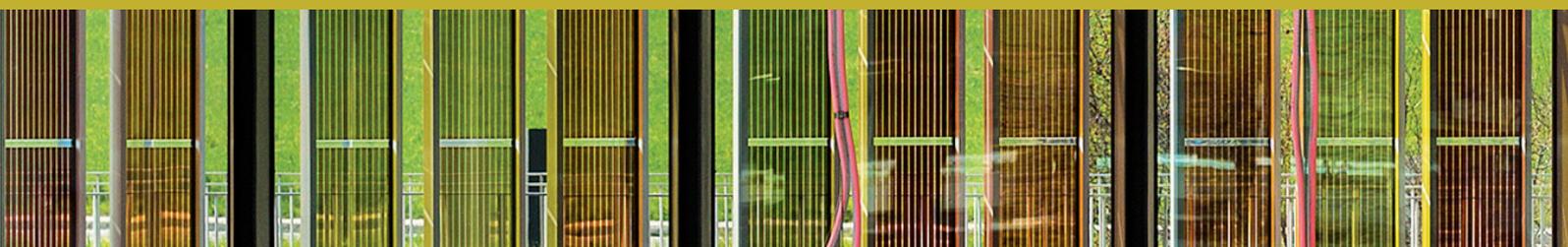


INSTITUTE OF CHEMICAL SCIENCES AND ENGINEERING

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MESSAGE FROM ISIC DIRECTOR PAUL DYSON

The past twelve months have been a period of considerable growth for ISIC, with seven new faculty members approved by the ETH board. These appointments have allowed ISIC to build on its strengths as well as to expand into new areas, and in so doing to consolidate its status as one of the top departments in Europe – a remarkable achievement, given the small size of our faculty compared to those of our competitors. Moreover, chemical engineering is not only back on track, but is now considerably stronger than ever with the arrival of Berend Smit, who also heads the EPFL's Energy Center, and two assistant professors, Ardemis Boghossian and Jeremy Luterbacher – the latter having graduated from our own Masters program in Chemical Engineering and Biotechnology a few years ago.

To maintain our world-leading position on dye-sensitized solar cells, we hired Anders Hagfeldt. And to quote the ETH board: 'EPFL strengthens its global leadership position in nuclear magnetic resonance spectroscopy and dynamic nuclear polarization in the long term', with Lyndon Emsley joining ISIC while continuing to head the Center for High Field NMR at the ENS-Lyon. We expand expertise in the coordination chemistry of f-elements with Marinella Mazzanti. And in the spring of 2015 Andreas Züttel's hydrogen research center at EMPA will relocate to the ISIC-Valais building in Sion.

This unparalleled period of growth, which shows no signs of stopping, has been made possible through both Federal and non-Federal resources. For example, a substantial donation from GAZNAT will allow us to continue to expand our activities in renewable energy. The new building for ISIC-Valais will open in Sion in 2015. And this year we saw the installation of the stunning large-scale Grätzel cell solar window facade on the new SwissTech Convention Center on the EPFL campus.



SWISS TECH CONVENTION CENTER BUILDING, EPFL, LAUSANNE

It is not only our research environment that improves with our carefully planned growth, but our teaching program is also strengthened. We are academically strong in areas of critical importance for the future. The connection between teaching and research at the Masters and Doctoral levels has been invigorated over the last few years, reinforcing a highly exciting and multidisciplinary learning experience for our students. Indeed, we are proud of our students, who enrich our environment and often go on to distinguish themselves once they have left. We should not overlook the contribution of our students to our continuous ascent in the world's academic rankings, although these rankings fully capture the essence of our community.

As always, we hope you enjoy reading about some of the highlights from yet another frenetic year. Please visit our website for more news and information concerning forthcoming events that might interest you, <http://isic.epfl.ch>. Your comments are always welcome, sent either by e-mail to secretariat.isic@epfl.ch, or by regular mail to the address below.

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ANDERS HAGFELDT AIMS FOR THE SUN



Anders Hagfeldt stepped into the world of dye-sensitized solar cells in 1991 and received his PhD from Uppsala University. He then joined Michael Grätzel as a postdoc, working on the development of the world-famous Grätzel cells. Today he is one

of the world's leading experts on mesoporous dye-sensitized solar cells and photoelectrochemical systems. His international impact was celebrated this year, when he was elected a member of the Royal Swedish Academy of Sciences (Kungl. Vetenskapsakademien) in chemistry. Now, taking up a new professorship at ISIC, Hagfeldt is bringing this arsenal to EPFL.

"I am a physical chemist. I got my PhD at Uppsala University, and during that time I began to work with dye-sensitized solar cells (DSSCs). I was visiting EPFL for the first time around 1991, and I got in touch with Michael Grätzel. Since then I've been doing research and development on DSSCs and various other types of solar cells and solar fuel devices."

Hagfeldt's research focuses on the molecular modification of nanostructured metal oxide electrodes for the development of efficient DSSCs. This means that first we must understand how DSSC systems function at a fundamental level. "I did my postdoc at EPFL with Michael Grätzel from 1993 to 1994, where – among other things – we looked into lithium ion batteries and also displays based on the same type of material as the solar cell." Upon returning to Uppsala University as an assistant professor, Hagfeldt also held a visiting professorship with the Royal Institute of Technology in Stockholm (KTH).

"My research is a fundamental search on the physical chemistry of this type of nanostructured solar cells. We have set up a longstanding research center here in Sweden between us in Uppsala, the KTH in Stockholm, and an engineering institute in Gothenburg. What we do is take basic research to materials development on solar cells, and also look at upscaling and production process development. We also have a spin-off company, *Dyename*, which we started two years ago with the purpose of commercializing solar energy materials and research."

A major breakthrough came in 2010, when Hagfeldt's group successfully replaced the common triiodide-based electrolyte of DSSCs with a cobalt-based one. "The traditional electrolyte component in the DSSCs has been and still is based on triiodide, and it's been very difficult to find an alternative. But in 2010, we did it. The cobalt-based electrolyte opened up a completely new direction for DSSCs in terms of improving the overall system and created new possibilities for higher efficiencies. Now, Grätzel's group has the world-record efficiency

of 13% for these DSSC's based on what we did in Uppsala with this type of new electrolyte and new dye modifications."

Of course, this is not the only milestone in Hagfeldt's career. "If we go back in time, very early on we presented the first description of charge transport in these materials. That's twenty years ago, more on the theoretical work of the solar cell, when we were the first to publish a description of how the electrons move in the system. We also advanced our understanding of charge separation in dye-sensitized systems by the end of the 1990s.

