2013.

Y. J. Tang, Zhelong; Xing, Guichuan; Li, Anran; Kanhere, Pushkar D.; Zhang, Yanyan; Sum, Tze Chien; Li, Shuzhou; Chen, Xiaodong; Dong, Zhili; Chen, Zhong, "Efficient Ag@AgCl Cubic Cage Photocatalysts Profit from Ultrafast Plasmon-Induced Electron Transfer Processes," Advanced Functional Materials, vol. 23, pp. 2932-2940, 2013.

Y. H. Wang, Jindui; Zhang, Wei; Xu, Rong, "Carbon nitride nanosheets for photocatalytic hydrogen evolution: remarkably enhanced activity by dye sensitization," Catalysis Science & Technology, vol. 3, pp. 1703-1711, 2013.

Y. W. Wang, Yongsheng; Xu, Rong, "Photochemical Deposition of Pt on CdS for H2 Evolution from Water: Markedly Enhanced Activity by Controlling Pt Reduction Environment," The Journal of Physical Chemistry C, vol. 117, pp. 783-790, 2013.

L. C. Xi, Sing Yang; Mak, Wai Fatt; Tran, Phong D.; Barber, James; Loo, Say Chye Joachim; Wong, Lydia Helena, "A novel strategy for surface treatment on hematite photoanode for efficient water oxidation," Chemical Science, vol. 4, pp. 164-169, 2013.

G. L. Xing, Yile; Wu, Xiangyang; Chakrabortty, Sabyasachi; Liu, Xinfeng; Yeow, Edwin K. L.; Chan, Yinthai; Sum, Tze Chien, "Ultralow-Threshold Two-Photon Pumped Amplified Spontaneous Emission and Lasing from Seeded CdSe/CdS Nanorod Heterostructures," ACS Nano, vol. 6, pp. 10835-10844, 2012.

G. L. Xing, Jingshan; Li, Hongxing; Wu, Bo; Liu, Xinfeng; Huan, Cheng Hon Alfred; Fan, Hong Jin; Sum, Tze Chien, "Ultrafast Exciton Dynamics and Two-Photon Pumped Lasing from ZnSe Nanowires," Advanced Optical Materials, vol. 1, pp. 319-326, 2013.

X. P. Zeng, Stevin S.; Batabyal, Sudip K.; Mhaisalkar, Subodh G.; Chen, Xiaodong; Jinesh, K. B., "Low temperature synthesis of wurtzite zinc sulfide (ZnS) thin films by chemical spray pyrolysis," Physical Chemistry Chemical Physics, vol. 15, pp. 6763-6768, 2013.

Q. L. Zhang, Xinfeng; Utama, Muhammad Iqbal Bakti; Zhang, Jun; de la Mata, María; Arbiol, Jordi; Lu, Yunhao; Sum, Tze Chien; Xiong, Qihua, "Highly Enhanced Exciton Recombination Rate by Strong Electron–Phonon Coupling in Single ZnTe Nanobelt," Nano Letters, vol. 12, pp. 6420-6427, 2012.

Y. T. Zhang, Yuxin; Liu, Xinfeng; Dong, Zhili; Hng, Huey Hoon; Chen, Zhong; Sum, Tze Chien; Chen, Xiaodong, "Three-Dimensional CdS–Titanate Composite Nanomaterials for Enhanced Visible-Light-Driven Hydrogen Evolution," Small, vol. 9, pp. 996-1002, 2013.

N. K. S. Elumalai, Amitaksha; Vijila, Chellappan; Jose, Rajan; Jie, Zhang; Ramakrishna, Seeram, "Enhancing the stability of polymer solar cells by improving the conductivity of the nanostructured MoO3 hole-transport layer," Physical Chemistry Chemical Physics, vol. 15, pp. 6831-6841, 2013.

X. H. Z. Huang, C.; Tay, C. B.; Venkatesan, T.; Chua, S. J., "Green luminescence from Cu-doped ZnO nanorods: Role of Zn vacancies and negative thermal quenching," Applied Physics Letters, vol. 102, p. 111106, 2013.

S. W. Zeng; Z. Huang; X. Wang; W.M. Lu, Z.Q. Liu, B.M. Zhang, S. Dhar, T. Venkatesan, and Ariando, "The influence of La substitution and oxygen reduction in ambipolar La-doped YBa2Cu3Oy thin films," Superconductor Science and Technology, vol. 25, p. 124003, 2012.

K. A. R. Stoerzinger, Marcel; Suntivich, Jin; Lu, W. M.; Zhou, Jigang; Biegalski, Michael D.; Christen, Hans M.; Ariando,; Venkatesan, T.; Shao-Horn, Yang, "Oxygen electrocatalysis on (001)-oriented manganese perovskite films: Mn valency and charge transfer at the nanoscale," Energy & Environmental Science, vol. 6, pp. 1582-1588, 2013.

Y. L. Xu, Jie; Mishra, Nimai; Chan, Yinthai, "Multifunctional Semiconductor Nanoheterostructures via Site-Selective Silica Encapsulation," Small, vol. 9, pp. 1908-1915, 2013.

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