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KAUST Solar Center News

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Message from the Director

Welcome to the first KAUST Solar Center (KSC) newsletter of 2019.

It has been a very busy and productive 2018 for our Solar Center, with over 140 publications arising from our research, as well as demonstrating significant technology advances, and we look forward to new challenges and opportunities in the upcoming year.

As our center continues the transition to a more applied focus, we are delighted to welcome new scientists and engineers that participate in KSC projects, as well as wishing our departing students and postdocs best of luck for their future careers.

Preparing our early stage researchers with the range of skills and knowledge to allow them to flourish in new career positions has been a particular focus during 2018. In addition to scheduling regular transferable skill seminars and workshops, we organised a very successful KSC summer school, offering not only a comprehensive series of fundamental lectures on photovoltaics, but also implemented our new solar teaching lab, more details of which can be found later in the newsletter. It is a source of great pride for us all to see the progress and impact made by our former group members, which we also highlight in this newsletter.

May I wish you all the very best for the coming year and hope to welcome many of you to our Center, whether joining us in our projects, participating in our conference or workshops, or perhaps just visiting.

Iain McCulloch,
Director of KAUST Solar Center
Professor of Chemical Science

"It is a source of great pride for us all to see the progress and impact made by our former group members."

KSC Research Highlights

P.h.D. student Hui-Chun Fu

Artificial photosynthesis for Net-Zero Carbon Fuels —By Hui-Chun Fu

Hui-Chun Fu is a Ph.D. student in Prof. Jr-Hau He's Nanoenergy group. Originally from Taiwan, she came to KAUST in 2014 after studying at National Taiwan University. Fu says that the most important factors in her decision to join KAUST were the state-of-the-art facilities and world-renowned faculty based here. At KAUST, she is working on the fabrication and application of photoelectrochemical (PEC) water splitting based on solar devices in artificial photosynthesis for Net-Zero Carbon Fuels. Instead of pursuing new materials, her attention has been attracted by the concurrent challenges of optical, electrical, and catalysis management of solar PEC cells. She believes that well-controlled, high efficiency and chemically stable PEC cells will be a key technological component of a hydrogen economy.

Replacing fossil fuels with renewable resources has recently received significant attention due to the alarming levels of atmospheric CO_2, which appear to be contributing to global warming. The sun is an abundant energy source, though its intermittent nature makes it difficult to capture. One way this resource can be made more accessible is to utilize sunlight to split water into hydrogen (H_2) and oxygen (O_2) generating hydrogen as a storable form of fuel. It can then react with oxygen to form water (H_2O) releasing energy. PEC cells use light-absorbing materials as photoelectrodes, mimicking natural photosynthesis to convert solar energy to a storable form of fuel. The overall PEC process consists of three parts: (i) light absorption and charge carrier generation; (ii) extraction of the excited carriers to the photoelectrode/electrolyte interface; and (iii) hydrogen evolution (HER) and oxygen evolution reactions (OER) driven by electrocatalysts. To effectively drive PEC water splitting, it is essential to harvest the majority of photons in the solar spectrum while also ensuring efficient charge separation/transfer and electrocatalysis. Therefore, a sustainable, low cost, and renewable energy cycle can be created.

Silicon (Si), the most investigated material for solar-to-hydrogen technology has great potential as the single photoelectrode. While some success has been achieved in Si-Based PEC systems, they suffer from low efficiency and short longevity. Moreover, in order for hydrogen to be commercially viable, the existing challenges of electrical, optical, and catalysis management must be addressed concurrently.

Together with CO_2 reduction, PEC water splitting is one of the most promising routes for the production of renewable energy hydrogen. KAUST is located next to the Red Sea, which is a favorable environment to realize solar fuel technology as it is rich in both solar and water resources. Fu's studies focus on the fabrication and application of PEC water splitting

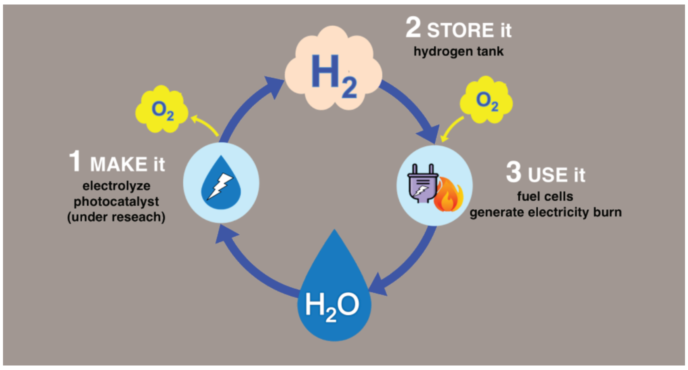


Figure 1. Renewable energy cycle

based on solar devices. In her preliminary work, she has demonstrated a high-efficiency solar cell that holds promise for stable and efficient water splitting.

Fu is now directing her work towards the further development of photoelectrodes to realize highly efficient PEC water splitting devices for practical applications to meet the needs of the Kingdom. She is investigating the simultaneous improvement in light harvesting, charge carrier separation/transfer, and catalysis management of Si-based photocathodes. By decoupling the light harvesting side from the electrocatalytic surface she nullifies parasitic light absorption. She has developed a Si bifacial (SiBF) PEC photocathode to absorb light on both sides of PEC devices, which exhibits a current density of 39.01 mA/cm^2. Unlike conventional monofacial PEC cells, her group's bifacial design demonstrates excellent omnidirectional light harvesting capability. Futhermore, another novel photon decoupling scheme has been implemented by fabricating back buried junction photoelectrochemical (BBJ-PEC) cells. This scheme enables maximum light-harvesting without any metal contact, which prevents the shading effect, while the electrochemical reaction occurs on the bottom side of the PEC cell. The resultant single-junction BBJ-PEC cell achieves a current density of 41.76 mA/cm^2 for hydrogen evolution, the best reported to date. By connecting the three BBJ-PEC cells in series, they have also realized unassisted photoelectrochemical water splitting. This efficient PEC cell design demonstrates promising performance, taking us a step closer to real-world solar-to-hydrogen production.

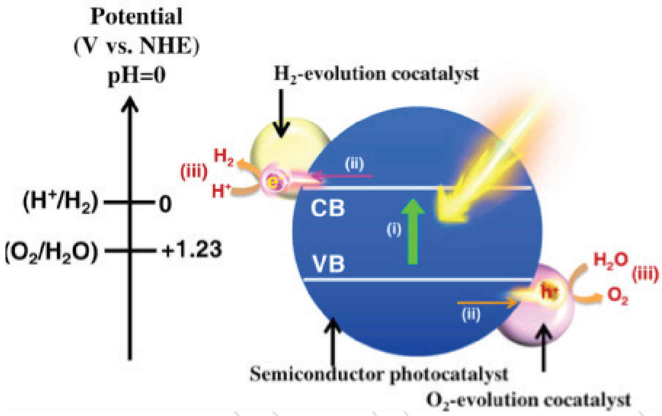


Figure 2. The schematic of the overall PEC process

Recently Fu won the Materials Today Rising Star Poster Award (Silver Awards) and Session Theme Poster Award at the Nano 2018 conference in Hong Kong. There were over 700 attendees at the Nano 2018 conference. Hui-Chun Fu's excellent work and awards are encouraging for the female scientists in STEM (science, technology, engineering and mathematics) community.

Adhesion lithography for nanoscale electronics

—By Hendrik Faber

The advancement of modern technology and computing power is driven largely by efforts to reduce critical feature sizes to ever smaller ranges, allowing, for example, faster processing speeds or higher resolution displays. This way, tremendous engineering accomplishments allowed the most advanced semiconductor companies to shrink down technology nodes for transistors in state-of-the-art silicon microprocessors down to 7 nm. It remains to be seen how much longer this miniaturization can be pushed and how long the famous Moore's Law can continue to hold true. In contrast to that, other technology trends have evolved in recent years, especially where applications do not require the fastest possible processing powers but rather benefit from new functionality or innovative fabrication techniques. Solution processing and digital printing techniques are envisioned to enable the cost-effective fabrication of flexible electronic devices on large scales in continuous processes.

