

KAUST Solar Center News

Table of Contents:



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KAUST
SOLAR
CENTER

Message from the Associate Director

KSC Research Highlights:

- Defect and contact passivation for perovskite solar cells opens a plateau towards Shockley-Queisser limits —By Erkan Aydin
- Towards the integration of fully printed green solar cells for self-powered biosensing applications — By Khulud Almasabi & Eloise Bihar

KSC: Developing in harmony with Saudi Arabia

KSC's Saudi students shape their own future

Faculty Focus:

- Prof. Udo Schwingenschloegl

International Partners:

- KSC Summer School offers 'global education' with our partners from TU Delft

Alumni Focus

- Mahesh Kumar Ravva

New Faces at KSC

PhD Profile

- Sanaa Alshammari

KSC News

KSC Highlight Paper

KAUST Research Conference 2020

Message from the Associate Director

Welcome to the 4th issue of the KAUST Solar Center Newsletter!

With this Newsletter, we intend to highlight some of our recent findings, provide insight into the current Center-based research projects, and share information about developments in the field of solar-energy conversion with you.

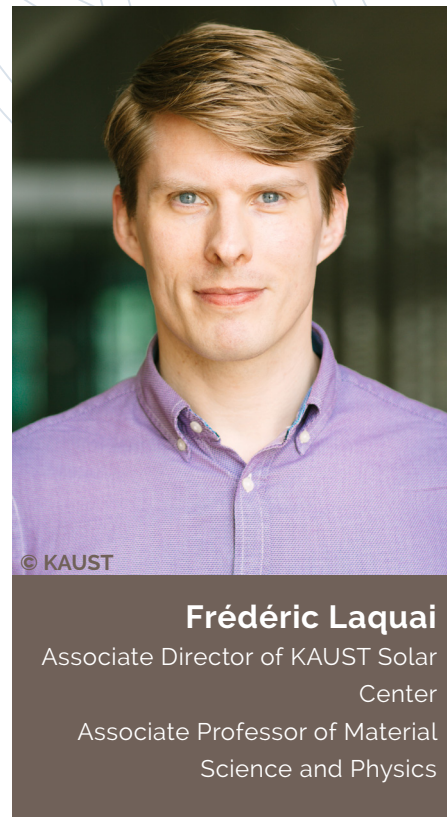
This issue features how defect and contact passivation can bring perovskite solar cells closer to the theoretical limit; how fully-printed organic solar cells can power biosensors; and how the KAUST Solar Center aligns with the Kingdom's Vision 2030 in the renewable energy and educational sector. Furthermore, we hear from Professor Udo Schwingenschlögl about his journey to KAUST and current research interests.

About a year ago, we launched a new set of goal-oriented, Center-supported research projects, aiming towards the advancement of existing as well as the development of new solar-energy conversion technologies. Recently, the Center has concluded the annual project cycle and we have reviewed the progress and achievements of our core and exploratory projects in a seminar series open to all KAUST members. I am excited to say that we have seen fast progress in all projects: the Center can now manufacture >22% efficient silicon heterojunction solar cells, organic solar cell efficiencies have gone beyond

16%, and combining traditional silicon technology with emerging perovskite materials we have realized >26.2% in tandem device structures. Certainly, such rapid and impressive progress has only been possible due to the joint effort of all Center-affiliated research groups and the excellent support our lab operations team provides every day. My sincere thanks to everybody in the KAUST Solar Center team for his or her hard work and motivation towards fulfilling our Center mission.

However, solar-energy conversion is not just photovoltaics. In the future, we aim to go beyond PV and, thus, have initiated a new core project led by Professor Vincent Tung, aiming to develop new materials and approaches towards efficient solar fuel generation, water splitting, and carbon dioxide reduction. We strongly believe that this is an area which still offers a lot of potential for both curiosity-driven and goal-oriented research and technology development.

Last, but not least, I would like to highlight our annual KSC Summer School. We have just had a busy week with morning lectures on PV-related topics presented by our collaborators from TU Delft and members of the KAUST Solar Center, while in the afternoons our lab team and Center researchers provided hands-on lab training sessions. With



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Frédéric Laquai

Associate Director of KAUST Solar Center

Associate Professor of Material Science and Physics

more than 50 people attending and 14 in-Kingdom and international participants staying now for 2-3 months internships in the Center, this has been a great success! Thanks to everybody involved in the organization, teaching, and training.

I hope you enjoy reading our KAUST Solar Center Newsletter!

KSC Principle Investigators

Iain McCulloch, Director, KSC
Professor of Chemical Science

Frédéric Laquai, Associate Director, KSC
Associate Professor of Material Science & Physics

Thomas Anthopoulos
Professor of Material Science & Engineering

Derya Baran
Assistant Professor of Material Science & Engineering

Stefaan De Wolf
Associate Professor of Material Science & Engineering

Udo Schwingenschlögl
Professor of Material Science & Engineering

Vincent Tung
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Muhammad M. Hussain
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Comments and suggestions regarding content can be sent to ksc@kaust.edu.sa

Defect and contact passivation for perovskite solar cells opens a plateau towards Shockley-Queisser limits —By Erkan Aydin

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Metal-halide perovskite-based solar cells have rapidly emerged as a high-efficiency photovoltaic technology that may enable high-performance solar cells. In the last ten years, tremendous progress has been recorded in terms of the power conversion efficiencies (PCE) of perovskite solar cells (PSCs) with PCEs in excess of 25% now being achieved, according to the recently updated NREL "Best Research-Cell Efficiencies" chart (Figure 1). Such device performance largely stems from the appealing optoelectronic properties of these materials.

The high absorption coefficient of perovskite absorbers enables photocurrents close to the theoretical maximum without the need for complicated light-trapping schemes. Nevertheless, similar to other thin-film PV materials such as gallium-arsenide (GaAs), copper-indium-gallium-selenide (CIGS) and cadmium-telluride (CdTe), the crystalline lattice of perovskites often includes defects such as interstitials, vacancies, and impurities at the grain boundaries and surfaces, dangling bonds can also be present, which all contribute to non-radiative recombination of photo-carriers. From a device perspective, such recombination undesirably inflates the open-circuit voltage deficit which, together

with detrimental effects on the fill factor (FF) of devices and thus the overall power output, creates significant roadblocks towards the theoretical efficiency limit of 30%. Taking inspiration from improvements made, it is obvious that a deeper understanding of the specific defect physics of perovskites, combined with the use of passivation strategies, will lead to performance improvements in PSCs.

To this end, different approaches have been developed to mitigate the voltage-limiting mechanisms in PSC such as non-stoichiometric chemistry, additive engineering, Lewis acid-base surface adduct approaches, as well as the use of 2D perovskites, polymers, dielectrics and fullerene derivatives as surface-passivation materials. While unintentional bulk defects may be eliminated by increasing the crystal quality and/or doping of the perovskite, extrinsic passivation methods are needed to minimize interfacial and grain-boundary recombination losses. Next, for enhanced device performance, such surface-passivating materials should be integrated into the contact stacks of the devices without introducing additional carrier-transport barriers.