"Another highlight was creating a solar cell with a plastic substrate, using a special pressure-based technique. Finally came the development of characterization methods, when we coined the term 'toolbox for DSSC measurements'. It comprises different simple techniques and is essentially a standardization of measurements."

This research trajectory has now put Hagfeldt in the forefront of the most recent breakthrough in solar cells, the perovskite solar cells. Spearheaded by EPFL and the University of Oxford, this is an initiative Hagfeldt is looking forward to join. "I have had a longstanding connection to EPFL since I did my postdoc there. And then I was asked if I was interested in joining ISIC – and of course, a position that builds on Michael Grätzel's activities at EPFL is something you must think about carefully!"

"THE MOTIVATION IS ENVIRONMENTAL, THAT'S CLEAR. THE PROBLEM IS TO FIND SOMETHING THAT IS AS EFFICIENT AS LEAD-CONTAINING PEROVSKITE CELLS, BUT WE'LL HAVE TO SEE. WITH THIS TYPE OF HYBRID ORGANIC-INORGANIC MATERIALS SEVERAL NEW DIRECTIONS OPEN UP."

"I can't say that I ever wanted to leave Uppsala, but on the other hand, making a life change like this at least once was too interesting to not do. EPFL is of course a renowned center of worldwide research, so it's a key place with a lot of opportunities. It is an honor to take on the position here and to continue to collaborate with Michael, who, of course, is staying on. I'm looking forward to that."

In this close collaboration with Michael Grätzel, Hagfeldt already has plans for the immediate future. "We will continue to work on perovskite cells, as there are some fascinating directions there. One is to find alternatives to the perovskite cell lead content, and also to find alternatives to the currently used hole conductor. We have some good ideas, which we intend to pursue."

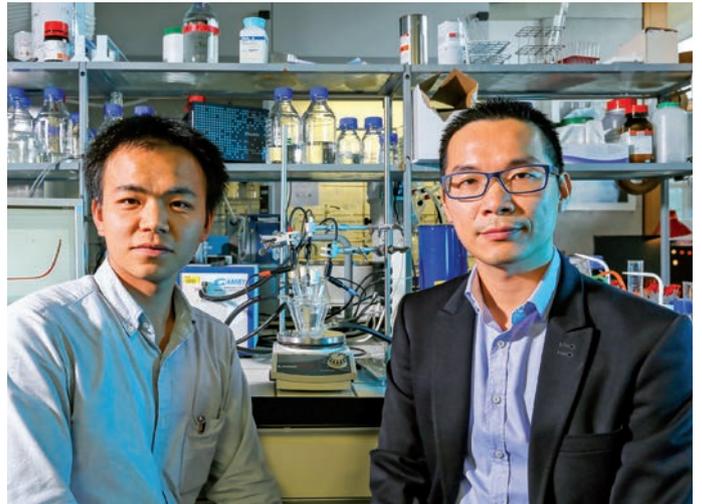
He is also looking forward to new collaborations for theoretical work. "We will also be carrying out fundamental studies because there are a lot of persisting questions about how the perovskite cell actually works. Perovskite solar cells have been such a tremendous and fast development that they are still lacking some research on basic understanding – for example, on the relationship between interface structure and efficiency. That direction will involve collaborations with other groups. I already know Michael Grätzel's and Jacques Moser's groups quite well, but I'm very excited to meet new colleagues and see what new possibilities open up."

IMPROVING THE COST AND EFFICIENCY OF RENEWABLE ENERGY STORAGE

And then is the question of lead content. “There are different opinions in the field. Some people say it’s not too much; it’s not a problem. Others think that even a little lead is a problem. I think it’s important, and I think that there are some new ideas in this area that have not been explored yet.”

Hagfeldt’s perovskite aspirations will not stop his work on DSSCs though. “I will also continue to work with DSSCs and new types of electrolyte components. I have a few ideas about continuing work not just on cobalt as a replacement, but on other redox systems. But all this has to be assessed on the basis on innovation; finding something that others aren’t working on at the moment. There are so many people in the field right now, so one has to be different.”

With all this lying just ahead, Hagfeldt can scarcely contain his enthusiasm. “I attended the HOPV 2014 conference, and that was really a big success, with state-of-the-art lectures and so on. Now at EPFL, we have entered this new chapter in research with great excitement.”



Scientists at EPFL have developed a method for improving the catalysis of water-splitting reactions used for storing wind and solar energy. The method chemically peels off the outermost surface of a catalyst, thereby maximizing its active surface for the reaction.

A major challenge in renewable energy is storage. A common approach is a reaction that splits water into oxygen and hydrogen, and uses the hydrogen as a fuel to store energy. The efficiency of ‘water splitting’ depends heavily on the catalyst. However, only the surface of the catalyst acts on the reaction, while its bulk is inactive. This restricts how much catalyst can be used, and limits the efficiency of water splitting in energy systems. Publishing in *Nature Communications*, Fang Song and Xile Hu developed a new method for maximizing the catalyst’s contribution by chemically ‘peeling off’ only its active surface and excluding its bulk from the reaction. Their data, which show 2.6- to 4.5-fold increase in water-splitting efficiency, pave the way for cheaper and more efficient renewable energy storage.

Because of the natural inconsistency of sunlight and wind, using them for energy purposes requires devices that can store that energy in the form of hydrogen for later use. These devices are based on a reaction called ‘photoelectrochemical water-splitting’, because it uses solar or wind energy to break water into molecular oxygen and hydrogen, the latter of which can be stored away as fuel for later use. But even though it is currently impossible to retrieve 100% of collected solar or wind energy, there are certain parts of the water-splitting reaction that can be improved to achieve much higher sustainable rates of storage.

Fang Song and Xile Hu have developed a novel method to increase the accessible active sites of the catalyst referred to as 'exfoliation' and is similar in principle to the method for obtaining graphene from graphite: wrap scotch tape around a piece of graphite, pull it off, and graphene from its outermost surface will stick to it. Exfoliation of metal oxides has already been used in electrochemical applications, e.g. batteries, chemical sensors and electrodes for supercapacitors, but this is the first time it has been implemented in the context of water splitting.

The exfoliating method developed by the EPFL scientists uses an organic solvent. Conventional metal oxide catalysts were incubated in the solvent, and a thin layer from its outer surface, 3 atoms-thick, peeled off. The single-layer surfaces retained their original structure, but when tested in the lab they showed increased catalytic properties.

The researchers tested several common metal oxide catalysts, including iridium oxide, which is an expensive material considered to be one of the most state-of-the-art catalysts for water splitting. Other catalysts included cheaper metal oxides based on iron, cobalt, and nickel. The data showed that exfoliated metal oxides increased the reaction rate by 2.6- to 4.5-fold compared to reactions containing the entire catalyst, meaning that if the exfoliation method is implemented in renewable energy systems, it could greatly increase energy storage. A few exfoliated cheaper catalysts even showed better efficiency than iridium oxide. The authors suggest that the enhancement of the reaction rate is mainly due to an increased number of the 'hotspots' on the catalyst where water molecules – in this case water – fit and undergo reaction.