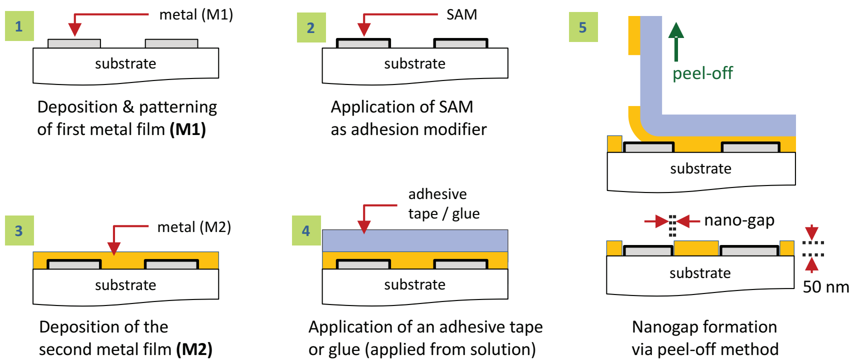
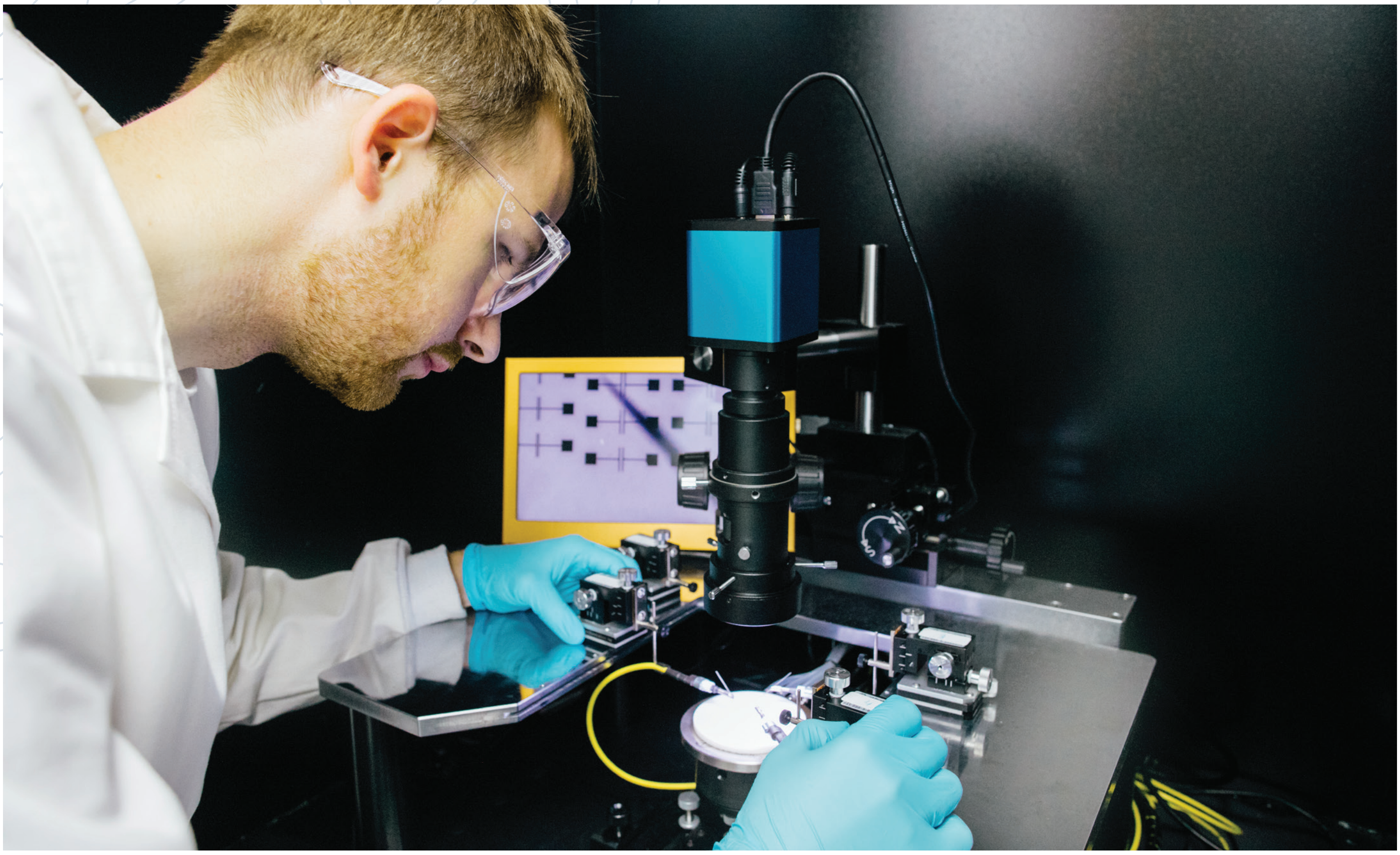


Figure 1. Schematic process chain for the fabrication of nanogap electrodes via adhesion lithography

The technique we are working on, adhesion lithography (a-Lith), is aiming to combine the best of both worlds by realizing the fabrication of electronic devices with nanometer small feature sizes within a simple processing scheme. Adhesion lithography allows us to create metallic electrodes that are separated by a nanogap of typically less than 20 nm, using a simple peel-off method based on tape or glue (outlined below). In devices such as diodes or thin-film transistors, the distance between the electrodes plays a crucial



Dr. Hendrik Faber; set-up of electrical device characterisation on the probe station

role especially where high operating speeds are targeted. A reduction of path length which a charge carrier needs to travel automatically translates to a faster signal transfer. Therefore, a-Lith is well suited to produce high performance devices such as fast sensors, rectifying diodes, or thin-film transistors.

So how does adhesion lithography work? It is based on the manipulation of adhesive forces between two metals that are deposited subsequently on top of each other. In the initial step, the first metal film (M1) is patterned into the desired shape using well-established standard lithography. Afterwards a self-assembled monolayer (SAM) is deposited on top of M1. The short molecule that forms the SAM is specifically chosen a) to only bond to M1 but not to the substrate material itself and b) to create a non-sticking hydrophobic surface on top of M1. The first property is decided by the chemical head groups of the SAM, for example thiols preferably bond onto noble metals while phosphonic acid groups form a strong bond on oxide surfaces such as native aluminium oxide. To fulfil the second criterion, molecules whose tail and end groups consist of short linear alkyl chains, such as in octadecylphosphonic acid (ODPA), are well suited to create a strongly hydrophobic surface property on metal 1.

When a second film of metal (M2) is now evaporated on top of a substrate with SAM treated and patterned metal 1, it interacts with two very different surface regions. Wherever there is just the bare substrate without a SAM, metal 2 has no problems to adhere to it. On the contrary, in all the areas where M1 and M2 overlap with each other, the altered surface properties due to the SAM treatment cause a drastically reduced adhesion of M2. When we then apply a liquid glue or pieces of tape over the whole substrate, the adhesive forces between M2 and the tape are stronger than between M2 and the SAM-treated M1. As a consequence, gently peeling off the tape removes M2 from all the areas where it was on top of M1 but otherwise leaves it present on the substrate. The applied shear forces during the peel-off cause the M2 film to fracture along the edge pattern of M1, leaving behind a small empty gap between the two metals. The minimum gap size is ultimately limited by the length of the SAM molecule. However, typically larger values on the order of 20nm are found, influenced by various factors including the peeling speed and direction or the edge profile of M1.

Adhesion lithography enables the fabrication of nanogap electrodes of either the same metal, say Aluminium-

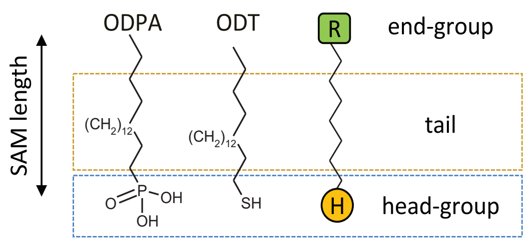


Figure 2. General breakdown of SAM-forming molecules into head-group, tail and end-group together with two specific examples: octadecylphosphonic acid (ODPA) and octadecane thiol (ODT)

Aluminium, or between dissimilar metals such as Aluminium-Gold. The latter is a major benefit, as it is very difficult to achieve with other techniques. Additionally, because there are no elevated temperatures during the fabrication process there are no restrictions when it comes to flexible substrates such as polymer films.

The gap formation happens all around the boundary line of M1, yet the gap size continuously stays in the low nanometer range. This feature effectively removes the requirement for highly specialized, costly or slow lithographic techniques such as e-beam lithography. It decouples the definition of the electrode shape from the magnitude of the critical gap dimension. In other words, M1 can be patterned into any arbitrary shape and the resulting nanogap follows along the full outline. This way it is possible to achieve extremely high aspect ratios (boundary length / gap size) in electronic devices. To give an example, an 80 meter long concentric spiral consisting of one continuous Al-Au nanogap over a 4-inch wafer could already be demonstrated.