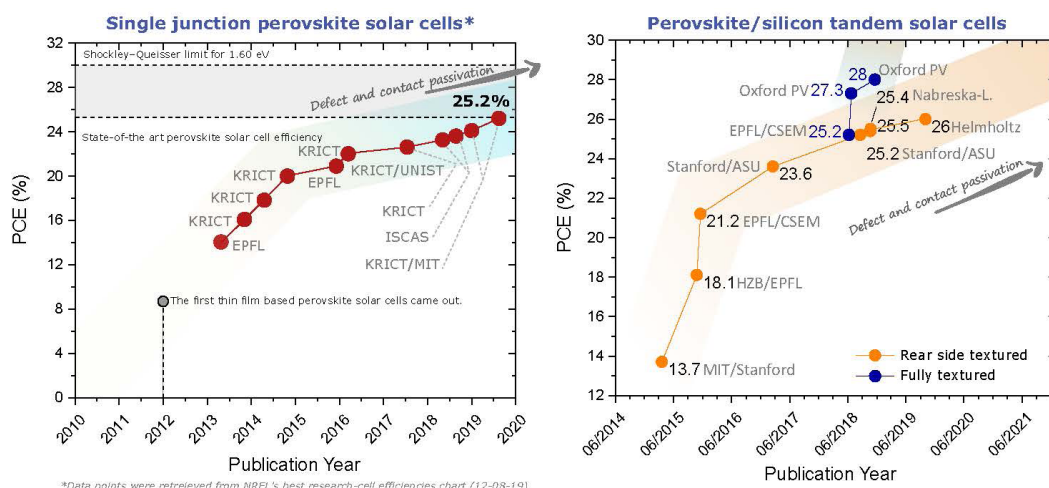


Figure 1. The evolution of the PCE values for the single-junction PSCs and perovskite/silicon tandem solar cells. Defect and contact passivation schemes are boosting PCE values toward the Shockley-Queisser limits for both configurations.

In this respect Erkan Aydin and coworkers recently published a comprehensive review in *Advanced Materials* with detailed explanations of the passivation schemes in PSCs and their influence on the device performances.⁽¹⁾

Although an increasingly wide spectrum of materials and techniques have been reported to reduce carrier recombination in perovskite materials and devices, so far, the majority of the reported passivation knowledge has been empirical. Quantifying the defects that are causing recombination still remains an open question. Exploring new and rapid spectroscopic and modeling techniques specifically geared toward understanding the passivation effect may be important in this direction.

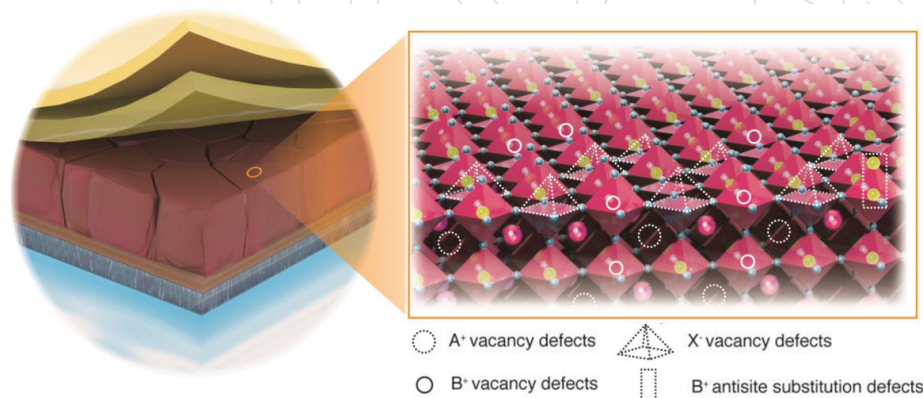


Figure 2. Schematic illustration of typical PSCs and detailed view of possible surface defects on perovskite crystals, e.g., interstitials, substitutional and vacancies.⁽¹⁾

On device level, the most critical parameter is arguably FF, which demands (passivating) contact stacks that simultaneously lead to low resistive and recombination losses. Taking inspiration from this point, a deeper understanding of factors that contribute to the contact resistivity of perovskite devices (such as Fermi-level pinning, the presence of thermionic barriers, as well the importance of chemical versus field-effect passivation) may give critical insights and lead the way to new types of contact stacks.

Long-term stability of perovskite devices is another sought after milestone if this technology aims to enter the conventional PV market. For commercialization, Pb-free perovskites, using Sn (or others) as a divalent cation, may be necessary. This change will raise new concerns regarding the passivation of defects originating from O-sensitive Sn^{2+} cations. Therefore, passivation of Sn-containing perovskites also should be considered. Besides this, scaling-up of perovskite solar cells requires large-area compatible deposition techniques; here vacuum-based deposition techniques can be considered to be particularly attractive. To approach market readiness, more realistic stability tests will also be required to further prove the effectiveness of passivation techniques.

KPV-LAB researchers also see benefits of the passivation schemes for the PSCs. Recently, the team has revealed the universality of PMMA passivation to improve the open-circuit voltage of the PSCs in collaboration with Australian National University.⁽²⁾ Additionally, the team observed that PMMA passivation has a crucial role in decreasing the hysteresis of the PSCs as well as increasing the open-circuit voltage.⁽³⁾ KPV-LAB researchers are currently developing novel passivation techniques for single-junction perovskite and perovskite/silicon tandem solar cells aiming to reduce open circuit voltage deficits.

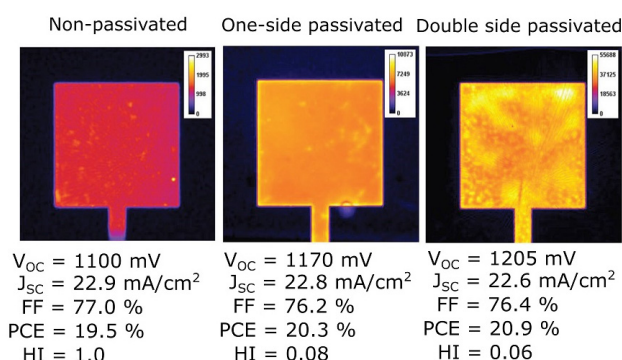


Figure 3. Photoluminescence images of the non-passivated, one side and double side PMMA passivated devices. The images clearly show the improved V_{oc} of the devices after each passivation step.⁽²⁾

Erkan Aydin earned his M.Sc. (2012) and Ph.D. (2016) degree in Micro and Nanotechnology Program from TOBB University of Economics and Technology, Ankara, Turkey. During his M.Sc. and Ph.D. he focused on the process development for cost-efficient and environmentally friendly fabrication of copper indium gallium sulfide (selenide) CIGS(Se)-based thin-film solar cells. Since 2016 he has been working on perovskite-silicon tandem solar cells at the KAUST Solar Center. His expertise lies in the process development and advanced characterization of high-efficiency perovskite solar cells for perovskite-based tandem PV devices by exploring thin films and engineering interfaces and contacts.



