



INSTITUTE OF CHEMICAL SCIENCES AND ENGINEERING

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MESSAGE FROM ISIC DIRECTOR PAUL DYSON

ISIC is a superb institute with a world-leading faculty and outstanding staff and students. Not surprisingly, 2015 saw ISIC continue to ascend rankings – coming in at first place in Europe in the National Taiwan University Ranking, which bases performance on scientific publications. According to the Web of Science, which ranks chemistry departments according to publications and citation data from the last decade, ISIC is now ranked at the top in Europe, having finally overtaken Cambridge towards the end of 2015, while also overtaking Harvard and Stanford in the same year. While these rankings are a reasonable measure of our academic achievements, we must also continue to respond to the needs of society around us. And it is exactly our ability to connect our scientific achievements with the wider world, both locally and internationally, that shapes our goals and helps us to translate fundamental science into new processes and products, as well as to create new companies that have a lasting impact on the world we live in.

The past year saw the opening of a new ISIC satellite at Sion, which is part of the *Energypolis*. The major focus is on renewable energy and sustainable chemistry, although other areas are also present including environmental protection and analytical chemistry. After considerable planning, the ISIC satellite has gotten off to a stellar start: 150 researchers are already occupying the 7000 m² of new labs and offices, with another 50 researchers expected to arrive over the next couple of years. The new faculty members bring new competences to ISIC, making it an exciting hub of learning, discovery, and knowledge.

This year's annual Newsletter emphasizes the nascent activities in Sion. But it's not like things have stagnated in Lausanne: the number of our researchers reached record levels, while 2015 witnessed the creation of the Lausanne Center for Ultrafast Science, a new ISIC-led interdisciplinary center conceived and headed by Professor Majed Chergui.



DR. ELENA VLADIMIROVA IN THE LABORATORY OF PHYSICAL AND ANALYTICAL ELECTRO-CHEMISTRY, SION

At its heart lies a unique, multifunctional platform for ultrafast photoelectron spectroscopy of gas, liquid and solid systems with capabilities that are not available anywhere else in the world. Finally, the NCCR in Chemical Biology – a joint initiative between EPFL and the University of Geneva co-directed by Professor Kai Johnsson – received an outstanding mid-term evaluation, leading the the Swiss National Science Foundation to renew it for another four years, notably with a 20% increase in funding.

We hope you enjoy reading this issue of our Newsletter, which contains only a few highlights of our successes in 2015. Far more news and information about ISIC are available on our website: <http://isic.epfl.ch>. Your comments are always welcome, which you can send either by e-mail to secretariat.isic@epfl.ch or by regular mail to myself at the address below.

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SION: RAFFAELLA BUONSANTI BRINGS NANOTECHNOLOGY TO SUSTAINABILITY



Raffaella Buonsanti heads up a new research group at EPFL Valais Wallis as tenure-track Assistant Professor. Her lab will be looking at combining nanotechnology with sustainability by synthesizing semiconductor and metal oxide nanocrystals, and integrating them

into energy devices. In addition, the lab will also look at new ways to interface nanocrystals with building blocks of a different nature (i.e. polymers and porous materials). Her work will open up new possibilities for combining hybrid and multifunctional nanomaterials in catalytic processes e.g. transforming solar energy into chemical energy.

“I hope to build an international team of young researchers with different scientific backgrounds,” she says enthusiastically. But her scope exceeds the confines of the lab. “My aim is to inspire students with my work and my classes. Ultimately, I want to help shape the next generation of scientists.”

After completing her PhD in 2010 with the University of Salento (Italy), at the National Nanotechnology Laboratory, Buonsanti joined the Molecular Foundry at the Lawrence Berkeley National Laboratory, in California. Whereas her doctorate work had focused on the synthesis of nanocrystalline heterostructures with magnetic and photocatalytic properties, her postdoc turned to the doping of metal oxides for smart windows, and assembling nanoparticle/polymers to build functional mesoporous electrodes.

After two years, Buonsanti was promoted to project scientist at the Foundry, a non-tenure track position that gave her the opportunity to engage the user community by sharing her considerable expertise on nanomaterial synthesis. In 2013, Buonsanti joined the Joint Center for Artificial Photosynthesis in the Materials Science Department at Lawrence Berkeley National Laboratory as a tenure-track staff scientist. That was where she began building her own research group, which has now moved to Sion.

“We are a very young and enthusiastic team,” she says.

“We are motivated by the challenges of energy technologies for a more sustainable society. I am just starting to build my group in Sion, so for now it is only me, my postdoc, Anna [Loidice] and my PhD student Esmail [Kamali]. But I expect us to grow quickly in the next few years.”