A large variety of electronic devices can be realized via a-Lith. So far, rectifying diodes, capacitors, LEDs, photodetectors, memory devices and TFTs are among those that have been demonstrated successfully. Other interesting applications include sensors for different gases, humidity, mechanical stress or bio-molecules. One of our focus topics at the moment are ultrafast diodes for radio frequency (RF) applications and wireless energy harvesting. Here, wireless AC signals from sources such as Bluetooth, WiFi or cellular networks are envisioned to be captured by an antenna and converted to DC output voltages that can supply e.g. low-power autonomous sensors as part of the growing Internet-of-things environment. A key part of the rectification circuit required for this will rely on ultrafast diodes that can operate in the frequency range of 1-30 GHz. The fabrication of these diodes is a challenge we believe adhesion lithography is well suited to take on successfully.

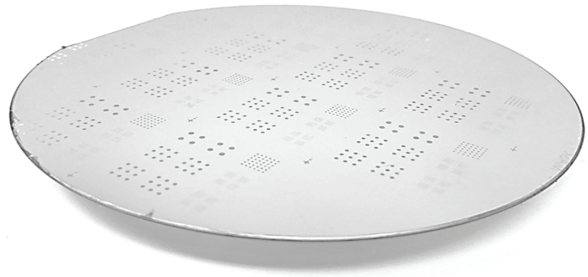


Figure 3. Nanogap electrodes fabricated via adhesion lithography on 4-inch wafer scale

Understanding the Physics of Organic Solar Cells

—By Ahmed Hesham Balawi

Ahmed Hesham Balawi joined the KAUST Solar Center in February 2015, supported by the KAUST Visiting Student Research Program (VSRP), after completing his Master degree in Materials Science and Engineering at the University of Toronto. Following the VSRP internship, he joined the group of Associate Professor Frédéric Laquai at KAUST as a PhD student to study loss processes in organic systems for photovoltaic energy conversion.

The power conversion efficiency of organic photovoltaics (OPVs) has gradually increased from 1% back in the early 1980s, to about 5% in 2007, and recently to more than 15%, thanks to the development of novel non-fullerene acceptors. Considering the recent progress, even higher efficiencies closer to those of silicon-based solar cells and other inorganic thin film technologies have come into reach. A key advantage of organic materials is their high absorption coefficient (typically around ~10^5 cm^{-1}), that is, three orders of magnitude higher compared to silicon. This property alongside the possibility of solution processing by roll-to-roll printing and other casting techniques gives the OPV technology an edge to be employed in thin photovoltaic modules at low production costs, if the key issues, performance and (photo) stability can be solved.

The photoactive layer in OPVs is comprised of an electron-donating material, which often is the main absorber, and an electron-accepting material that facilitates charge separation at the interface. Fullerene-based derivatives (PC61BM or PC71BM) have dominated as electron acceptor materials for a long time due to their outstanding electron-accepting and charge carrier transport properties. However, fullerene molecules absorb little of the solar light, which sets a ceiling to the photocurrent generation, while in addition their energetic disorder and low LUMO energy level causes energy losses and thus low solar cell voltages. Hence, novel materials are needed to replace the fullerene acceptors. Here, non-fullerene electron acceptors come into play: they absorb a larger fraction of the solar light with minimum energy losses during charge generation. While new materials have already led to an impressive enhancement in performance of OPV devices, a precise understanding of the photophysical mechanisms of charge carrier generation is still lacking.

That is precisely the focus of my thesis, to track the journey of photogenerated excitons and quantify the losses along

Ph.D. student Ahmed Hesham Balawi

the way to charge carrier extraction in non-fullerene OPV systems. Organic solar cells are called 'excitonic' devices, since excitons are formed upon photo-excitation of organic materials. An exciton is an excited electron-hole pair, in which the two carriers (electron and hole) are strongly bound by Coulomb attraction, and it is not easily separated to free charges. In my work, I use ultrafast transient absorption (TA) spectroscopy and time-resolved photoluminescence (TRPL) techniques to track the photo-physical processes such as exciton and charge recombination following photon absorption. Often contributions from singlet excitons, charges, and also triplet excitons spectrally overlap and thus we need to apply advanced data analyses techniques such as multivariate curve resolution alternating least squares (MCR-ALS) analysis to the obtained datasets to separate their contributions. This analytical tool allows me to access the individual kinetics of photogenerated states and to apply photophysical models to extract important parameters such as the efficiency of free charge generation and the rate (constant) of charge recombination (see Figure 1a). Furthermore, knowing the spectral contribution of each species, one can also determine the densities of singlet excitons, charges, and triplet excitons (see Figure 1b) in the organic thin film. The combination of these ultrafast techniques and analytical methods provides insight to what limits the short-circuit current (J_{SC}) and the quantum

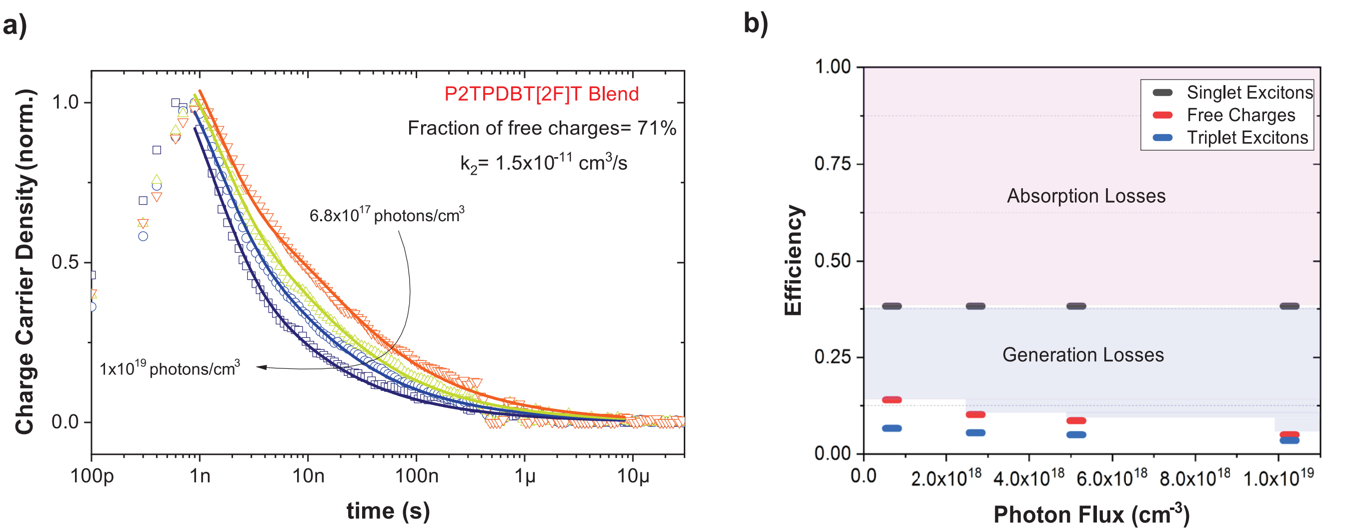


Figure 1. (a) Photon flux (excitation density) dependent charge carrier kinetics of an all-polymer blend (PBDT-TS1:P2TPDBT[2F]T) fitted with a photophysical model and (b) efficiency of singlet exciton (black), free charges (red), and triplet exciton (blue) generation as a function of the photon flux for the same blend after excitation at 532 nm.

efficiency of photovoltaic devices.

However, we have to not only consider charge carrier (quantum efficiency) losses, but also energy losses occurring in solar cells, which we can monitor by a combination of steady-state electro-optical measurements. Sensitive external quantum efficiency (s-EQE), photo-thermal deflection spectroscopy (PDS), and electroluminescence (EL) measurements (see Figure 2) help to probe the energetic landscape of the bulk heterojunction, from the energy of photogenerated excitons and interfacial charge transfer (CT) state energies to the energy of free charge carriers, which determines the experimentally observed open circuit voltage (V_{OC}) of the devices. These techniques can answer the question why a solar cell is efficient and further what still limits its performance. Ideally, the results can be related to the chemical structure of the materials and the thin film morphology of the blend, which then allows synthetic chemists and device engineers to develop more efficient organic materials and device structures.