Erkan Aydin

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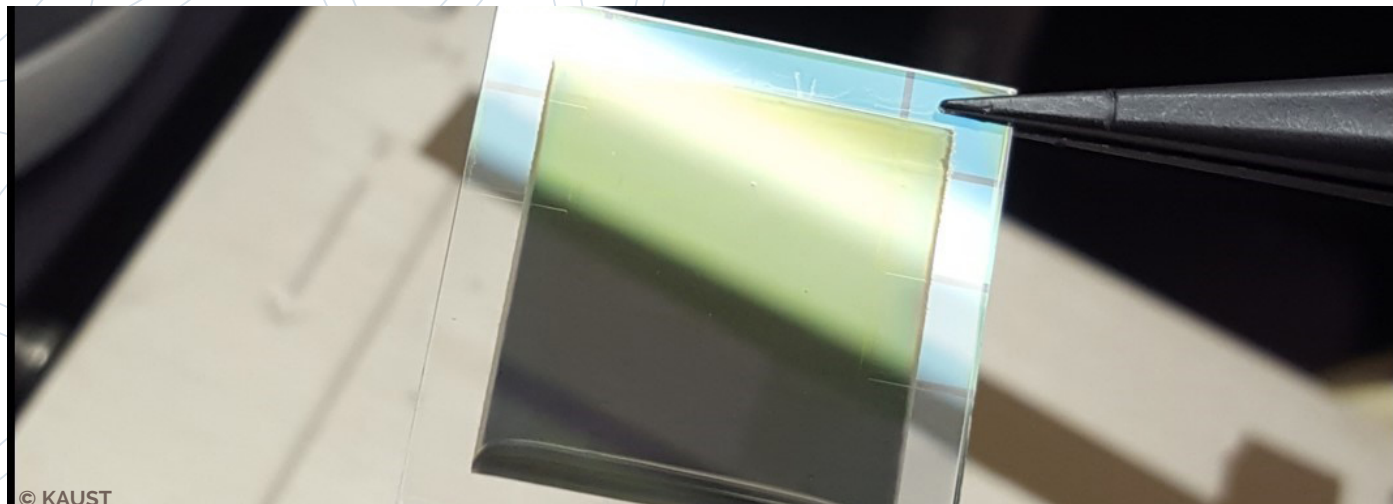


Figure 1. Inkjet-printed active layer processed using green solvents

Towards the integration of fully printed green solar cells for self-powered biosensing applications — By Khulud Almasabi & Eloise Bihar

Khulud Almasabi is an MS/Ph.D. Material Science and Engineering (MSE) student in Derya Baran's group. She completed her undergraduate studies at Taibah University in Medina, majoring in applied physics. Her thesis work focused on solar energy which was one of the reasons she was interested in pursuing her Master's research in this area. This summer Khulud has completed her Master's thesis on the development of highly efficient inkjet-printed organic solar cells processed using environmentally friendly solvents.

'As a Saudi I am from a country which has the potential for solar power. With the increase in energy consumption and energy demand, solar photovoltaic research seems a promising field.' said Khulud Almasabi.



Khulud Almasabi

Eloise Bihar obtained her PhD degree in bioelectronics from Ecole des Mines de Saint Etienne in Gardanne in France under the supervision of Prof. George Malliaras where her work focused on the development of printed biomedical devices for electrophysiology. She joined KAUST, as a postdoctoral fellow in July 2017 in Prof. Derya Baran's group (KSC, PSE) in collaboration with Prof. Sahika Inal (BESE) and later on with Prof. Khaled Salama (CEMSE) and is currently working on combining inkjet-printed biosensors with solar cell



Eloise Bihar

technologies.

Currently, organic solar cells are still limited in terms of their power conversion efficiency in comparison with the performance of inorganic solar cells but their reduced fabrication costs render them attractive for certain applications. Organic solution processable materials are promising candidates as alternatives to inorganic materials as they present undeniable advantages such as their soft nature, low cost, and suitability for low-temperature processing, making them appropriate for integration into roll-to-roll processes with different printing techniques.

The development of printing technologies for photovoltaics is a promising field, especially inkjet printing as it offers endless possibilities in terms of customization, freedom of design, and the ability to use flexible substrates for large-scale production.

However, one concern regarding organic solar cells is the common use of chlorinated solvents such as Chlorobenzene (CB), Dichlorobenzene (DCB) and Chloroform (CF) during the ink formulation process. While these solvents suit the inkjet printing process due to their high boiling points, suitable

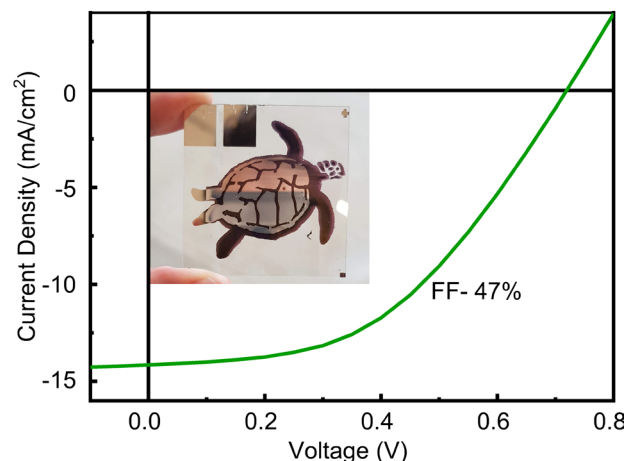
viscosity, and excellent solubility of the organic donor and acceptor compounds, they still pose some risks for both human health and the environment, excluding them from being the ultimate choice for large area production. Hence, research to find suitable non-toxic hydrocarbon solvent alternatives that meet the requirements for the fabrication of solar cells is on-going.

Khulud's research focuses on the engineering of environmentally friendly inks using a blend of non-halogenated benzene derived solvents optimized to meet the rheological property requirements of the inkjet printing process. Khulud is studying the influence of the parameters affecting the printability, such as viscosity, surface tension, boiling point, and solubility for different green solvents. She also works on the optimization of other key parameters for obtaining uniform and continuous layers, a prerequisite for improving the fill factor and PCE of the devices, by adjusting drop spacing and the printer bed temperature for each functional ink.

Recent ongoing efforts are concentrated on the study of new materials which can outperform fullerene acceptors such as PCBM, one of the most studied materials used as the active layer in combination with P3HT for organic solar cell fabrication. While fullerene derivatives have been at the heart of research so far due to their excellent electron transport properties, they still have significant drawbacks such as poor light absorption properties, limited tunability of energy levels and instability.

One of Khulud's recent achievements was the successful printing of an active ink comprising a novel non-fullerene acceptor (NFA) O-IDTBR (rhodanine-benzothiadiazole-coupled indacenodithiophene) and commercially available P3HT (poly(3-hexylthiophene)) processed using environmentally friendly solvents. These cells in a solar cell device demonstrated an efficiency of up to 4.73% – the best efficiency achieved so far by a P3HT:O-IDTBR system processed with all non-halogenated solvents. Khulud recently presented her results at the e-MRS spring meeting which was held on

Figure 2.
J–V of freeform inkjetprinted solar cell in the shape of a marine turtle on top of ITO glass.



27th–31st of May 2019 in Nice, France. She is currently working on printing other highly efficient material systems that could boost the device performance as well as increase the cells' transparency.

Baran's printing team recently published their first outcomes in the journal *Advanced Material Technologies* titled 'Digital Inkjet Printing of High-Efficiency Large-Area Nonfullerene Organic Solar Cells on the P3HT:O-IDTBR system'. They demonstrated that through engineering the composition of the active inks they could fabricate printed organic solar cells using inkjet-printing technology and that these could compete with other traditional coating technologies, such as spin coating and blade coating, in terms of device performance reaching over 6.4% PCE, one of the highest efficiencies reported in literature to date.

Together, Eloise Bihar, Daniel Corzo, and Khulud Almasabi, aka the "Baran Printing team", are working on developing the next generation of fully printed organic solar cells on flexible substrates, ITO-free, via the superposition/deposition of successive printed organic layers towards the realization of high performance solar cells.