The authors state that the new method represents a "top-down" approach in the development of oxygen evolution reaction catalysts", with a significant impact on energy research. The relatively simple exfoliation method and the increased catalytic properties of low-cost, abundant materials can open the way for cheaper and more efficient storage of energy obtained from renewable sources.

REFERENCE

Song F, Hu X. Exfoliation of layered double hydroxides for enhanced oxygen evolution catalysis. *Nat. Comm.* 5:4477 (17 July 2014). DOI: 10.1038/ncomms5477



Ardemis Boghossian, newly-appointed tenure-track assistant professor at ISIC, works at the intersection of two very distinct fields: nanotechnology and protein engineering. This is not accidental, as Boghossian developed her interest in nanotechnology and its applications during her PhD in Michael Strano's group at MIT. There she explored the development of biomimetic materials for photovoltaic cells, engineering nanoparticles to stabilize proteins for light-harvesting applications.

Her research continued with her postdoc work in the Frances Arnold lab at Caltech, where she currently focuses on a complementary approach: engineering proteins and biological cells to interface with synthetic materials, including nanoparticles and electrodes, for energy applications. "I've worked a lot with single-walled carbon nanotubes", she says. "I used them for biosensing applications and sensing applications in general. I also interfaced them and other nanoparticles with proteins, with a focus on light-harvesting applications."

Single-walled carbon nanotubes (SWNTs) are cylindrical tubes of graphene a single-atom thick and about 1 nm in diameter – though their length can vary. Because of their unique electrical properties and their ability to give out fluorescent signals, SWNTs are currently being explored in a wide range of applications. Boghossian's focus has been mainly in energy sources and sensing technologies such as biosensors that can be used inside the human body to detect physiological changes.

"Single-walled carbon nanotubes make excellent sensors. They are indefinitely photo-stable, meaning that their fluorescent signal lasts for a long time. They are also very, very sensitive to their environment, and small changes will result in a measurable change in fluorescence. This makes them really great sensors, specifically for the body." And because SWNTs absorb in the near-infrared rather than the visible region of the optical spectrum, their optical signals are not affected by tissue, water or blood.

This research path can be a game-changer for prevailing diseases like diabetes, where patients have to constantly monitor their blood glucose levels by pricking their finger on external devices. SWNT biosensors can help create devices that can automate this process. "One application is to create an artificial pancreas where, for example, you could continuously monitor your blood glucose level and have your insulin automatically dispensed depending on the amount of glucose in your blood."

Such technologies are currently limited due to the cost of glucose-monitoring biosensors. "This is a problem that I think that we can address through both nanotechnology and protein engineering.

COMBINES BIOLOGY WITH NANOTECHNOLOGY

We developed a glucose sensor based on SWNT fluorescence, which interfaces a SWNT with a glucose-binding protein. When this protein binds glucose, it changes conformation, which in turn changes the SWNT's environment and causes it to emit a fluorescent signal when the glucose concentration in the blood changes."

Another aspect of Boghossian's research is the interface of biological organelles with nanotechnology. The idea is to create hybrid constructs that can be used to improve the light-harvesting properties of photovoltaic materials used in solar cells. "Chloroplasts are very easy to access. If we can isolate them by just grinding up the plant, we can have a construct that has the benefits of a purified protein and a living organism."

"Cyanobacteria are the hot thing in the field, but in order to harness energy using biofuels, they have to be specifically engineered. Besides, you're not going to walk around in your back yard, pick up some cyanobacteria from a pond and expect them to naturally be able to produce biofuels in an efficient, competitive manner." The advantage of using chloroplasts for energy applications is that they offer more stability than isolated proteins, which usually last at most a few days.

"MUCH OF THE CRITICISM AGAINST USING BIOLOGY FOR ENERGY APPLICATIONS IS THAT BIOLOGICAL CONSTRUCTS HAVE NOT EVOLVED TO MAKE DEVICES; THEY HAVE NOT EVOLVED TO HARNESS ENERGY EFFICIENTLY. THEY'VE ONLY EVOLVED TO SURVIVE. USING DIRECTED EVOLUTION AS A TOOL, I'M TRYING TO CHANGE THAT. WHAT WILL HAPPEN IF WE CAN EVOLVE ORGANISMS THAT ARE UNDER SELECTIVE PRESSURE FOR MAKING GOOD DEVICES?"

Chloroplasts also offer advantages in both light harvesting and maintenance. "Chloroplasts already contain the machinery to repair or regenerate damaged proteins. In addition, they produce glucose, and glucose can be readily processed for energy. You don't have to engineer them to produce usable fuels."

Of course, chloroplasts are not as stable as whole cyanobacteria. When chloroplasts are exposed to light, reduction reactions increase and they start forming reactive oxygen species, which begin attacking proteins, causing the chloroplast to eventually degrade. "Isolating a chloroplast is basically like taking an organ out of your body, and trying to keep it alive. What we did was ask if there is something we can do to keep chloroplasts from being unstable and prolong their activity."

The answer lies in nanotechnology and specifically 'nanoceria', which are nanoparticle forms of cerium oxide that act as antioxidants by scavenging for reactive oxygen species. In a 2014 *Nature Materials* paper of which Boghossian was an author, Michael Strano's group demonstrated that nanoceria complexes were able to suppress reactive oxygen species inside extracted chloroplasts. "To keep these reactive oxygen species from accumulating inside the chloroplast, we use

nanoceria, which actively scavenge for them. They can do this over an extended period of time because their nano-scale nature allows them to regenerate. So, in theory, nanoceria can scavenge for reactive oxygen species and prolong chloroplast activity over time."

Boghossian's current work takes a different approach. "My focus is, rather than trying to engineer nanoparticles to interact with biomaterials, to engineer proteins and living constructs so that they can interact with nanoparticles. Specifically, I'm engineering new constructs to allow whole cells to interface with SWNTs and electrodes." This is a challenging proposition since the proteins found in nature tend to be very specific to their biological functions, but Boghossian is undeterred. "When a protein binds to something we're trying to sense in the body, it undergoes a conformation or electrical change. This is something we can interface with SWNTs to send out a fluorescent signal, turning the whole system into a biosensor."