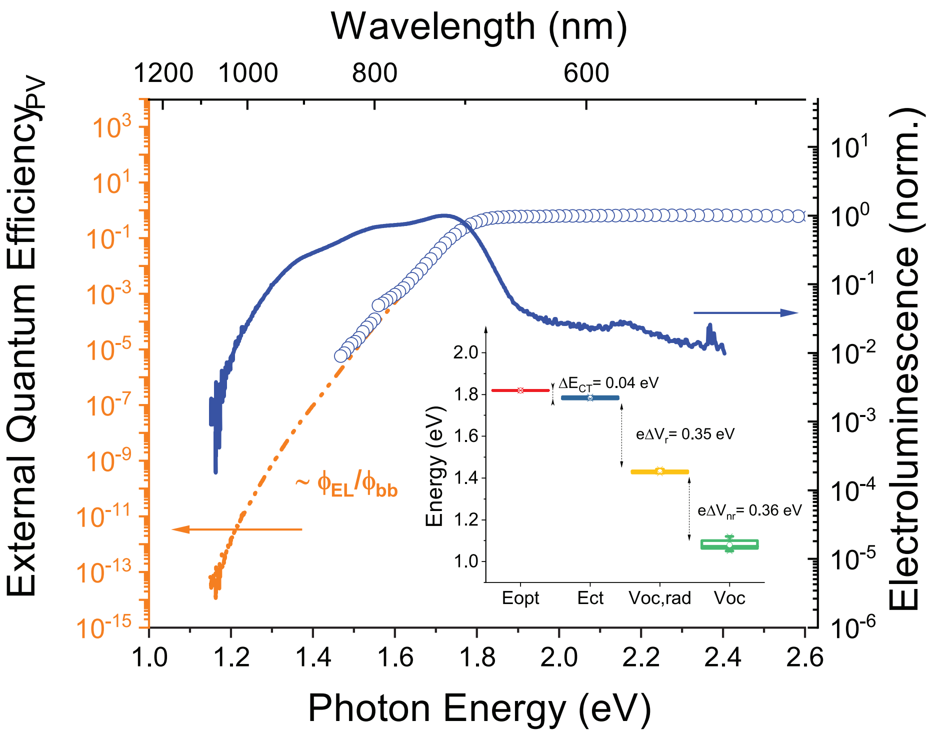


Figure 2. Quantification of energy loss processes: sensitive EQE (open dots) and electroluminescence (EL) data (blue solid line) of a 2F-DRCN5T:PC71BM device. EQE_{PV} spectra (orange dashed-dotted line) evaluated from EL data and blackbody radiation of the device. Inset: energy levels of singlet states (red), CT states (blue), radiative V_{OC} (yellow), and device V_{OC} (green).

KAUST Research Conference: 3rd Generation photovoltaic technologies and beyond

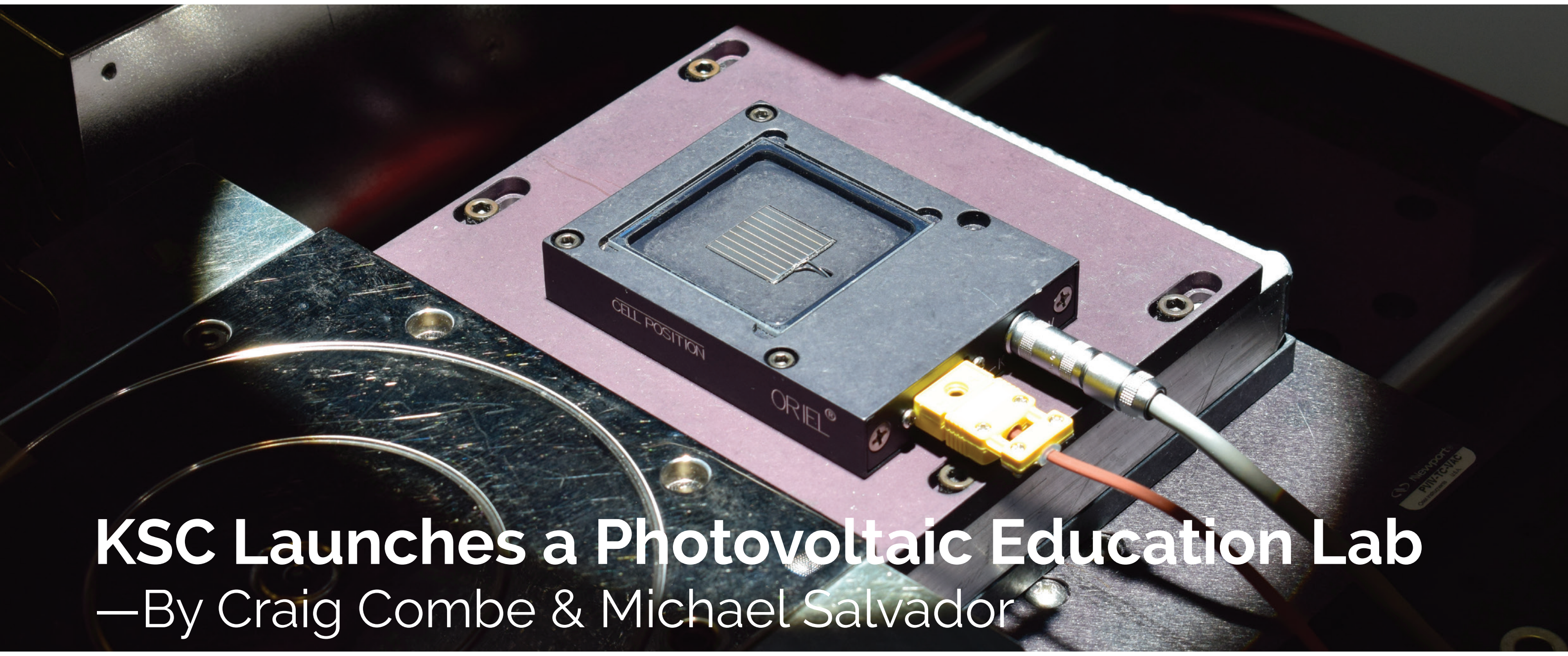
February 10 - 12 2019

The main program on February 11-12 will focus on three major themes:

- Novel materials and devices for 3rd generation PVs
- Manufacturing, upscaling and commercialization of PV technologies
- Technologies and concepts beyond PV

On 10 February there will be a workshop for young scientists addressing the fundamentals of solar energy conversion, including the associated economics.

ksc.kaust.edu.sa/Conference-2019



KSC Launches a Photovoltaic Education Lab

—By Craig Combe & Michael Salvador

Silicon reference solar cell under a solar simulator

Educating and inspiring young minds to tackle the scientific challenges associated with light-to-energy conversion will bring about the intellectual ability and skills to solve those challenges. The Kingdom of Saudi Arabia's Vision 2030 builds on this idea. It defines important goals for the future of the country; notably an economy less dependent on fossil fuels and the expansion of private sector industries. Solar energy will play a key role in the realization of both these goals given Saudi Arabia's ideal sunshine duration indicator (3,600 – 3,800 hours of bright sunshine annually) and the industry required for it to be harnessed, stored and processed.

With numerous solar projects in development throughout the Kingdom a large effort is required from academia and industry alike to provide large numbers of solar energy experts. One way that KSC is rising to the challenge is through the launch of a Photovoltaic Education Lab.

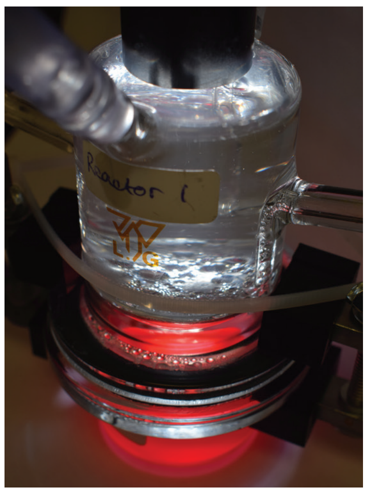
Through the PV Education Lab, we provide a platform to learn about fundamental science as well as state-of-the-art developments in photovoltaics and other solar energy applications. We engage with people from a variety of backgrounds with differing experiences and the PV Education Lab enables KSC to host national and international training programs, for example the KSC Summer School. The lab provides facilities for academics to give practical, experimental lessons, building upon the theory from lecture courses. The PV lab provides hands-on experience with device fabrication and characterization techniques in a more settled setting than fast-paced research labs.

Within the lab there are a variety of instruments that cover the broad scope of solar energy research. The experiments range from providing general understanding of the relevance of the spectral composition of sunlight to more sophisticated device physics.

Spectroscopy experiments can be conducted, so users can obtain a fundamental understanding of how light interacts with relevant semiconducting materials in thin film and in solution. A complete device fabrication line allows users to build fully functioning thin film solar cells from scratch, using different fabrication techniques such as spin coating, ink-jet printing, and slot-die coating, demonstrating the translation from lab scale devices to more industry relevant, high throughput standards. These techniques are set up in air or in a glovebox. The latter providing users with their first experience of fabricating devices under inert conditions. A solar simulator and a tool for measuring light to electron conversion efficiency allow participants to measure the photovoltaic performance of solar cells.

A solar fuels experiment shows participants how to prepare organic nano-particles that harness light to split water and make hydrogen gas, a highly versatile fuel that could be an answer for long term energy storage. Both the synthesis and characterization of novel photocatalytic materials are thus of high technological relevance.