Eloise's current research focuses on the fabrication of solar-powered electrochemical sensors for monitoring human metabolites fabricated via inkjet printing. Eloise recently published her latest work on inkjet-printed biosensors on paper for the detection of glucose in saliva in the journal *Nature Flexible Electronics*. This is a project led by Prof. Sahika Inal which is ongoing in her "Organic Bioelectronics" laboratory in BESE. Eloise printed all the components of the sensor from the electronics to the biorecognition elements. The study showed that the sensor could measure physiologically relevant glucose concentrations in human saliva based on enzymatic electrochemical detection up to 1 month after fabrication. Eloise and Prof. Inal are now working to commercialize this sensor via the Taqadam program.

'Printing all layers for the fabrication of solar cells is very challenging as it requires a lot of optimization to match the surface tension of all the inks deposited successively while preserving their properties. One of the difficulties we face frequently while printing is short circuits,' says post-doctoral researcher Eloise Bihar.

She is currently trying to integrate cutaneous biosensors with solar technology. Towards that end, Eloise is working in collaboration with Baran's printing team on the development and optimization of the printing process for the realization of highly efficient semi-transparent solar cells integrated in polymeric biocompatible substrates that could be used in daily life.

'The ultimate goal is to print high performance solar cells in order to replace batteries as the source of power for biomedical devices. Eventually, these solar cells would be integrated into conformable substrates, and would provide a sustainable power source for biomedical devices, and why not in the near future integrate them into smart garments' says Eloise.



KSC: Developing in harmony with Saudi Arabia

— By Christine Rueping

With the exciting developments in Saudi Arabia promoted by the Kingdom's Vision 2030 initiative for the advancement of the country, we are experiencing vibrant times. KAUST Solar Center is well positioned to seize the opportunities that the Kingdom and Vision 2030 afford. Notably for KSC, Vision 2030 promotes an economy less dependent on fossil fuels, as well as the expansion and localization of private sector industries, and the advancement of the Kingdom's educational system.

KSC intends to utilize its core strengths, characterized by a breadth of expertise covering the full spectrum of solar energy conversion technologies (organic photovoltaics (PV), Perovskite and silicon heterojunction technologies) to serve the Kingdom and simultaneously build a strong international reputation. Furthermore, we will expand our application focus into solar fuels and storage. KSC promotes interaction amongst researchers and drives this through collaborative project based research to derive maximum benefit from collective expertise. With a culture that fosters innovation and collaboration, we seek to rapidly transfer lab based research results to produce prototypes and demonstrators for fast adoption by the energy sector.

The geography of our region shapes us too. The benefit of Saudi sun hours for solar energy generation is self-evident but conversely the exceptionally high temperature conditions that solar panels in the region need to operate under, cause energy conversion efficiency losses. Addressing the need for improved high temperature performance is a key area of KSC research. Thanks to KAUST Office of Sponsored Research funding, one of our flagship research projects is 'High-Efficiency Perovskite/Silicon Tandem Solar Cells' in which a multidisciplinary team lead by Stefaan De Wolf is achieving

world class efficiencies.

Perovskite solar cells (PSCs) are rapidly emerging as a high-efficiency photovoltaic technology, with low-cost manufacture potential. As they can also achieve a relatively large bandgap, PSCs are particularly suited for use as top cells in conjunction with well-established silicon bottom cells to create tandem solar cells. In such a configuration, the PSC harvests the blue part of the solar spectrum while allowing low energy light to pass through, to be absorbed in the silicon bottom cell. In this way, the power conversion efficiencies of traditional silicon solar cells, with a Shockley-Queisser and Auger recombination limit of 29.4%, can be improved.

Our second flagship research project is focused on organic photovoltaic (PV) technologies. We have developed organic PVs that are flexible and either transparent or colored, which can be deposited by high throughput and additive printing techniques such as ink-jet and slot-dye coating. This leads to a wide range of new design possibilities and applications. In particular, building integrated photovoltaics is an exciting development area for KSC: architecturally enhanced, solar power generating buildings, in the smart cities of the future. To accelerate progress, our team is focused on developing stable, record efficiency organic solar cells via research into molecular design and interface engineering.

Stemming from the organic PV research conducted at KSC, Professor Derya Baran and her coworkers have formed a startup company, iyris. Based on an ink that captures infrared light, iyris makes transparent solar windows, producing electricity and blocking heat from entering a building.

In addition to solar electricity generation, KSC is developing

technologies for the solar driven production of fuels and chemical feedstocks which could potentially be a key technology to reduce reliance on fossil fuels as an energy source. Over the past decade, solar generated hydrogen has garnered attention but advances are still required to enable it to be cost competitive with fossil fuel derived hydrogen. At KSC, researchers are also focusing on organic semiconductors which are proving to be promising light absorber materials for solar driven fuel generation. From summer 2019 these efforts will be enhanced by a collaborative project between Professors McCulloch, Tung and Laquai together with coworkers, exploring new concepts and materials for photocatalytic water splitting and carbon dioxide reduction.

The research conducted at KSC is outward looking and we actively seek to work together with industry. In addition to multinational companies, KSC works with local companies to support their development efforts to meet the Kingdom's need for industrial diversification and growth.

Our collaboration with industrial partners is enhanced by cooperation with KAUST's outdoor testing facility, the NEO Solar Park. This on-campus technology park provides outdoor testing and monitoring facilities, attracting both regional developers and larger international companies keen to test their technology and generate data. KSC plans to utilize this data to gain improved understanding of the extreme outdoor conditions that solar panels are exposed to in Saudi Arabia and the long term effects on efficiency.

As part of a thriving university, KAUST Solar Center's greatest asset is its people, and educating the next generation of researchers in an environment of excellence is at the heart of what we do. 40% of the students at KSC are Saudi nationals who will be able to focus their knowledge back into the Saudi economy. Student numbers at the KSC will swell over the summer, as we host interns from universities across the Kingdom and abroad. International Masters and PhD students further enhance the diversity and expertise of our center and together with their Saudi counterparts they are able to form global networks for the future.

KSC's Saudi students shape their own future

At KAUST Solar Center we aim to support the advancement of the Kingdom through both our research and the empowerment of our Saudi students, enabling them to contribute to the country's long-term development. We asked Saudi students based in our various research groups to share the impact of their research.

Introduction by Wejdan Alghamdi, PhD Student

Over the last two decades, scientific research in Saudi Arabia has significantly increased. Along with awareness of the critical role that research plays in guaranteeing the nation's continuity and development, the country aims to shift the oil-based economy to a knowledge economy and diversify energy resources towards a renewable energy base. Recently, Saudi Arabia's government, underpinned by its Vision 2030 strategy, committed to generating 9.5 gigawatts of renewable energy by 2023 and 60 gigawatts by 2030.

There are still many obstacles to meet the Vision 2030 targets that young scientists are challenged to deal with. At KSC many young Saudi students have chosen to focus their research work on solar energy technologies under the guidance of global experts. Students are involved in projects that cover different aspects from material synthesis, device fabrication, photophysical analysis, and computational modelling. This variety of projects gives us a chance to participate in the development of solar energy research and to actively contribute to the Kingdom's development.



Salman Alsharif

Salman Alsharif, Masters Student, Chemical Science (McCulloch Group)

"I was surprised when I learned about KSC for the first time not only because of its state-of-the-art facilities but also its direct contribution to the development of Saudi Arabia. I see this in two ways: The first is the development of next generation Saudi scientists. As young Saudi researchers in the center, we are given the freedom to choose and tackle challenging problems in variety of fields. Also, we have the chance to work on sophisticated and advanced instruments

that help us to gain fundamental understanding of the underlying science and to publish our findings in prestigious journals. The center's unique interdisciplinary environment encourages discussion and collaboration, which improves our communication skills and encourages us to come up with creative solutions to challenging problems.