This is the kind of work she intends to pursue at EPFL in her new position at ISIC as tenure-track assistant professor. "In my professorship, I'm trying to combine two fields to exploit their complementary advantages: Nanoparticles have amazing optical photophysical properties, but are not so good in recognizing biological molecules. On the other hand, we have biological constructs that are really good at recognizing biological molecules, but their photophysical properties outside the body are not so great. I'm hoping to combine the optoelectronic properties of nano-materials with the molecular recognition and robustness of biological materials to make a new generation of devices specifically for biosensing and energy applications."

But Boghossian's vision doesn't stop there. "I'm also interested in interfacing SWNT fluorescence and using this as a tool to evolve and engineer new proteins. I'm hoping that I can use SWNTs as a sensor to engineer new proteins. What I'm ultimately interested in is taking this to the next level where, in addition to engineering nanomaterials that will enhance stability, to also engineer biomaterials like living cells and systems so that they can interact with biomaterials and transfer energy through these mechanisms."

LYNDON EMSLEY USES NMR TO BREAK OPEN MOLECULAR STRUCTURES



As scientific director of the Centre for High Field NMR (CRMN) in Lyon, Lyndon Emsley campaigned for seven years to install a 1 GHz NMR spectrometer at his institute. The milestone machine is the most powerful of its kind, and has opened up avenues

for exploring biological structures like large and membrane-bound proteins. Now, Emsley is bringing his immense expertise to EPFL by taking up a professorship at ISIC.

“The objective of our research is to find out how molecular systems, especially in the solid state, work. To do that, we need to determine atomic-level structures and dynamics. And since these objects are obviously beyond direct visualization, we need to use indirect methods of detection. The key methods for detection are often based on NMR spectroscopy. By developing new methods, we can determine atomic and electronic structures and measure dynamics or even thermodynamics in detail in an increasingly wide range of systems.”

NMR spectroscopy works by exploiting the resonance frequencies of atomic nuclei in molecules and compounds when they are placed in a strong magnetic field. Despite being a relatively lengthy process, NMR often has an advantage over rival structural approaches like X-ray crystallography, which can demand months or even years to grow suitable crystals of substrates before it can resolve their structures. NMR can, for example, yield useful information about proteins that are poorly defined or that would have to bind to another protein in order to crystallize.

“A lot of this science is based on diffraction of X-rays. But today we’re seeing an increasingly large number of problems, including biological machines or membrane proteins in the bio area, or surfaces of titanium dioxides involved in solar conversion in the materials area, where what we’re looking at is neither crystalline nor regular – or we might be looking at an interface or the edge of the material. In such cases, X-ray crystallography doesn’t provide clear answers.”

Emsley intends to use the power of NMR in crystalline solids such as drug molecules used in the pharmaceutical industry. But he is also interested in developing methods to look at molecules outside crystalline environments like those on surfaces, often used in a wide range of applications today, including catalysis, energy conversion and gas storage. “Most industrial processes today that involve molecular transformations occur at the surface where you either have a catalytic event or some other interaction between molecules on the surface. The processes depend heavily on the precise arrangement of atoms on the surface.” Structurally resolving such arrangements is key in optimizing industrial processes, and this is where NMR comes into play.

“Today there is much development of alternative methods to determine surface arrangements of atoms. One example is electron microscopy, and our lab has developed NMR spectroscopic methods to work with it. What we like to do is try to work out exactly what is the surface arrangement or the shape of a material, e.g. titanium dioxide”.

But that means first overcoming the current challenges that NMR faces, namely sensitivity and resolution. Sensitivity has to do with obtaining an observable signal from molecules. “Increasing sensitivity is a big challenge. One of the key ways that we are addressing it is by developing new methods that involve quantum-mechanical processes. Here, we take electronic degrees of freedom and combine the high sensitivity arising from their high polarization to strongly polarize the NMR transitions.” The approach can potentially strengthen signals by hundreds of times, which can lead to experiments that are ten thousand times faster and more sensitive.

The other NMR challenge is resolution. “If we are looking at a complex molecule on a surface, such as biological machine, there will be thousands, or maybe even tens of thousands of different signals coming from all of the different atoms. One of the big challenges in NMR is to observe and identify, in a given spectral window, all of these thousands of transitions, and then to associate the data with the properties of the molecule.”

“OUR RESEARCH IS REALLY CENTERED ON THE QUESTION OF HOW WE CAN DETERMINE STRUCTURES IN SYSTEMS WE PREVIOUSLY COULD NOT.”

To address resolution in NMR, Emsley’s group is developing a technique called ‘multi-dimensional NMR’, which can identify each of the single atomic resonances. “We can see exactly ‘who’s doing what’, thus gaining the resolution we need in the spectrum to build a detailed structural model of the system.”

The alluring possibility of exploring novel NMR avenues is what drew Emsley to EPFL, where he will be sharing his time with ENS-Lyon. “This seemed to me to be a unique chance to capitalize on the infrastructure and resources of both institutions – both of which have a strong history of advanced NMR research – in such a manner that the result will obviously be greater than the sum of the parts. I think that the chemistry and materials science [in ISIC] is simply among the best in the world, and given the opportunity to be able come and join that department, it was very hard to say no. There’s a very, very good group of people working on the kinds of chemistry and materials problems that we are very interested in providing these tools for. So I jumped at the opportunity!”

In the immediate future, Emsley is planning to develop what he calls a ‘dynamic mixture of polarization methods’, which aims to enhance NMR sensitivity of surfaces. Ultimately, he wants to use these to study technologically relevant surfaces and develop similar approaches towards solving structures in bulk systems, e.g. pharmaceutical formulations. “We’d like to be able to look at structures and interfaces in intact formulations, and explain the behavior of drug release inside the complex formulations that have been developed in the pharmaceutical industry today.”

JEREMY LUTERBACHER'S RESEARCH IS FUELLED BY BIOMASS



It seems almost inevitable that the future of renewable energy will include biomass-derived fuels. However, turning plant material into liquid biofuels such as ethanol requires breaking down cellulose molecules into their component sugars. So far, protocols for doing

this involve concentrated acids, ionic liquid solvents, and cellulase enzymes. But Jeremy Luterbacher, who joined ISIC in August as a Tenure-Track Assistant Professor, has broken through with a different path.

"I've done a lot of research on biomass upgrading to fuels and chemicals. That has been my starting perspective, and that's what drew me to pursue a PhD and continue working as a postdoc," says Luterbacher.

As a Postdoctoral Research Fellow in James Dumesic's lab in the University of Wisconsin-Madison Department of Chemical and Biological Engineering, Luterbacher made headlines in early 2014 when he published a paper in *Science* demonstrating that a renewable biomass-derived compound called γ -valerolactone, or GVL, can help break down cellulose selectively and efficiently. Using GVL, Luterbacher and his colleagues showed that biomass sugars can be obtained in a single step using this renewable easily produced from compounds already present in biomass, and without aggressive treatments or additional chemicals.