The PV Education Lab and its users are supported by KSC's operational team of engineers and scientists with rich experience in solar cell technology and materials design. We believe that the PV Education Lab can provide users with a unique learning experience that will make them literate in solar technology, allowing them to make informed decisions about their professional future as well as to contribute to future energy solutions for the Kingdom and the world.



Photocatalysis reactor for water splitting

Faculty Focus

Interview with Assistant Prof. Derya Baran

Derya Baran is Assistant Professor of Material Science and Engineering in the University's Physical Science & Engineering (PSC) Division, who joined KAUST and KSC in January 2017. She studied chemistry at the Middle East Technical University, Turkey, where she was awarded her B.Sc. in 2008 and her M.Sc. in 2010. She was awarded the Bavarian Science Foundation Scholarship to pursue her doctoral studies, receiving her doctoral degree in 2014 from Friedrich-Alexander Erlangen-Nürnberg University, Germany. As a recipient of the Helmholtz Association's postdoc grant, Prof. Baran conducted postdoctoral research into the characterization of non-fullerene acceptors and microstructure/recombination correlation in solution processed solar cells at Imperial College London, UK. In 2016 she took up an additional position as a Research Associate at Jülich Forschungszentrum, Germany. Her current research interests include solution-processable organic/hybrid soft materials for printed electronics.

What was your motivation to join KAUST and KSC?

I first heard about KAUST during my PhD in Germany when my supervisor visited KAUST. We students heard stories about the facilities and it was beyond our imagination. During my fellowship at Imperial College London, UK and Julich Research Center, Germany, I had the opportunity to visit KAUST as a speaker at the KSC Solar Conference in 2015. I was impressed by the facilities and the international culture - it certainly lived up to the stories we'd heard before! I knew from then on that KAUST was something I wanted to be a part of. Fast-forward three years and now, as a new faculty member, I have the great opportunity to utilise the KSC facilities for my own research group.

Please tell us about your research interests and how you see them fitting with the Center's mission.

My research is focussed on organic optoelectronics and how we can make them better, cheaper and more stable. In that respect, my research is one of the driving forces behind the Center's mission to develop the next generation and building integrated photovoltaic (PV) technologies. As an engineer at heart, I always want my research to find industrial and real-world application. Therefore, my group focuses on printing and coating techniques for organic materials; device structure; efficiency optimisation; and ultimately how all these parameters affect the degradation of a device. More recently my work has focussed on organic PV that absorbs in the IR, allowing for transparent solar cells that can be coated on windows. This not only gives rise to a PV technology that can be truly building-integrated but, by blocking the heat from entering a building, it is also highly relevant for the Middle Eastern region. Aside from PV, we are finding new and novel uses, not only for the materials we research but also the techniques we use to deposit them. This is allowing us to develop new devices in the field of organic thermoelectrics, and self-powered optoelectronic devices. The most interesting part for me is being able to see a research idea become a real device and it is exciting to be part of a Center with the same mission. Whether it is through our large area processing or device engineering, giving commercial reality to the research is what drives me.

How does your position support your short and long term research goals?

The biggest support that my position in KAUST provides is the immediate network of faculty that I have the opportunity to work with. I've always been a firm believer in team work and collaborations and being able to work with the great members of KAUST and KSC enables not only better research but also faster breakthroughs. I have found my work to be very complementary to research within the Center and also the university as a whole, for example utilising materials from another group or working with other research groups to measure our devices in innovative ways. Combining the world-leading facilities within the departments; the Core-labs; and the expert equipment operators, the support between everyone in KAUST is invaluable. In the long run, my position in KAUST gives me the opportunity to diversify my research and to have the freedom to work on very high-risk high-gain projects for my future career through grants such as the Competitive Research Grant (CRG) scheme.

Please tell us about your five year scientific vision.

Scientifically my longer term vision is to accelerate the development of new organic electronic devices using the knowledge and experience we have from organic PV research. Within my group, 'OMEGALAB', we are finding new areas such as thermoelectrics and self-powered wearable electronics that today are still in their infancy, but one day could revolutionise the world around us. By beginning to work on these areas now, we are finding many similarities and crossovers with more well-established technologies. Now that this is happening in my OMEGALAB research group, I would like to graduate students who will be peers and colleagues in the future and help at least a little to create a scientific community with integrity and a passion for science and technology.

What do you see as significant challenges and how will you address them?

One of the biggest challenges with this kind of research and development is being able to synchronise the commercial readiness of a technology with the market readiness for that technology. Too often great research ideas and concepts never make it to the real world as the market wasn't ready. Similarly technologies regularly fail as the market is ready but the technology still has too many flaws. I focus my research on market areas holding back technology but that are ready for innovation and on promising technologies without a market, my research is focussed on longer term developments. For areas holding technologies back, in our field, we find stability and cost to be significant and recurring challenges. By studying the fundamentals, learning and understanding the materials from their basic principles, we are able to overcome the challenges, but we need to do it fast enough to not miss the market!

What do you like to do beyond research?

When I moved to KAUST, I thought I would have a lot of time to do my own things due to the close proximity of work and home. Well, I'm not sure that's how it's working out but I try to snap out from my research mood when I have time (or maybe I should create time). One of my big loves is music and playing instruments. From just listening through to playing it myself, I surround myself with music. I love that it does not have any language. I like to spend time playing flute, classical guitar and alto-saxophone. Plus I've just bought a trumpet if there are any teachers in KAUST!

What is your advice to young scientists?

I am not sure what big advice I can give to young scientists, as I feel I am still one too. But I can share my motivation and how I see things in life: I think it is very important to know yourself, and what you want, or I should say you want to achieve. You can do this for certain time frames of course, and it can be a small or a very big thing in your life. If you believe in it, and work hard enough you will make it, for sure. And if you don't achieve it, you did not want it that much. It doesn't matter if you're young or old, you should never stop learning. This comes from listening to others. Never be afraid that you don't know something or to ask questions. The smartest people are the ones who know what they don't know, then do something about it.

Ph.D. Profile

Maryam Alsufyani

"

...I have the passion to design polymers for solar cells. ..."

Maryam Alsufyani is a Saudi national who completed her undergraduate studies in chemistry at Taibah University in Madina. She recently completed her Master in Chemical Sciences at KAUST under the supervision of Prof. Niveen Khashab, AMPM, where she focused on inorganic host-guest chemistry which resulted in an Angewandte Chemie paper, https://doi.org/10.1002/anie.201884061.

During her undergraduate studies Maryam began to realize her dream of pursuing a career as a synthetic chemist and applied to carry out a Ph.D. in Prof. Iain McCulloch's group at KSC where she is now working on the design and synthesis of semiconducting polymers for use in organic electronic devices.

Ph.D. student Maryam Alsufyani

"I'm really interested in synthesizing polymers that are suitable for bioelectronics. At the same time, I have the passion to design polymers for solar cells. I think that by joining the solar center, I'll have the chance to learn from the many different people and faculty members and I've already seen how strongly they collaborate with each other. There is a high degree of communication and that is absolutely going to fit with my extroverted character and help me to learn deeply by discussing with the solar center members", said Maryam.

International Partners

KSC benefits greatly from the scientific expertise of other research groups outside KAUST (as do they from ours) and, in addition, these collaborations create valuable channels for student exchange, postdoc recruitment, and placement of our own graduates and postdoctoral associates after their auspicious time at KAUST.

Denis Andrienko

is a group leader at the Max Planck Institute for Polymer Research working on the development of multiscale simulation techniques for charge and exciton transport in conjugated polymers as well as small molecular weight organic semiconductors.
www.mpip-mainz.mpg.de/~andrienk/

In September 2018 Denis came to KAUST for a six month stay on the Physical Sciences & Engineering Division's Visiting Faculty Program. He is based within KAUST Solar Center and has been teaching in the Material Science & Engineering program.

Dr. Denis Andrienko

Enjoying 1 Sun
-By Denis Andrienko

Frédéric Laquai's email about the PSE Division's Visiting Faculty program at KAUST excited me in less than a femtosecond. The enthusiasm instantaneously dissociated into pluses and minuses: moving with 1.5 kids (my second daughter, Mila, had yet to be born) and my wife, Natacha, to a foreign country versus the opportunity to work in, literally speaking, the "imperial" KAUST Solar Center (KSC). A few days later, I filed the proposal, with full support from Natacha and Prof. Kurt Kremer, the head of the theory department at the Max Planck Institute for Polymer Research, MPIP.