"Secondly, the center contributes by pushing the frontier of science and technology to solve solar energy challenges, helping to make Saudi Arabia an appealing destination for solar energy companies. Also, the center assists with the foundation of startups that work on the commercialization of the center's technology and patents, e.g. iyriss. I am very proud to be a part of KSC, since I am expanding my knowledge and contributing to the development of my country."

Wejdan Alghamdi, PhD Student, Material Science & Engineering (Anthopoulos Group):

"During my undergraduate studies at King Abdulaziz University, the work that most stimulated me was my research on the optical properties of nanoparticles. Self-education, through many online open courses focusing on the properties of materials and featuring case studies from industrial applications of advanced materials to nanotechnology, gave me some insight into research work. I visited KAUST during the last year of my undergraduate studies and I was amazed by the campus, labs, all the working facilities and the environment.



Wejdan Alghamdi

"Coming from a university that is not research directed to one of the world's largest academic centers for solar energy research was a big change for me. However, the lab operation staff in the center provided me with much training and helped me gradually to improve my skills. KSC's working environment is beneficial: people are here to help you with information or the running of experiments."

Areej Alzahrani, PhD Student, Material Science & Engineering (De Wolf Group)

"I have experienced first-hand the incredible research environment KAUST Solar Center has to offer. Advanced facilities and opportunities to share research through seminars and lecture series have made conducting research at KAUST an experience I feel lucky to have had. The uniquely diverse community provides the possibility for me to collaborate with international researchers both within and outside of KAUST.

"In particular, I wish to use the skills developed throughout my PhD to contribute to the furthering of research and the use of solar cells. This research is pivotal for the efficiency and application of solar cells to advance sustainable energy sources needed for the in-kingdom development planned in Vision 2030. I believe this research will enable me to fulfil the duty I have to others as it will shape the future of communities; as well as developing my knowledge which will enable me to inspire and educate future generations.

"The chance to meet people at conferences who are pioneering research within my field has allowed insightful scientific discussions which help shape my research focus. This, along with the skills and experience gained throughout my PhD will provide a starting point to continue my research in the future."



Shahad Sulaimani

Shahad Sulaimani, Masters Student, Chemical Science (McCulloch Group)

"When I first joined the Solar Center at KAUST I was fascinated by the great facilities available and this motivated me to conduct solar energy research to benefit and support my country in the dramatic changes that we are going through (Vision 2030). As a young Saudi I am encouraged to research and discover more about the problems that we face in the future regarding energy. At KSC we seek solutions to these problems ... KAUST provides great opportunities and is a great place to learn. We can discover hidden secrets in science and be creative in finding answers."



Maryam Alsufyani

Maryam Alsufyani, PhD Student, Chemical Science (McCulloch Group)

"As a Saudi student, I couldn't be more proud and confident than doing my research in the KSC. I have the chance to study; contribute and discuss the world's vision with the very diverse KSC members; and to work towards replacing fossil fuel energy with cheap clean solar energy. In the lab, by using organic polymers and small molecules, we're trying to improve the efficiency as well as the cost and flexibility of solar cells.

"It's now been a year since I joined the solar center and I've already gained a lot of knowledge and experience. Nothing has given me more confidence to stand up to the demands of my country and the world, than contributing to the research of the KSC. Located in the so-called sun-belt of the world, Saudi Arabia is well positioned to be one of the largest solar energy producers and, of course, that should be so important to every Saudi researcher wanting to contribute and improve the research of solar photovoltaic (PV) energy. I believe that this will definitely open up chances and paths for us in the future, as many companies are now concentrating on solar energy research.

"As a Saudi female, it's now the perfect age to rise, and I choose to pursue that through contributing to my country's demands via the KSC."

Wejdan Alsufyani, Masters Student, Material Science & Engineering (Laquai Group)

"My current research focuses on fabricating organic solar photovoltaics for industrial applications. My journey at KAUST has helped me grow on both a personal and professional level. This can be attributed to many things starting with the outstanding environment that KAUST has where diversity is essential to our growth. We work in a teams with people of different backgrounds, with many skills and perspectives, who offer unique ideas to find a broader range of solutions.

"I feel very privileged to be part of the KSC as it gives me the opportunity to participate in major projects that addresses essential challenges for the Kingdom and the world, such as solar energy. KSC empowers young Saudis to be part of the Saudi Vision 2030 by providing the inspirational laboratories that equip us with the necessary tools to promote and develop research towards the solar energy applications that suit the Kingdom for conversion of solar energy into electricity, reducing the economy's reliance on oil.

"History is measured by developments in materials that meet society's demands. It is my career goal to solve a major problem and to be part of this global development. Our responsibility as Saudi scientists starts with spreading awareness of the importance of solar energy and its application in the community. I plan to pursue a PhD degree in MSE to achieve my dream career in an academic field so that I can pass on my knowledge and experience to younger generations."



Wejdan Alsufyani, picture courtesy of Khulud Almasabi



Faculty Focus

Interview with Prof. Udo Schwingenschloegl

Udo Schwingenschloegl is a Professor of Material Science and Engineering with the university's Physical Science and Engineering (PSE) Division. He joined KAUST as an Assistant Professor when the university was founded in September 2008 and in 2011 was promoted to the rank of associate professor. From 2012 to 2015 he served as Associate Dean for the PSE Division and has been a full professor since 2014. Udo Schwingenschloegl's research interests concentrate on the electronic and structural properties of nanostructured systems, in particular those including surfaces and interfaces.



Please briefly describe the subject of your PhD research and what lead you to enter academia?

I received my PhD from the University of Augsburg, Germany. During my PhD, I used first-principle calculations to evaluate the common features and differences between the metal-insulator transitions in VO_2 and V_2O_3 by studying the so-called Magneli phases $\text{V}_n\text{O}_{2n-1}$.

After spending four years as a secondary school teacher in Bavaria, Germany, I developed an interest in combining scientific research with the education of students in cutting-edge subjects. My first university position was as a Visiting Professor at the University of Brasília (ICCMP), Brazil.

When and how did you first become involved with KAUST and how does being at KAUST support your research goals?

I applied for a faculty position at KAUST in Summer 2008 and assumed duties in September 2008. As the university was still under construction, I was initially located at Imperial College London until KAUST campus opened in September 2009.

KAUST provides me with access to excellent high performance computational facilities vital for my research, particularly the super computer Shaheen II, and supports both fundamental and applied research projects.

Please tell us about your current research interests?

My current research interests lie in condensed matter physics and first-principles materials modeling, focusing on 2D materials, materials for solar cell applications, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport.

You are currently working with KSC on collaborative projects. What is the role of your research group in these project?

My group aims to provide insights into physical and chemical processes playing a determining role in solar cell materials, both to support experimental efforts in the collaborative projects and to advance fundamental understanding of current and future material classes. Currently, we are looking into interfaces of $\text{Fa}_{1-x}\text{Cs}_x\text{PbI}_{3-y-z}\text{Br}_y\text{Cl}_z$ and crystalline Si with NiO_x , using the evolutionary crystallography approach. We also investigate three-divalent perovskites by first-principles calculations to establish the structure-property relationships, focusing on the size of the band gap and the structural stability.

What advice do you have for young scientists?

I always suggest to students and postdoctoral fellows that they should pursue what they enjoy in science, as this is the only way they will find the creativity and endurance to solve important problems.