"I think it's a topic that's generating a lot of interest right now because if you think of the world in which we live, we're highly dependent on fuels, and that's something a lot of people realize. There's going to be a tremendous demand for biomass-derived products in the future because biomass is really the only large-scale source of carbon that's renewable – besides atmospheric CO₂, which isn't very easy to convert."

In certain countries, biomass is burned in stoves, making it the dominant energy source. Other countries co-fire biomass and coal in power plants. However, using biomass to produce liquid biofuels is still experimental in most countries. "One of the reasons that biofuel solutions are not implemented is because they are either not quite economical enough or not green enough," says Luterbacher.

Luterbacher aims to address both these issues by developing cost-effective and ecologically benign biofuel production methods as it has been shown that in Switzerland a significant proportion of its fuel could come from waste biomass. A primary focus of his research is scaling up biomass systems to bring them out of the lab and into the real world.

"You can get beautiful results if you work with model compounds or very dilute systems that are completely unrealistic industrially," he says. "So, I have systemically run experiments and determined

what yields would look like under conditions that are relevant to the real world. That means using real plant materials that may be challenging to work with when they are processed according to industrial standards."

Another part of Luterbacher's research focuses on understanding the mechanisms behind the relative efficiency of different biofuel processes.

"One of the highlights of my PhD was to explain the link between increasing access to plant matter and the ease with which you can convert it to biofuel with enzymes," says Luterbacher.

"It has long been known that there is a correlation between access and ease of conversion, but I developed mathematical models to describe that correlation. The old way of biofuel production was to treat biomass with chemicals and heat, and then add enzymes without truly understanding the theoretical link between these two steps. I showed how increasing the available surface area of the plant matter during the initial stage improved conversion by allowing the subsequently added enzymes to access and attack. So, you're really not doing anything special to the chemical properties of biomass—you're just increasing access to it."

The third and final aspect of Luterbacher's research was highlighted in his *Science* paper. "We showed that GVL exhibited remarkable properties in terms of enhancing acid-catalyzed reactions, and dissolving some parts of biomass that have been difficult to dissolve until now, such as lignin. Converting biomass to sugars is the first step in many processes to make anything from plants, so the method has tremendous potential."

"WHEN WE DEVELOP BIOMASS CONVERSION METHODS, WE HAVE TO THINK ABOUT MAKING RENEWABLE PROCESSES MORE EFFICIENT AND MORE ECONOMICAL."

As an alumnus of EPFL, Luterbacher was drawn back to Lausanne by more than just his passion for biofuels. "EPFL is just a high-quality institution, and its location in Lausanne, which is a nice place to live, is a great combination. The quality of the science at EPFL now rivals the major US institutions.

"EPFL's funding model allows you to take risks that you just couldn't take when you're always trying to satisfy a funding agency."

Luterbacher also finds ISIC ideal for his future research plans. "There are few departments in the world where they have a combined chemistry and chemical engineering programs, and I think that's smart and exciting because there are a lot of overlapping themes."

So how does he plan to divide his research time at ISIC? "I hope to develop a larger theme of making processes greener and more sustainable. We're going to start by doing what we know, working on converting plants, but I'd like to expand into sustainability and green chemistry: making processes more environmentally benign, more efficient, more atom-efficient, less wasteful, etc.

"I plan to work on several areas in biomass conversion research. One area I'm excited about is combining biological and chemical

SIMULATION AND CREATI BEREND SMIT SEARCHES

catalysis within the realm of biomass conversion. If we're going to swap petroleum for biomass, we need to figure out how to make a lot of different things because there's just a huge amount of molecules right now that we're making from petroleum.

"I also want to continue improving catalytic processing of biomass. Proteins and inorganic salts from plants can cause a lot of problems in a biomass conversion system, and so one area I'd like to get into is designing better catalytic materials that can target specific molecules and remain active even when working in messy systems. When you work with natural systems such as plants, there are many challenges but also endless possibilities for research."



Berend Smit studied Chemical Engineering and Physics in the Netherlands, where he first became interested in the field of molecular simulations and using classical force fields to predict the properties of materials. Following that, his focus turned to thermodynamic

properties and phase behaviors of hydrocarbons, which gradually moved him towards catalysis – an area that would become his research domain during his years in Berkeley. Now, he joined ISIC as a head of the newly-founded Laboratory of Molecular Simulation.

Smit's name has become associated with carbon capture and sequestration, and particularly in the discovery and development of materials that can be used in this area. "I spent quite some time trying to understand the behavior of hydrocarbons in zeolites. This is important in the context of catalysis, e.g. refining; the conversion of oil-related molecules into more useful molecules. If you want to increase your octane number, you want to convert linear hydrocarbons into branched hydrocarbons. So it's all about energy-related applications."

Berend Smit's research has encompassed materials known as zeolites. These are aluminosilicate minerals with exceptionally consistent microporous structures, and are used in the petrochemical industry as catalysts and molecular sieves. In attempting to create computer models of the interactions between zeolites and hydrocarbons, Smit found that size was an important consideration.

"From a molecular simulation point of view it is relatively easy to do small molecules because they move faster. So if you're doing molecular dynamics, you're just mimicking the time evolution of these systems, i.e. how they move into the pores of zeolites. If the hydrocarbons move slower, then the diffusion slows down, which increases simulation time by 8 to 10 orders of magnitude. Simulating at this rate quickly becomes impossible, so we have developed techniques to deal with long-chain hydrocarbons. These proved to be extremely successful: we can now predict the adsorption isotherms of linear hydrocarbons, branched hydrocarbons, in all kinds of different zeolites, and that has given us crucial insights into why certain materials are better for some processes than others."

It was his interest in pursuing research in energy that led Berend Smit to EPFL. "In particular, I want to see whether chemical engineering can evolve around the theme of energy rather than the traditional chemical industry, and that is something which resonates very well with EPFL. EPFL is one of the best institutes in Europe, and the way they support research is really outstanding."

Smit will take up two positions at EPFL: one as Professor at ISIC and one as Director of the EPFL Energy Center (<http://energycenter.epfl.ch>). His dual role seems to fuel his ideas for the immediate future of his

ON: FOR THE BEST MATERIAL

research. “EPFL has an excellent computational infrastructure with many excellent groups, so I’m hoping to take advantage of that position. Because of my interest in energy, I’m planning to focus on what we would call the ‘materials genome’, which is a recent initiative that started in the US, where they’ve realized that it takes an extremely long time for novel materials to be implemented in practical applications.”