At the end of August we landed in Jeddah - at probably ideal 1 sun illumination conditions. Within two weeks all formalities were settled: housing (including a snake in the garden, two visiting cats and a chicken of unknown origin), my new office with a 24-core workstation, my daughter Zoe's place in KAUST daycare (at least as well equipped as the KAUST core labs), the number-crunching supercomputer access, phones, and picture IDs. It was a long to-do-list but thanks to the helpful and friendly administration, all went well. To us it seems like the KAUST community makes everybody happy, in the supermarket, on the campus' streets, in the daycare, or at the recreation center.

The dream of any hardworking scientist, KAUST is a paradise for a computer simulator like me. The University provides fantastic computing resources: without mentioning the numbers, think of what you were always dreaming of... and then double, triple or quadruple it. System admins fix all issues practically instantaneously. There must be a software KAUST does not have a license for – but I have still to work out which. Now add air conditioning to your office (which easily defeats my 24-core computing oven), 24/7 campus diner, coconut trees along research buildings, palm trees along roads, bananas and papayas in private gardens, a view of the Red Sea from almost everywhere, and a fancy security robot wheeling around with a craving for selfies. For someone who spends most of the day watching computer screens, this is paradise on Earth.

To complete the picture, people here are in love with molecules, electrons, excitons, polarons, devices, path integrals, data mining, artificial intelligence, biodiversity, startups... Students here are dedicated, curious, and engaged. I enjoyed lecturing, even though I had a 50% drop-out rate. Don't get me wrong, it was a tough computer simulation course, I normally teach over two semesters. Designed for PhD students, packed with math, it requires a deep understanding of advanced statistical and quantum mechanics. I myself would have had difficulties following it, when I was a postgraduate student.

It is impossible to get bored at KAUST: Research topics, projects, and problems literally flood you. My initial humble goal was, apart from escaping the cold, rainy, and cloudy German winter, to establish collaborative projects with the faculty at the KAUST Solar Center. However, this quickly branched into a number of activities, from understanding energy and charge transfer between donor and non-fullerene acceptors in organic solar cells, to the design of absorption spectra of small molecules, to the correct accounting of light recycling in perovskite solar cells. Let me briefly summarize my activities at KAUST, hoping that the list will justify the – sometimes slower than expected – progress from my side.

To begin with, together with Frédéric's group, I studied the photophysical properties of rather sophisticated donor-acceptor-donor complexes synthesized back at the MPIP. Such dyads are excellent model systems that help to elucidate elementary processes in organic solar cells: light absorption, creation of a charge transfer state, and geminate charge recombination. It turned out to be an unexpectedly challenging task to rationalize the experimental results: we had to dig into peculiarities of dipolar and quadrupolar excitations, Marcus theory of charge transfer, non-equilibrium solvation models, and even statistical perturbation theory for free energy differences, which dates back to the work of Zwanzig from the fifties.

At the same time Iain McCulloch and his team were eager to learn how to chemically control the shape of the absorption spectra of D-A-D dyads. In other words, given the donor, the acceptor, and the bridge blocks, would it be possible to reconstruct the entire spectra of a conjugated complex? The answer to this 'simple' question is the key to the design of colorful (or transparent) solar cells.

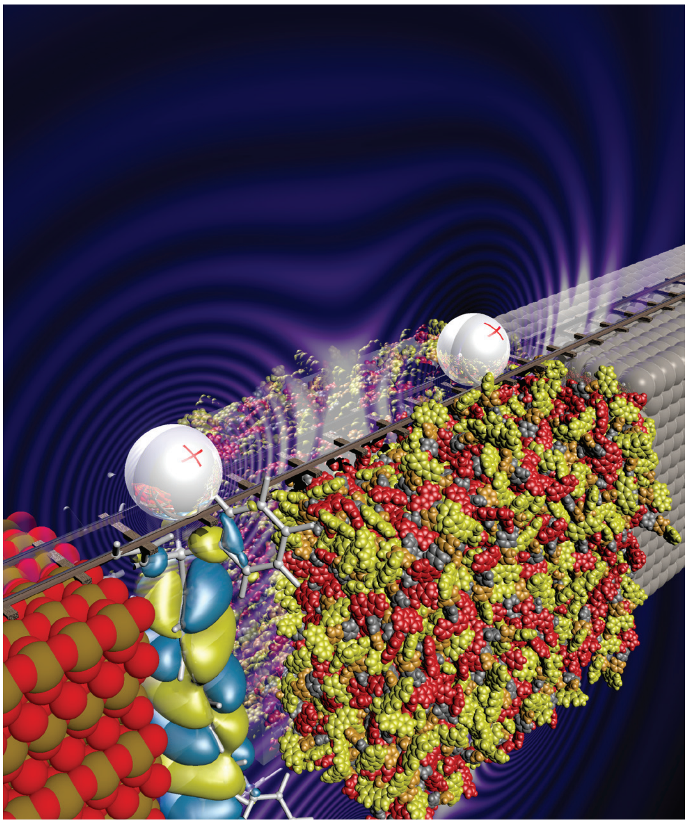
Thomas Anthopoulos and his group wanted to know whether doping changes the crystal structure/orientation of organic semiconductors in thin organic films that are used to prepare field-effect transistors. We have tried to answer this question by evaluating the mobility tensor of the supercell crystallized in Derya Baran's group.

Derya's group in turn are curios to understand why non-fullerene acceptors split charges so efficiently. In fact, some of these materials can even do the job of both the donor and the acceptor: There must be some kind of 'magic' going on in these systems that effectively screens the Coulomb attraction of holes and electrons. This observation turned out to be closely related to studies conducted in Frédéric's group, performed on a large number of combinations of different donor and acceptor molecules. I believe together we will be able to link these results to the underlying chemistry.

Overall, my family and I have had a busy and exciting schedule here at KAUST. However, what is more important, these collaborations will last longer than just my visit: with Derya and Frédéric we will start a research project between the MPIP and KAUST in April 2019 funded by the Office of Sponsored Research (OSR) at KAUST.

All this would not have been possible without the support from friends and colleagues, as well as the amazing administrative support we received. I would like to thank Frédéric for talking me into this adventure and signing tons of forms, Iain for being so lenient about my misspellings of his name(s), Julien for the baby chair, which made my daughter Zoe feel at home, as well as for the organization of private snorkeling trips, Ahmed for explaining the difference between fresh, dried, and frozen dates, and other facts related to Saudi's traditions and culture, Thomas for gardening advice, and Jafar for enrolling me into the Solar Center's football team.

Thanks everybody for hosting us and for being so welcoming, friendly, and helpful! Let's work together toward the 42% efficient transparent, single-component, flexible, water-resistant, and x-ray stable solar cell! ;-)

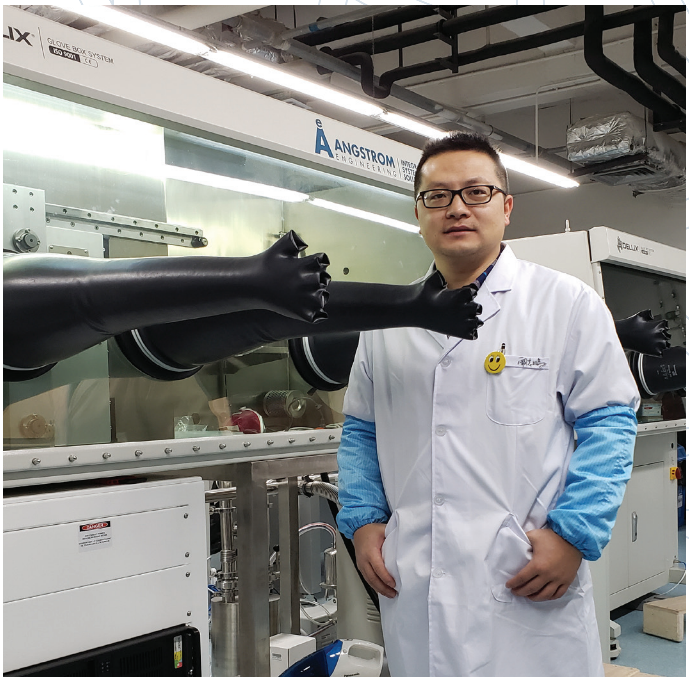


Computer-aided design of organic semiconductors: from charge injection to exciton formation to transport.

Feature Article

Successfully stepping into academia

For many young researchers their time at KSC is a stepping stone to an academic career but the path to academia is often ambiguous. We spoke to former KSC postdoc Dr. Zhipeng Kan to find out how he successfully entered the world of academia.



Dr. Zhipeng Kan

Kan recently joined the Chongqing Institute of Green and Intelligent Technology (CIGIT) at the Chinese Academy of Sciences as a professor. He is now establishing his group in the area of optoelectronics of organic materials. From 2011 to 2015 he obtained his PhD from the Department of Physics, Politecnico di Milano, conducting all his experiments in the Center for Nano Science and Technology Istituto Italiano di Tecnologia before joining KSC as a postdoctoral fellow, firstly with Prof. Pierre Beaujuge and subsequently with Prof. Frédéric Laquai's Ultrafast Dynamics Group.