KSC Summer School participants: talented students from across the Kingdom and around the world

International Partners

KSC Summer School offers 'global education' with our partners from TU Delft

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.

Over the last two years we have had enjoyed a successful partnership with Professors Miro Zeman and Olindo Isabella from the Technical University of Delft, Netherlands. The collaboration with delivering our summer school has benefited our center members, international interns and invited students from across the Kingdom who have profited from their wealth of expertise.

Following the success of the initial summer school held in 2018, July 1st-4th 2019 saw the launch of the second KSC Summer School and Internship Program. Aimed at undergraduates in their final year, interested in pursuing a career in the field of solar energy conversion, this year's program attracted students from across the Kingdom (King Abdulaziz University, Taibah University, Islamic University of Medinah) as well as internationally (UC Berkely, Imperial College London and the Universities of Washington, Bologna, Petras, Glasgow).

The four day summer school comprises lectures on photovoltaic (PV) fundamentals as well as silicon, perovskite and organic PV technologies with practical lab sessions addressing device fabrication & characterization and the properties of light. In addition to the KSC summer interns, the lectures are opened up to the broader KAUST research community. Selected students then go on to complete summer internships, conducting research projects in our laboratories. The whole summer program is made possible

by KSC faculty, postdocs and operational lab staff who mentor the students not only during the short summer school but throughout the summer. To complement our in-house capability we also draw upon external expertise and this year we again welcomed to the KSC summer school Professors Miro Zeman (MZ) and Olindo Isabella (OI) from the Technical University of Delft.

Professors Zeman and Isabella have been running a photovoltaic summer school for a number of years at their home university and we took the opportunity to ask them about the value of such educational programs.

When did you first become aware of KAUST?

OI: It was in 2012 during my time as a postdoc in Japan. Friends of mine moved to KAUST and since then I have been aware of the university's development. I am also aware of the progress being made by KSC in photovoltaics through numerous presentations given by Stefaan De Wolf at global

conferences.

MZ: Several years ago there was a KAUST call for international projects and many colleagues in the broader field of solar energy conversion were excited about the prospect of making a joint application due to the ideal and different weather conditions in Saudi Arabia. KSC is now much more visible and known to me for material science, engineering and processing aspects of PVs.

Why is it important to you to provide PV courses beyond standard university educational offerings?

MZ: Global education is about all our futures. We all share a hope for a better future. We need a vision about how people treat each other and the need to live in balance with nature. Education serves both of these goals and I consider myself fortunate to be involved with a technology that can provide answers. Our motto is: 'Reliable, sustainable and affordable electricity for everyone'. We truly believe that PV technologies can deliver this and we are happy to pass on our knowledge because it serves our overall vision for the future.

OI: Our vision about 'global education' includes bachelors, masters and postgraduate research, both on-campus and online, but also extends to courses for PV engineers to keep abreast of processing and system design, as well as in-the-field training. In a university setting it is worth remembering that most postdocs don't stay in academia but pursue industry careers, so it is important to provide them with relevant on-going training. In Delft we run courses that are didactically aligned: Courses are provided every quarter, building up along a logic chain of theoretical knowledge.

We were pleased to be invited back to support this year's KSC summer school. Didactically Miro started the lectures with the broader picture of the importance of solar energy and fundamental aspects. I was able to build on this, lecturing on PV technologies and the week was rounded off by KSC lecturers addressing topics such as Perovskites and organic photovoltaics.

As part of Saudi Arabia's Vision 2030 the country is looking to shift away from an oil based economy. What role can we play?

OI: To achieve a sustainable economy any nation needs knowledge. As a university, KAUST can help shape the change and make it possible. The university needs to take on this responsibility to contribute to the shift and bring young people together to rise to the challenge.

MZ: I like the quote from Robert Kennedy: "Some men see things as they are, and ask why. I dream of things that never were, and ask why not." I would challenge students at KAUST to dream and make their futures come true. Dreaming is necessary to achieve change and young people are full of dreams that can be realized.

How can the younger generation be empowered?

MZ: It is important that they recognize the issues and realize that they can be part of the change. This is the job of global education. We need young people to recognize that what they can achieve together is exciting and to be motivated by that.

OI: To empower young people, I would encourage them to see the world and to look at what different societies are doing and achieving. The young students I've met this week from both Saudi Arabia and abroad have had their interest in future solar technologies ignited and I hope we have created a hunger for global education.

Finally, what impressions will you take home with you?

OI: It has been most natural to wander around the campus. The campus facilities and education are fantastic and there is the infrastructure here for world class research. I enjoy each visit to Saudi Arabia and take home to Europe very positive images for the future.

MZ: That we can come and support the KSC summer program shows me that this university takes its global role importantly and I look forward to continued collaboration.



TU Delft Professors Olindo Isabella (l) and Miro Zeman (r) during the KSC Summer School 2019

Alumni Focus

Mahesh Kumar Ravva



Mahesh Kumar Ravva, picture courtesy of Mahesh Kumar Ravva

Mahesh Kumar Ravva received his Master of Science degree in Chemical Sciences from Pondicherry University, Puducherry, India in 2008 and his Ph.D. degree in Chemistry from the University of Madras, Chennai, India in 2013. After a brief postdoctoral appointment at the Georgia Institute of Technology, USA he joined as a postdoctoral fellow at King Abdullah University of Science and Technology in the Solar and Photovoltaics Engineering Research Center (now KAUST Solar Center) in the group of Jean-Luc Brédas. Mahesh Kumar Ravva is now Assistant Professor in the Department of Chemistry at SRM University, AP, India.

What were your research interests at KAUST?

My research activities at KAUST were directed towards the application of a range of computational methodologies to study challenging problems in the field of organic electronics and photonics. I was particularly interested in design and reengineering of organic/polymer materials and the study of their structural, electronic, optical and interfacial properties. My research work focused on establishing chemical structures, electronic properties, morphology, and device performance relationships by understanding a number of fundamental issues like charge generation and charge transport in organic materials.

Looking back, what were the benefits of having been at KAUST?

As I mentioned, I am a computational chemist and I need computational resources to solve problems related to my research. The extraordinary facilities available on campus, including the KAUST Supercomputer (Shaheen II), helped me a lot to conduct my research.

During my stay at KAUST, I also used to have very

good discussions with my experimental colleagues and distinguished professors which helped to understand the research problems much more clearly. In fact, the KAUST research seminars were very useful to learn about the research activities of other group members and help to form networks among students and post-docs.

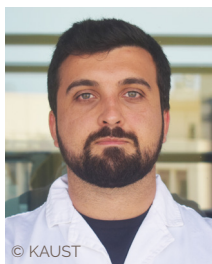
My journey at KAUST taught me how to overcome the challenges and situations that made me who I am today. Personally, I found fun to live in a compound with people from different nationalities and cultural background.

What is the current focus of your research at SRM University, AP, India?

My research group activities focus on understanding the electronic and optical properties of organic materials for organic electronics applications. Apart from these, we are also interested to understand the stability and reactivity of reactive intermediates, locating precise transition states for complex chemical reactions, kinetics, and thermodynamics aspects of chemical reactions by collaborating with experimental colleagues.