To address this, Smit aims to mimic novel materials using computational techniques, trying to shorten the time it takes from fundamental research and discovery to practical applications. “For example, we are looking for ways to screen millions of possible materials in order to identify the best one for carbon capture. So we have to make a model of the carbon-capture process and see what are the important material properties we need to predict with sufficient accuracy. Then we go back to the genome aspect, which sounds a bit crazy because it’s really biology, but the idea is that DNA uses from four simple ingredients, and about 20 amino acids can make thousands of different proteins.”

These biological principles can be translated into the synthesis of nanoporous materials. “For example, I’m looking at metal-organic frameworks where you can change the metal or the linker, and with these ingredients you can make millions of different materials. Practically, we can synthesize only a small fraction of those. But in a computer we can actually generate all these hypothetical materials and evaluate them beforehand to determine whether they’re good enough for a certain property.”

to go to the fundamentals of actually being able to exactly rapidly predict those properties sufficiently and accurately.”

To achieve this, Berend Smit is looking forward to working with CECAM at EPFL. “There are many beautiful opportunities to collaborate there. Not only for computational research, but for research related to energy in general. From the Energy Center perspective, I think for EPFL there will be, in the future, a lot of money for various organizations available for energy research. It’s very important that EPFL makes a coordinated effort to create proposals and plans that show its strength. Since all these energy calls are very multidisciplinary, across the boundaries of research schools, the Energy Center should be able to coordinate these kinds of things, and make sure that we coordinate coherent proposals in which all the relevant groups participate.”

“WHAT IS INTERESTING TO DO IS TO BRIDGE THE GAP BETWEEN WHAT PEOPLE ARE DOING IN THE MATERIAL SCIENCES USING FUNDAMENTAL QUANTUM CALCULATIONS, AND WHAT’S ACTUALLY GOING ON IN CHEMICAL ENGINEERING.”

This is what lies behind the concept of a ‘materials genome’. “We use computers to generate millions of hypothetical materials to identify which ones are the best for practical applications. When we look at carbon capture, methane or hydrogen storage, or the many energy-related issues, it’s there where we want to be able to screen different materials so we can focus your experimental effort on the most promising ones. Having said that, we also want to predict the properties of a material before it’s synthesized. From a computational and scientific point of view that is an extremely interesting challenge – how can we guarantee that we’ll predict accurately enough?”

An important practical question is the definition of a best material. “From a chemistry point of view, we can look at the best performing materials that we can synthesize today and analyse. What I really would like to do is to reverse that situation, to actually go to the practical applications, to talk with chemical engineers and ask them how they would rank materials, which can be very different. I think the best way is to both analyze a process to identify the key factors that determine the performance of a material, and then try

NEW MOLECULE ENABLES QUICK DRUG MONITORING

Kai Johnsson's team invented a molecule that can easily and quickly show how much drug is in a patient's system. The molecule, now the basis of a start-up company, is expected to enable point-of-care therapeutic drug monitoring.

Monitoring the drug concentration in patients is critical for effective treatment, especially in cases of cancer, heart disease, epilepsy and immunosuppression after organ transplants. However, current methods are expensive, time-consuming, and require dedicated personnel and infrastructure away from the patient. Published in *Nature Chemical Biology*, scientists at EPFL introduced novel light-emitting sensor proteins that can quickly and simply show how much drug is in a patient's bloodstream by changing the color of their light. The method is so simple that it could be used by patients themselves.

Effective drug treatment relies on balancing the efficiency and toxicity of the drug, which lies at the core of personalized medicine. But as each patient differs from another, this requires constant monitoring in order to best customize drug dosage and prevent side-effects or even poisoning. Current drug-monitoring methods rely on techniques that require specialized personnel and expensive devices, and have to be carried out in diagnostic labs away from the patient's point-of-care. Developing quick, low-cost methods could improve drug therapy at the patient's bedside or home, especially in areas with poor medical infrastructure.

A NEW MOLECULE FOR MONITORING DRUG CONCENTRATION

Kai Johnsson's team at EPFL has developed a novel biosensor molecule that can quickly and accurately measure drug concentration in a patient's system without requiring anything more complicated than a regular digital camera. The molecule is the result of innovative protein engineering and organic chemistry, and has been shown to work on a range of common drugs for cancer, epilepsy and immunosuppression.

The sensor molecule works by binding the drug circulating in the patient's bloodstream and changing color accordingly. The molecule itself is made up of four components. One component is a receptor protein, which can bind the molecules of the target drug. The second component is a small molecule similar to the target drug, which can bind the drug receptor. The third component is a light-producing enzyme

called luciferase, and the fourth is a fluorophore molecule that can modify the color of the luciferase's light when it comes close to it.

When there is no drug around, the receptor and the drug-like molecule bind together. This brings the fluorophore close to the luciferase enzyme, and the system produces a red light. But in the presence of a drug, e.g. in the blood of a patient, the drug molecules bind the receptor more efficiently and therefore "push" the drug-like molecule off it. The whole sensor molecule system opens up, taking the fluorophore away from the luciferase. As a result, the emitted light turns gradually from red to blue in proportion to the concentration of the drug.

The doctor or the patient can record the signal very easily by putting a drop of sample, e.g. blood, onto a piece of paper, placing it in a dark box and photographing it with a conventional camera. The photograph can then be analyzed by color-measuring software to generate an average measurement. By comparing this measurement to a standard drug-concentration curve, it is easy to calculate the drug concentration in a sample or a patient's bloodstream. The sensor molecule can be used with virtually any kind of drug, as it simply requires changing the receptor protein on one end and the drug-like molecule on the other.

SUCCESSFULLY TESTED AGAINST ANTI-CANCER AND OTHER DRUGS

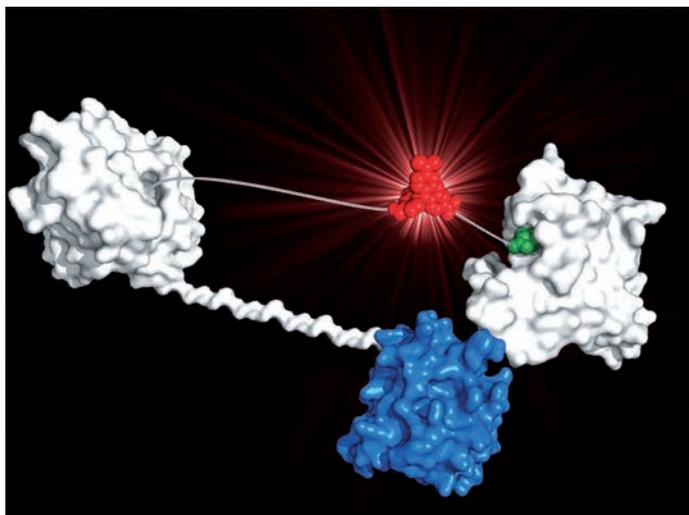
The EPFL scientists have called their new class of biosensors "LUCiferase-based Indicators of Drugs", or LUCIDs. To test their versatility, they developed LUCIDs against six commercially available drugs, including three immunosuppressants, one anti-epileptic, one anti-arrhythmic, and one anti-cancer drug. The drugs were successfully tested in vitro, and the anti-cancer one was also tested against actual human blood-plasma samples. The signal from all six LUCIDs was shown to be accurate and very stable.