When did you first realize that you wanted to pursue an academic career?

I dreamed of doing research during my childhood but I clearly made up my mind to do research after I started to work in a company: I had gained experience of how research work was conducted in both an institute and a company and realized that industrial research was not what I wanted to do for the rest of my life so I started to apply for PhD positions overseas.

Why did you chose to come to KAUST - Did you already have your academic career in mind?

Yes, before joining KAUST I was hoping to pursue an academic career. I had already visited several places in China and looked into potential work opportunities but in the end I joined KAUST.

I chose to do my postdoc at KAUST based on the advanced lab and characterization equipment that was available – this hardware was really important for my experimental work. Also the PI's at KAUST are young and creative. They also work at the frontier of science which gave me even more chances to learn; be trained in the latest techniques; and gain new ideas.

At KAUST the living conditions for postdocs are cool. After suffering the rental market in Milan for four years, I very much appreciated the wonderful housing that KAUST is able to provide. The health service is also excellent. Finally, the remuneration was good. I was actually able to save and this helped me when I returned to China - everyone knows the crazy apartment prices in China!

How did your time KAUST help you achieve your career goals? Was there support?

In addition to the great working environment, I was involved in amazing collaborations with both internal and external partners – I had not expected these opportunities before I joined KSC. Also KAUST were supportive with my career development as a whole.

When did you first start to apply for positions? How long did it take?

I started to apply for faculty positions from the beginning of my third year in KAUST - it was time. During the first half year, I didn't receive any good feedback, but from October 2017, I got many positive replies. The interview for my current position was done in the middle of October 2017. So the process doesn't take long. Of course, it also depends on what kind and the level of position you want to get, i.e. the support and the salary, and you may have to hold out if you want more but for me, I am very satisfied with the position I got and I believe I entered at the right level.

What particularly attracted you to your new position?

Independence and freedom.

How was the interview / selection process and how did you prepare?

There were two parts to the interview: free discussion and an oral presentation.

The free discussion was done with the president, the head of the institute and the vice head, and included questions on my research background, experiences, and future work plan – about15 minutes for each.

There was an interview team of 10 professors working in the institute to whom I presented my current work and future plans for about 18 mins. I'm glad to say that the interview team were unanimous in their hiring decision.

Actually, it's worth mentioning that the preparation of the powerpoint slides took me quite some time because I not only had to present in Chinese but also the style needed to follow the customary Chinese format with regards to what information the reviewers would want to hear about. I suggest to anyone in a similar situation that they ask a friend who has gone through the process for help with regard to the panel's likely expectations as this helped me a lot.

What experiences/skills did you have that helped you stand out from your peers?

It was really a combination of things: My PhD degree from Polimi, postdoc experience in KAUST, and the research ability gained throughout these years.

What is the focus of your work now?

I still need to pass an evaluation in order to get the full start up package, so I am still very much focused on my research which is related to organic semiconductors.

I am also working on recruiting group members. It is currently quite difficult to hire people, especially postdocs, because they all want to gain overseas experience or enter permanent positions but I do have several joint students from local universities.

What has surprised you about getting started in academia?

The bureaucracy and, actually, it's difficult to spend research funding. There are so many rules that need to be followed when buying equipment or consumables, and I am still getting used to it.

What tips do you have for young researchers wishing to pursue an academic career?

Being able to critically evaluate your own CV is important in my opinion. Also, I only looked for jobs that would match what I was able to offer.

Chongqing Institute of Green and Intelligent Technology at the Chinese Academy of Sciences

Recent Ph.D. Graduates

Weiyuan Du, Maha Alamoudi

Weiyuan Du

Dr. Weiyuan Du defended his Ph.D. dissertation entitled, 'Side Chain Modifications of Conjugated Polymers for Bioelectronics and Biological Applications' under the supervision of Prof. Iain McCulloch.

Maha Alamoudi

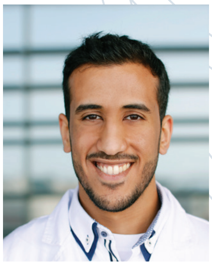
Dr. Maha Alamoudi defended her Ph.D. dissertation entitled, 'Spectroscopy of Polymer: Non-fullerene Small Molecule Acceptor Bulk Heterojunction Organic Solar Cells' under the supervision of Prof. Frédéric Laquai.

New Faces at KSC

Sarah H Al- Abdullatif

MS Student
with Iain McCulloch

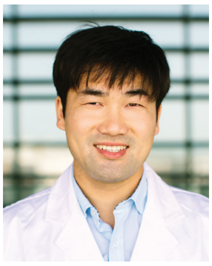
From – University of California, Berkeley, USA



Salman A Alsharif

MS Student
with Iain McCulloch

From – Dalhousie University, Halifax, Canada



Xingxing Chen

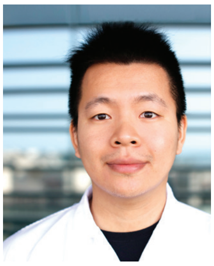
Postdoc
with Iain McCulloch

From – Changchun Institute of Applied Chemistry, Chinese Academy of Science, China

Furkan Halis Isikgor

Postdoc
with Stefaan De Wolf

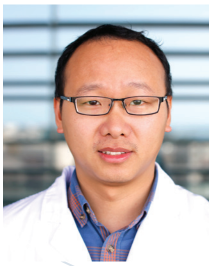
From – National University of Singapore, Singapore



Yuanbao Lin

Ph.D. Student
with Thomas Anthopoulos

From – Jinan University, Guangzhou, China



Jiang Liu

Postdoc
with Stefaan De Wolf

From –Tsinghua University, Beijing, China

Abhinav Sharma

Postdoc
with Thomas Anthopoulos

From – Ulsan National Institute of Science and Technology (UNIST), Ulsan, South Korea.

Alumni Focus

Rahim Munir

Dr. Rahim Munir

Rahim Munir is a KAUST Material Science and Engineering Ph.D. graduate (2017) who is now pursuing his research career as a postdoctoral fellow at the Helmholtz Zentrum Berlin, Germany.

Munir joined KAUST in 2012 after completing his undergraduate studies in Metallurgy and Materials Engineering at Ghulam Ishaq Khan Institute in Pakistan and obtaining his Masters in Materials Science and Engineering from Korea Advanced Institute of Science and Technology (KAIST).

Recalling his time at KAUST, "I experienced a steep learning curve. I worked on the understanding of solution processing of different types of semiconductors for energy applications. However, my prime focus was towards solution processing of perovskite materials for solar cell applications." Munir said.

"The various research groups at KSC have created a friendly and cooperative environment where new or experienced researchers can thrive when pursuing their goals of creating new knowledge. As a scientist, it is essential to understand the concepts, discuss the original hypothesis and perform experiments to reveal novel aspects of the topic and KSC provides an environment where anyone can feel comfortable presenting their ideas openly to both their colleagues and faculty. These open discussions helped me to identify my passion and choose a career path of research."

During his time at KAUST, Munir was not only an enthusiastic researcher but also an active member of on-campus societies. Based on his own experiences, Munir had the following advice, "Involve yourself in one or two societies such as the Materials Research Society (MRS), American Chemical Society (ACS), etc. I was involved in the MRS student chapter at KAUST." Together with KSC's Ahmed Mansour, Guy Olivier, Maha Alamoudi and Sanaa Alshammari, Munir organized the first ever student-organized symposium at the Fall 2016 Meeting of MRS in Boston, USA, under the guidance of Prof. Husam Alshareef. This experience enabled Munir to gain insight into how to approach sponsors and to convince them to support ideas. This student group was ultimately able to enjoy the reward of overseeing an event that was well received with full house sessions.

At KAUST Munir took full advantage of the opportunity to attend international conferences: "I would also strongly recommend attending at least one international conference a year. It will open up your horizons to learn from the scientists around the world and get their insights on your work."

Reflecting on his personal development during his time at KAUST, Munir stated that he learnt to be more open to accepting criticism in order to grow: "There is nothing wrong in someone critically reviewing your work... use it to your advantage and learn from it. It will improve you scientifically as well as personally."

Studying at KAUST also provided Munir with opportunities to conduct research in collaboration with other universities. "I collaborated with research groups in the USA, Canada, Italy, India, and China which resulted in publications in high impact journals. These activities have helped me to grow my global network which is essential for every scientist... The bonds I have formed while at KAUST are forever", said Munir.