New Faces at KSC

Welcome to:

*Alberto Scaccabarozzi*

Postdoctoral Fellow with
Thomas Anthopoulos

From - Imperial College London, United
Kingdom

*Catherine De Castro*

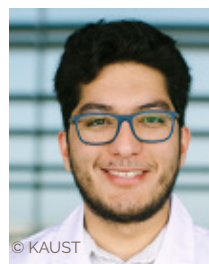
Postdoctoral Fellow with
Frédéric Laquai

From - University of Coimbra, Portugal

*Anand Subbiah*

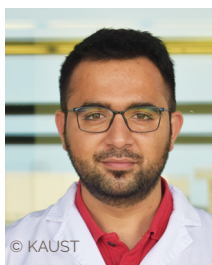
Postdoctoral Fellow with
Stefaan De Wolf

From - Indian Institute of Technology
Bombay, Mumbai, India

*Fahad Bokhari*

Master Student with
Frédéric Laquai

From - Purdue University, West Lafayette,
USA

*Anirudh Sharma*

Postdoctoral Fellow with
Derya Baran

From - Flinders University, Adelaide,
Australia

*Jules Bertrandie*

PhD Student with
Derya Baran

From - ENSCBP, Bordeaux, France

*Calvyn Howells*

Postdoctoral Fellow with
Iain McCulloch

From - University of St Andrews, United
Kingdom

*Luis Huerta Hernandez*

Master Student with
Derya Baran

From - Guevara Intellectual Property,
Sonora, Mexico



KAUST Research Conference: 3rd Generation photovoltaic technologies and beyond

Organized by KAUST Solar Center, chaired by Professors Iain McCulloch and Thomas Anthopoulos, and with financial support from the KAUST Office of Sponsored Research (OSR), this year's conference was held on campus from February 10th-12th.

The conference provided an exceptional opportunity to invite international experts from a wide range of institutions, including Georgia Institute of Technology, UC Santa Barbara, Imperial College London, EPFL and the Universities of Washington, Valencia and Groningen, to address exciting developments in the field of third generation photovoltaic (PV) technologies with emphasis on approaches for improving cell performance and manufacturing. Leading scientists and engineers from different disciplines, as well as key industrial contacts, came together to share and discuss their latest discoveries. This enabled researchers and students from KAUST and the Kingdom to receive a comprehensive overview of PV developments from other high calibre academic groups and entities, helping to generate new ideas and providing motivation for their own research and collaborative projects.

With over 20 representatives from external Saudi institutions and 38 international delegates, topics could be viewed from diverse perspectives. As such, the conference provided over 200 researchers, postdocs and students with a unique opportunity to attend presentations and join discussions with the speakers. The evening poster session not only allowed the young scientists to showcase their work to an international audience but also provided them an ideal opportunity to enter into dialogue with the visitors.

Industrial sessions with speakers from Dupont, Armor SAS and Sunew, mirrored KSC's efforts to focus on applied research so that more industrially relevant outcomes can be achieved. Young regional companies, namely iyris, HAALA Energy and Nomadd Desert Solutions were also provided with a platform to reach out to our delegates and guests.

An auxiliary half-day workshop addressing was also held to introduce students to diverse extra-curricular topics such as intellectual property, entrepreneurship and scientific publishing.

Finally, congratulations to Zhao Chao (PhD student, National University of Singapore), Nessler Kattan (Assistant Professor, Taibah University) and Dimitra Tsokkou (Postdoctoral fellow, University of Bern) who were award recipients for their poster contributions and to Jan Kosco (PhD student, KAUST Solar Center) who won the award for Best Young Scientist Talk.



PhD Profile

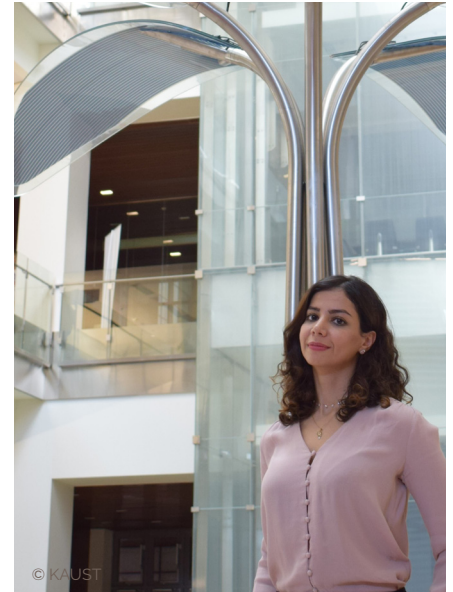
Sanaa Alshammari

I am currently a PhD student in the Material Science and Engineering program (MSE), working in the Laboratory of Advanced Materials and Applications (LAMA) under the supervision of Professor Thomas Anthopoulos.

I am working on multi-layer metal oxide electron transport layers in organic photovoltaics, as a novel structure to increase the performance of the devices. By studying their optical and electrical properties I aim to understand the mechanism of charge extraction and charge transport through metal oxides from the active layer to the electrodes. Additionally, I am researching the effect of doping and surface modifications of the metal oxides on the device performance.

Working in KAUST gives me the opportunity to learn and to sharpen my research skills by offering me the chance to work with experts here in KAUST and with cooperation partners worldwide.

KSC provides a collaborative environment for researchers with use of state-of-the-art facilities. In bi-weekly meetings there is interaction with faculty and researchers to discuss on-going projects, monthly social events to network with all members and their families outside of our labs and study groups for different activities.



Sanaa Alshammari

CARF Project Review

From July 2019 to June 2019 KAUST Solar Center was fortunate to receive 'Center Applied Research Funding' (CARF) from the KAUST Office of Sponsored Research to support research initiatives focussed on end applications.

In December a mid-cycle review was held, followed by an end-of-cycle review in June. In each of these review sessions the researchers active in each project presented their findings to KSC members and the wider KAUST research community. Open question sessions prompted dialogue, generating ideas for further development and refinement of the projects. Faculty also scored the performance of the projects with the ranking serving as the basis for project continuation.

The 2018-19 project 'Stable organic solar cells for building integrated photovoltaic and greenhouse applications' will be continued in 2019-20 in broader terms in the project 'Stable record efficiency organic nonfullerene solar cells via molecular design and interface engineering'.

The project, 'High-Efficiency Perovskite/Silicon Tandem Solar Cells' will also continue as a major flagship project for KSC and will be expanded to include elements of the 2018-19 project 'Highly transparent, stable, and highly conductive inter-layers for solar cells'.

In 2019-20 a new project entitled 'Advanced Carrier Selective Passivation Layer for c-Si solar cells with nano-gap interdigitated back contacts' will be undertaken and KSC will also look to further diversify its portfolio by introducing a new project, 'van der Waals heterostructures: new device concept for solar fuel applications'.

KSC welcomes industrial partners

The start of the year, KSC supported Kaneka Corp and GEC's Silicon Heterojunction installation at KAUST's NEO Solar Park facility. Together with KAUST Core Labs and Aramco, KSC's Prof. Stefaan De Wolf and Dr. Michael Salvador co-hosted the team from Japan who will test their technology under the local climatic conditions as part of a project subsidized by the Japanese Ministry of the Environment.

February saw a delegation from the Chinese solar energy sector, visit KSC for exploratory talks, together with the local Jeddah company, Desert Technologies.

In May we hosted a delegation from Saudi Aramco's Industrial Services Department, introducing them to our research and lab facilities.



Visitors from Kaneka Corp and GEC visit KAUST's NEO Solar Park with support from KSC, KAUST Core Labs and Saudi Aramco.

News



Dounya Barrit
picture courtesy of Dounya Barrit

Dounya Barrit wins best presentation award at ICAMSEC

Congratulations to KSC PhD student Dounya Barrit who won the best presentation award at ICAMSEC 2019: International Conference on Advanced Materials for Solar Energy Conversion that took place in Dubai from 30-31 January.