"This system is a cheap, effective solution for customizing drug dosage in patients across a whole array of diseases", says Rudolf Griss, one of the authors. The successful achievement has encouraged him and co-author Alberto Schena to develop a start-up company in order to streamline and commercialize the innovation. "We envision a simple, hand-held detector where the patient can take a pin-prick of blood and can have an immediate reading of free drug concentration in their system – much like diabetics do now for blood glucose."

This work involved a collaboration between EPFL's Laboratory of Protein Engineering and the National Centre of Competence in Research (NCCR) in Chemical Biology with the Clinical Chemistry Laboratory (Service of Biomedicine) at the Centre Hospitalier Universitaire Vaudois (CHUV) who donated the human blood plasma samples, and the University of Washington's Department of Biochemistry.

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UNCOVERING THE 3D STRUCTURE OF A KEY NEURORECEPTOR

Horst Vogel's team revealed for the first time the 3D structure of a crucial neuroreceptor. The achievement has great implications for understanding the basic mechanism of electrical signal transmission between neurons and might help to design novel medicines to treat various neurological diseases.

Neurons are the cells of our brain, spinal cord, and overall nervous system. They form complex networks to communicate with each other through electrical signals that are generated by chemicals. These chemicals bind to proteins on the surface of neurons that are called neuroreceptors, opening or closing electrical pathways that allow transmission of the signal from neuron to neuron. One neuroreceptor, called 5HT3-R, is involved in conditions like chemotherapy-induced nausea, anxiety, and various neurological disorders such as schizophrenia. Despite its clinical importance, the exact way that 5HT3-R works has been elusive because its complexity has prevented scientists from determining its three-dimensional structure. Publishing in *Nature*, EPFL researchers have now uncovered for the first time the 3D structure of 5HT3-R, opening the way to understanding other neuroreceptors as well.

NEURORECEPTORS: STRUCTURE AND FUNCTION

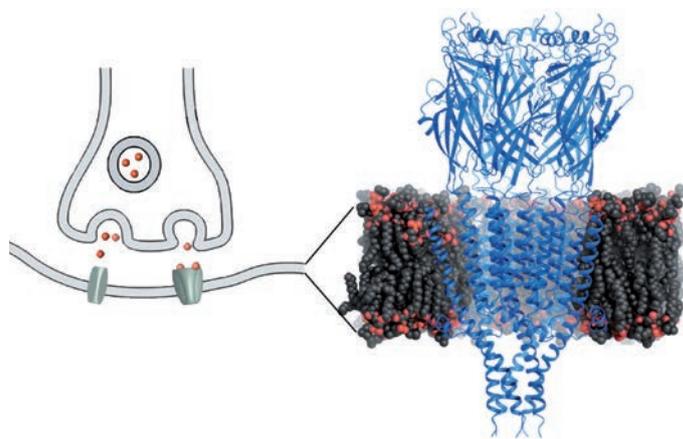
Communication between the neurons of our body is mediated by neuroreceptors that are embedded across the cell membrane of each neuron. Neuronal communication begins when a neuron releases a small molecule, called a 'neurotransmitter', onto a neighboring neuron, where it is identified by its specific neuroreceptor and binds to it. The neurotransmitter causes the neuroreceptor to open an electrically conducting channel, which allows the passage of electrical charges across the neuron's membrane. The membrane then becomes electrically conducting for a fraction of a millisecond, generating an electrical pulse that travels across the neuron. The family of neuroreceptors that work in this way is widespread across the nervous system, and is referred to as the "ligand-gated channel" family.

The mystery is how the binding of the neurotransmitter can induce the opening of an electrical channel to transport a signal into the neuron. The understanding of these molecular machines is of great medical importance, especially since neuroreceptors are involved in many neurological diseases. Currently, none of the mammalian ligand-gated channel neuroreceptors have been structurally described, which significantly limits our understanding of their function on a molecular level.

UNCOVERING THE STRUCTURE OF 5HT3-R

The team of Horst Vogel at EPFL has used X-ray crystallography to determine the 3D structure of a representative ligand-gated channel neuroreceptor, the type-3 serotonin receptor (5HT3-R). This neuroreceptor recognizes the neurotransmitter serotonin and opens a transmembrane channel that allows electrical signals to enter certain neurons. The 5HT3 receptor was grown in and then isolated from human cell cultures, and finally crystallized.

But before obtaining the 5HT3-R crystals, the EPFL team had to overcome a number of challenges. First, the relatively large size of the membrane-embedded 5HT3-R, like that of other similar channel neuroreceptors, makes it notoriously difficult to purify in sufficient



quality and quantity. After years of painstaking work, the EPFL scientists succeeded in obtaining a few milligrams of 5HT3-R, which was still not enough to grow crystals using conventional methods.

Still, the crystal quality was insufficient. To address this, Vogel's team used small antibodies, so-called nanobodies, which were obtained from llamas after the animals were injected with purified 5HT3-R. From a large library of isolated nanobodies, a particular one was found to form a stable complex with the 5HT3-R, and this complex eventually yielded crystals of exceptional quality.

After this, the procedure was straightforward: The crystals for X-ray crystallography were investigated at the synchrotron facilities at the Paul Scherrer Institut in Villigen and the European facilities in Grenoble.

The X-ray diffraction experiments yielded the 3D structure of 5HT3-R at an unprecedented resolution of 3.5 Ångstroms (0.35 millionths of a millimeter). The resulting 3D image shows a bullet-shaped 5HT3 receptor with its five subunits symmetrically arranged around a central water-filled channel that traverses the neuron's cell membrane. The channel can adopt two states: a closed, electrically non-conducting state or, after binding a neurotransmitter, an open, electrically conducting state that allows the flow of electrical charges in and out of the neuron to generate an electrical signal.

"We have now elucidated the molecular anatomy of a receptor that plays a central role in neuronal transmission," says Horst Vogel. "It is the first 3D structure of its kind and may serve as a blueprint for the other receptors of this family. In the next step, we have to improve the resolution of the structure, which might give us information on how to design novel medicines that influence this neuroreceptor's function."