His latest research, at the Helmholtz Zentrum Berlin in Dr. Eva Unger's group, focuses on scaling up the printing process of perovskite material and gaining insights into the changes and phase transformations occurring during the process. "It is a unique combination of efforts towards scaling up while keeping a close eye at the fundamental understanding of the processes", concluded Munir.

News

Desert Technologies host KSC

KAUST Solar Center's research activities span the value chain in solar energy from molecule synthesis to module prototype testing, including solar fuel and solar thermal. These activities are aimed at addressing real world challenges and it is imperative that research output is both scalable and applicable to industry and market demands. Therefore, KSC continually seeks to engage with industrial partners.

In November KSC faculty and management, together with KAUST Innovation & Economic Development, were delighted to be invited by Dr. Nabih Cherradi, Chief Technology Officer, to visit the Desert Technologies (DT) facility in Jeddah.

The KSC Management Team are warmly received at Desert Technologies' facility in Jeddah

DT is a global platform for sustainable development including investment development & management and an engineering, procurement and construction platform for large-scale renewable energy projects. DT has solar panel manufacturing capability with a 110MW capacity Reis Robotics crystalline silicon assembly line in Jeddah, which the KSC PIs were keen to view.

Exploratory talks regarding technology verification; transitioning from solar cell to module; and out door testing were extremely encouraging and both partners were keen to enhance R&D efforts within the Kindgdom.

KSC postdoc Dr. Michele De Bastiani awarded prestigious Eni Award 2018

President Sergio Mattarella presents Dr. Michele Di Bastiani with his Eni Young Researcher of the Year Award

On October 22nd Sergio Mattarella, President of Italy, presented KSC postdoc Michele Di Bastiani with his Eni Young Researcher of the Year Award for his research towards a new class of photovoltaic systems: "The stability of conversion processes to transform light into power is one of the key challenges facing emerging solar technologies".

The Eni Award was launched in 2007 to recognize the best studies on efficiency, sustainability and environmental protection. The annual Eni Award is a prestigious international prize for applied research in the field of energy and the Young Researcher of the Year category is awarded to researchers aged under 30 who have received a PhD from an Italian university.

Michele conducted his PhD in the School of Material Science and Engineering of the Universita' degli Studi di Padova, in co-tutelage with the Center for Nanoscience and Technology (CNST) of the Istituto Italiano di Tecnologia, in Milan. In 2016 Michele joined Prof. Osman Bakr's group and since 2017 has been conducting research in Prof. De Wolf's KPV Lab at the KAUST Solar Center.

Congratulations: iyris goes from strength to strength

The young startup company, iyris, was established by KSC co-founders Derya Baran, (KAUST assistant professor); Daniel Bryant; Nicola Gasparini; and Joel Troughton. Based on an organic photovoltaic formulation that captures infrared light, iyris makes transparent solar windows, producing electricity and blocking heat entering the building, reducing the building's cooling load.

In mid-2018 iyris was selected to take part in KAUST's startup accelerator program, TAQADAM, a Saudi Arabian startup accelerator for ideas that are pushing the boundaries of science and technology. After completing the program, iyris was one of six finalists awarded $100,000 follow-on funding which they plan to use to produce bigger prototypes.

iyris (l-r: Daniel Bryant, Derya Baran, Joel Troughton and Nicola Gasparini) receive their TAQADAM funding award.

Following on from this success, in October iyris went on to compete in StartupIstanbul, securing third place in the conference and exhibition that brought together around 4,000 leading entrepreneurs, innovators, venture capitalists and investors.

In addition to the numerous conferences and exhibitions that iyris has been invited to, the team has been selected from over 4,500 applications as one of the Hello Tomorrow Top 500 deeptech startups and will participate in the Hello Tomorrow Summit in Paris from 14-15 March 2019.

KSC Highlight Paper

"Controlling Blend Morphology for Ultrahigh Current Density in Nonfullerene Acceptor-Based Organic Solar Cells"

In the past decade, the urge for fullerene replacements for higher Voc while maintaining high Jsc has been of significant interest to synthesis groups in the field of organic solar cells. Recently, small-molecule nonfullerene acceptors (NFAs) emerged as superior alternatives to fullerene derivatives.These materials provide strong absorption coefficients along with energy level tunability that can maximize the Voc and Jsc when low band gap derivatives are used to harvest photons matching the solar flux in the NIR region.

In KSC's recent Letter published in ACS Energy Letters, Xin Song et al. report a system with a well-known polymer donor (PTB7-Th) blended with a narrow band gap nonfullerene acceptor (IEICO-4F) as the active layer and 1-chloronaphthalene (CN) as the solvent additive. Optimization

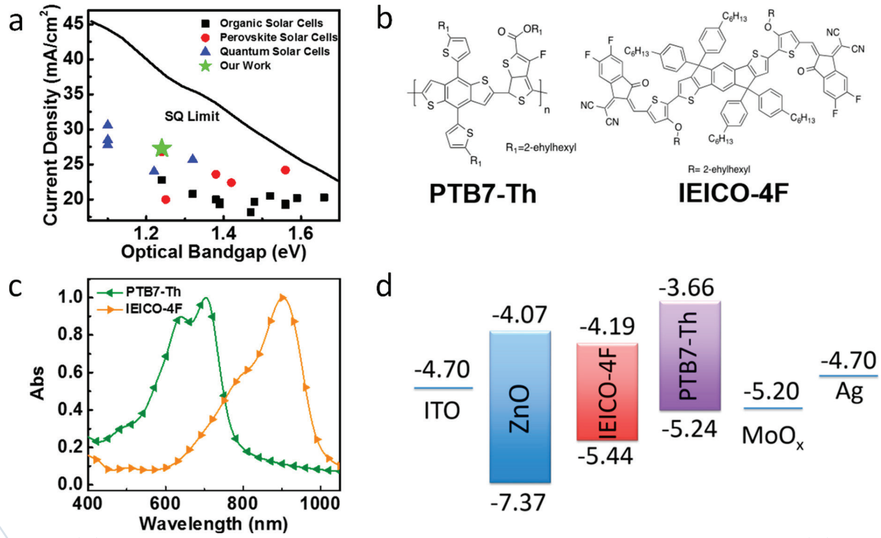
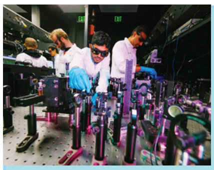


Figure 1. (a) Map of the band gap vs current density with the lines of the SQ limit; (b) chemical structures of PTB7-Th and IEICO-4F; (c) normalized thin film absorbance of PTB7-Th and IEICO-4F; (d) energy alignment of the materials used in the inverted solar cell.

of the photoactive layer nanomorphology yields a short-circuit current density value of 27.3 mA/cm^2, one of the highest values in organic solar cells reported to date, which competes with other types of solution-processed solar cells such as perovskite or quantum dot devices. Along with decent open-circuit voltage (0.71 V) and fill factor values (66%), a power conversion efficiency of 12.8% is achieved for the champion devices. Morphology characterizations elucidate that the origin of this high photocurrent is mainly the increased π–π coherence length of the acceptor, the domain spacing, as well as the mean-square composition variation of the blend. Optoelectronic measurements confirm a balanced hole and electron mobility and reduced trap-assisted recombination for the best devices.

Events

KSC Summer School







KSC Summer Internship Program

If you're a talented final year undergraduate student considering a research career addressing the challenges of solar energy conversion, why not apply to ksc@kaust.edu.sa for a stipend to attend the KSC Internship Program?

We have 15 stipends available which cover travel and accommodation, as well as a living allowance.

Awardees will attend the **KSC Summer School** *from* **1st – 4th July:**
Experts from KSC and TU Delft will guide you through tutorial lectures on:

- *PV fundamentals*
- *Design of materials for solar energy conversion*
- *Electrical characterization tools for PV devices*
- *Silicon Solar Cells*
- *PV Systems*

Develop your practical skills in the KSC laboratory sessions:

- *Silicon preparation and characterization*
- *Organic Photovoltaics: preparation and characterization*
- *Semi-conducting thin film and material characterization*

After completing the summer school you can then put your skills to use during an extended stay as an intern with a summer research project in the world-class KSC laboratories from July to September.

Located next to the Red Sea you'll be able to participate in the full range of recreational activities available on campus.

"The opportunity to come to KAUST has been nothing short of incredible – not only have I had the chance to work on novel research in world-class facilities, I've been given the chance to experience a culture which not many people get to engage with first-hand... Because of this experience, my horizons have been broadened, and the world has become smaller."

- Chimdi Igwe, KSC Internship Program 2018, student, Materials Science & Engineering, Imperial College London

Challenge yourself this summer!

KAUST Solar Center

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