Assistant Professor Derya Baran named an 'Innovator Under 35 in the MENA region'

In 1999 MIT Technology Review began to honor young innovators whose work is shaping our world. The Innovator Under 35 List is now recognised globally as a unique platform for individuals who strive to make a disruptive and impactful change in the world. Following the launch of 'MIT Technology Review Arabia' in 2018, the region's young innovators are now also honored, including KSC's Prof. Baran for the technology behind her start-up, iyris, which enables windows to function as solar cells. Moreover, the technology also blocks heat from passing through, reducing the need to cool buildings, a particularly pertinent feature in the MENA region.



Derya Baran



Abdullah Al Ajmi
picture courtesy of Abdullah Al Ajmi

Abdullah Al Ajmi wins Gold Medal at the World Young Inventor Exhibition

Congratulations to Abdullah Al Ajmi winner of the World Young Inventor Exhibition's Gold Medal at ITEX 19 for "A novel organic solar cell using the polymer K37". Abdullah was an SRSI student in Prof. Laquai's Ultrafast Dynamics Group.

Congratulations to our Center Staff

In April Faisal Wali, KSC's Strategic Partnership & Lab Operations Manager, received his 10 year service award from KAUST President, Dr. Tony Chan and Acting Dean PSE Division, Dr. Ravi Samtaney.

In June Gumana Habis successfully completed the KAUST Administrative Program (KAP) following a six month placement with KSC, during which she took on the organization of the KSC Summer School. KAP develops young Saudi graduates and prepares them for their future careers. We are delighted Gumana's decided to stay with us at KSC to support the business administration team.



Top picture: (l-r)
KAUST President,
Dr. Tony Chan, Dr.
Faisal Wali and
Acting Dean PSE
Division, Dr. Ravi
Samtaney



Lower picture:
Gumana Habis

KSC Highlight Paper



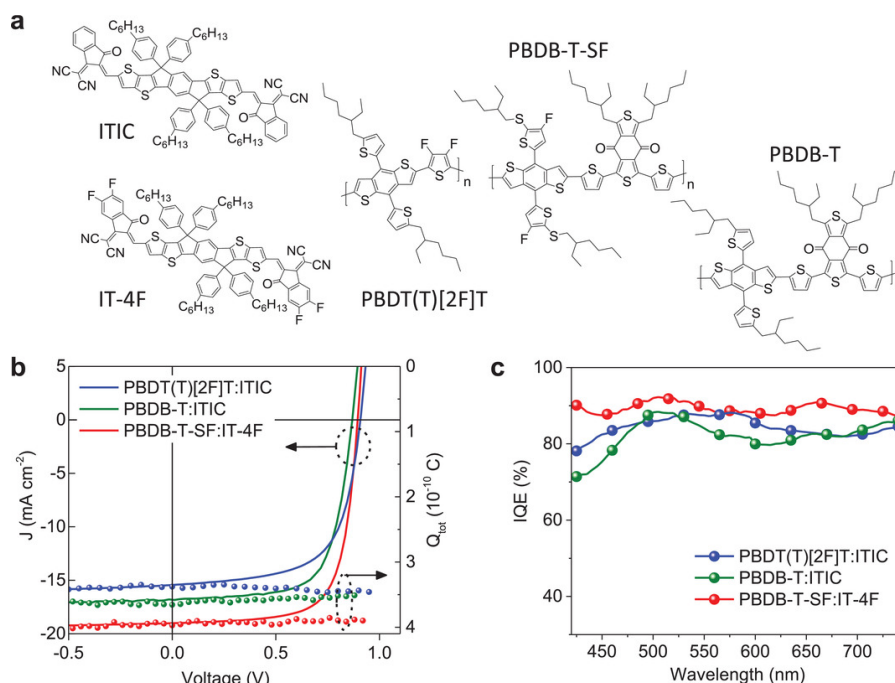
Key parameters requirements for non-fullerene-based organic solar cells with power conversion efficiency >20%

Since it was first published in March 2019, this paper from Yuliar Firdaus and coworkers has garnered much public attention. The paper formed the basis of a KAUST Discovery article, '[Benchmarks to better catch the sun](#)', following which it was promoted by Nature Research on social media where engagement was strong.

The team has used a computational approach to calculate cell efficiency targets for organic photovoltaic design.

Authors: Yuliar Firdaus, Vincent M. Le Corre, Jafar I. Khan, Zhipeng Kan, Frédéric Laquai, Pierre M. Beaujuge, Thomas D. Anthopoulos

Abstract: The reported power conversion efficiencies (PCEs) of nonfullerene acceptor (NFA) based organic photovoltaics (OPVs) now exceed 14% and 17% for single-junction and two-terminal tandem cells, respectively. However, increasing the PCE further requires an improved understanding of the factors limiting the device efficiency. Here, the efficiency limits of single-junction and two-terminal tandem NFA-based OPV cells are examined with the aid of a numerical device simulator that takes into account the optical properties of the active material(s), charge recombination effects, and the hole and electron



a) Molecular structure of donor (D) and acceptor (A) materials used in this study. b) J-V characteristics and total amount of charge (Q_{tot}) extracted from the device as a function of prebias (V_{pre}) measured by time delayed collection field (TDCF) experiments (10 ns delay time, -4 V collection bias, laser pulse fluence: $0.1 \mu\text{J cm}^{-2}$). c) IQE spectra of PBDB-T[2F]T:ITIC, PBDB-T:ITIC, and PBDB-T-SF:IT-4F BHJ cells.

mobilities in the active layer of the device. The simulations reveal that single-junction NFA OPVs can potentially reach PCE values in excess of 18% with mobility values readily achievable in existing material systems. Furthermore, it is found that balanced electron and hole mobilities of $>10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in combination with low nongeminate recombination rate constants of $10\text{--}12 \text{ cm}^3 \text{ s}^{-1}$ could lead to PCE values in excess of 20% and 25% for single-junction and two-terminal tandem OPV cells, respectively. This analysis provides the first tangible description of the practical performance targets and useful design rules for single-junction and tandem OPVs based on NFA materials, emphasizing the need for developing new material systems that combine these desired characteristics.



Yuliar Firdaus and colleagues have developed a computational approach to predict efficiency limits and propose design rules for nonfullerene organic solar cells.

Advanced Science, 1802028 (2019)

<https://doi.org/10.1002/adv.201802028>

Events



جامعة الملك عبد الله
للعلوم والتقنية
King Abdullah University of
Science and Technology

KAUST
SOLAR
CENTER

KAUST Research
Conference:

Emerging Concepts in Solar Energy Conversion - from Computation to Implementation

February
10 – 12, 2020

Save the date: Our 2020 conference will address solar energy concepts of global importance and with relevance to the Kingdom of Saudi Arabia:

- Photovoltaic solutions tailored to hot climate conditions
- High-efficiency silicon-based (tandem) solar cells
- High-efficiency solution-processed organic and perovskite photovoltaics
- Solar-energy conversion to solar fuels

The conference will also provide an opportunity for PhD students and postdocs to present their work in a poster presentation on the evening of Monday February 10th.

Travel Fellowships: A limited number of students and postdoctoral researchers will be awarded a travel fellowship to cover conference attendance, airfare and accommodation. The travel fellowships will be awarded by the scientific committee based on merit.

Further details will be published online: ksc.kaust.edu.sa/Conference-2020

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