This work is supported by the Swiss National Science Foundation (www.snf.ch) and represents a collaboration between EPFL's Laboratory of Physical Chemistry of Polymers and Membranes; the Center for Cellular Imaging and NanoAnalytics of the University of Basel; the Swiss Light Source and the Laboratory of Biomolecular Research of the Paul Scherrer Institute; the Architecture et Fonction des Macromolécules Biologiques of the Centre National de la Recherche Scientifique; the Université Grenoble Alpes; and the Unité de Dynamique Structurale des Macromolécules of the Institut Pasteur.

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VASSILY HATZIMANIKATIS RECEIVED THE IMES AWARD



Vassily Hatzimanikatis has been named the recipient of the 2014 International Metabolic Engineering Award.

The International Metabolic Engineering Society (IMES) is a community within the American Institute of Chemical Engineers' (AIChE's) Society for Biological Engineering. Every two years, IMES recognizes "an outstanding career contributor to the field of metabolic engineering" with an award.

This year, IMES has given the award to Vassily Hatzimanikatis, Professor of Chemical Engineering and Bioengineering and head of EPFL's Laboratory of Computational Systems Biotechnology (LCSB) and Fellow of the American Institute for Medical and Biological Engineering. His research interests are in systems biotechnology, bioinformatics, and the complexity of biological systems. He is also Editor-in-Chief of *Metabolic Engineering Communications*, Senior Editor of the *Biotechnology Journal*, Associate Editor of the journals *Metabolic Engineering*, *Biotechnology and Bioengineering*, and *Integrative Biology*, and a founding director of IMES.

Hatzimanikatis is being honored "for developing new methods to model and analyze large metabolic networks, and for demonstrating how such networks can be used to study biosynthetic pathways." The Metabolic Engineering Award was presented at the IMES-sponsored Metabolic Engineering X conference, in Vancouver (June 15–19), along with a lecture by Hatzimanikatis.

ELENA DUBIKOVSKAYA RECEIVED THE LEENAARDS AWARD 2014



The work of **Elena Dubikovskaya** in targeted breast cancer chemotherapy was recognized with the prestigious Leenaards award for 2014.

The Leenaards Foundation, founded in 1980, awarded this year a total amount of CHF 1,750,000 to two prestigious projects in translational biomedical research. This field combines clinical research and basic science, and aims to rapidly translate basic discoveries into therapeutic applications.

One of the two awards was given to a collaborative project between Elena Dubikovskaya who heads the Laboratory of Bioorganic Chemistry and Molecular Imaging at EPFL, Anita Wolfer at the CHUV, and Yann Siembille at the HUG. The project develops a new method for precise targeting of breast cancer tumors with potent chemotherapeutic agents. This can be achieved by adding a peptide that specifically targets chemotherapeutic drugs to cancer-specific receptors expressed in tumors.

By improving drug specificity, the researchers hope to minimize systemic toxicity, while significantly increasing therapeutic dose at the site of the tumor, providing breast cancer patients with more efficient treatment.

Elena Dubikovskaya received her PhD in the field of Organic Chemistry and Drug Delivery from Stanford University and joined EPFL in 2011 as a tenure track assistant professor.

TWO EPFL PROFESSORS WIN THE SCS WERNER PRIZE 2014



Professors Clémence Corminboeuf and Jérôme Waser were each awarded the Werner Prize 2014 from the Swiss Chemical Society.

Two ISIC professors have been awarded the prestigious Werner Prize from the Swiss Chemical Society. The Prize is awarded annually to promising young Swiss scientists or scientists working in Switzerland (under 40 at the time of the award) in order to recognize their outstanding independent chemical research.

Clémence Corminboeuf was awarded for developing and applying state of the art computational and theoretical methods for interpreting and solving chemical problems in complex systems.

Jérôme Waser is recognized for the development of novel synthetic methods and strategies to construct complex structures of potential biological interest.

HUBERT GIRAULT RECEIVES THE CHARLES N. REILLEY AWARD



Professor Hubert Girault has been selected by the American Society of Electroanalytical Chemistry for the 2015 Charles N. Reilley Award.

The Award is given in memory of Charles N. Reilley, one of the most renowned analytical chemists of the 20th century. Like his own work, the award celebrates scientists who eschew mere empiricism in favor of fundamental understanding.

Professor Girault's research focuses on electrochemistry in particular of charge transfer reactions at soft interfaces, biosensors for allergy research, off-gel electrophoresis for protein fractionation and ionization methods for mass spectrometry. He is currently Associate Editor of *Chemical Science*, the flagship journal of the Royal Society of Chemistry.

The award ceremony will take place at the Pittcon conference in March 2015 in New Orleans.

MICHAEL GRÄTZEL: THREE AWARDS



Michael Grätzel received the 2013 Benoist prize, as well as the first Lee-Anne Conn prize in renewable energy from the University of Kentucky and the 2014 Eric and Sheila Samson award. In addition, he published two papers in *Science* this year.

The first, with the Michael Grätzel Center for Mesoscopic Cells of Huazhong University (China), developed a perovskite solar cell that does not require a hole-conducting layer (July 2014). The novel solar cell achieved energy conversion efficiency of 12.8%, and was stable for over 1000 hours under full sunlight. Two months later, in September 2014, he published another paper in *Science*, combining a pair of solar cells made with a mineral called perovskite and low-cost electrodes to achieve 12.3% conversion efficiency from solar energy to hydrogen. The conversion percentage is a record for earth-abundant materials compared to rare metals. Both stories have gathered considerable media attention.

In addition, Michael Grätzel was the recipient of two prestigious awards: The Marcel Benoit prize and the Eric and Sheila Samson Prime Minister's Prize for Innovation in Alternative Fuels for Transportation.

The Marcel Benoit prize has been awarded annually since 1920 to scientists working in Switzerland who have made, as stated in its founder's testament, "the most useful scientific discovery or study, in particular in disciplines which are of significance for human life." It is administered and awarded by the Marcel Benoit Foundation, and remains one of the highest distinctions of science in Switzerland.

The Eric and Sheila Samson Prime Minister's Prize for Innovation in Alternative Fuels for Transportation is the world's largest monetary prize (\$1 million) awarded by Israel to pioneers in the field of alternative fuels. It is given each year to scientists who have made critical advancements in the field, selecting from a long list of candidates in Israel and the world. Grätzel will share the prize with another winner, Professor Thomas Meyer from the University of South Carolina, known for his work in artificial photosynthesis and water splitting. The award ceremony took place on December 3, 2014 in Tel-Aviv during the 'Fuel Choices Summit', an international conference on fuel alternatives organized by the Fuel Choices Initiative of Israel's Prime Minister's Office.

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