Her lab’s focus is on developing novel synthetic routes for tailoring hybrid materials. The design is based on atomically defined nanocrystals. The group seeks to achieve superior control on the structure and composition of nanocrystals, and to do so at multiple length-scales. This means that her research must be based on

a fundamental understanding of the chemical transformations that drive nucleation, growth and assembly.

“The nanomaterials we make can be used in many different applications,” says Buonsanti. “Achieving such high tunability is essential to build meaningful relationships between structure and properties, which constantly improve the current state-of-the-art.”

Trying to reimagine the future of global energy, researchers are seeking alternative means of energy production. Currently, our dependence on fossil fuels requires us to capture and store CO₂ in order to keep in from reaching dangerous levels in the atmosphere. Recycling CO₂ by converting it into useful chemicals, such as fuels for transportation, is becoming a critical research field, since its ultimate aim is to wean us off fossil fuels and petroleum and onto clean, sustainable energy sources.

“PLANTS TRANSFORM WATER AND CO₂ INTO SUGAR. WE ARE BUILDING ATOMS-BY-ATOMS NEW ARTIFICIAL MATERIALS WHICH WILL TRANSFORM WATER AND CO₂ INTO FUELS AND USEFUL CHEMICALS TO MOVE TOWARDS A MORE SUSTAINABLE SOCIETY”

That is the research plan of Buonsanti’s lab for the next five years. “Using nanochemistry, we will try to answer questions such as: Can we make materials that can store energy into chemical bonds, like plants do? And materials that capture and convert sunlight, water and CO₂ into useful chemicals, such as fuels for transportation, in a more efficient manner?”

These are the questions Buonsanti will pursue as she begins her journey at Sion, which she aims to take full advantage of. “I expect to create a highly collaborative environment; I strongly believe that collaborative science is key to advancing the knowledge and addressing problems in society.”

SION: MOHAMMAD NAZEERUDDIN SETS UP A LAB FOR PEROVSKITE SOLAR CELLS



Professor Mohammad Nazeeruddin heads up one of two industry-funded labs at Sion, focusing on functional materials and photovoltaics. Born out of Professor Michael Grätzel's lab at EPFL, Professor Nazeeruddin's lab has gathered world-renowned expertise on perovskites, which are solid mineral pigments with promising photovoltaic properties.

His new lab at Sion is funded by Abengoa, a company specializing in the solar industry. Abengoa is funding two researchers at EPFL Valais Wallis at Sion, offering two million Swiss francs across five years, with additional licenses for almost half a million Swiss francs. The funds will be shared by two research labs at Sion and two at Abengoa's site at Seville.

Abengoa has been working with EPFL since 2012. Now, the two partners are investing in the EPFL-Abengoa Research Center, which will focus on research and development of perovskite-based photovoltaics. The joint effort aims to facilitate the transition from lab to production.

Nazeeruddin's lab will build on their expertise in perovskites, which are semiconducting materials that can absorb light and generate electron-hole pairs. The electrical charge can be collected at cost-effective prices.

Perovskites are applied on a very thin layer on solar panels, using methods that will greatly reduce the cost of solar cell fabrication. "Perovskite pigments are very simple to apply, which cuts down on costs," says Nazeeruddin.

At Sion, Nazeeruddin leads a research group of 23 involving 12 postdocs, 6 PhD students, and technical assistants. "I am lucky to have high-level scientists with diverse expertise working in my group. The team is international, with people from various countries and cultural backgrounds. And we are very pleased with the state-of-the-art facilities provided by EPFL and the city of Sion. Now that our laboratories are fully equipped, our research activities are in full swing."

Nazeeruddin's research bears an important highlight: he was involved in Michael Grätzel's now-famous development of highly efficient, ruthenium-based sensitizers designed for solar energy applications. Today, this discovery forms the basis for the multicolored photovoltaic panels of the SwissTec Convention Center in Lausanne, while EPFL has licensed the technology to several industrial partners. "I must confess that I feel very proud when I see them every day," he says.

Currently, Nazeeruddin focuses on perovskite solar cells, light-emitting diodes, and photo- and X-ray-detectors. Perovskite technology has recently experienced an impressive rise in terms of photovoltaic efficiency, from 3.8% to 20.2%, which has revolutionized ideas about photovoltaic devices. This high efficiency is the product of new molecularly engineered charge-transporting materials. "I am very

passionate about perovskite solar cells," says Nazeeruddin. "Unlike silicon-based solar cells, they can be developed through a variety of low-temperature solution-process techniques by using inexpensive raw materials."

But a low market price is not the only advantage of perovskites. The materials also feature broad absorption in the visible and near-infrared spectrum, high optical absorption coefficients, extremely low exciton-binding energy, long carrier-diffusion lengths, and very high open circuit potentials.

The main drawback of perovskite solar cells is their sensitivity to humidity, heat and UV light, all of which affect their reliability under real operating conditions. "Finding solutions to these problems is our main objective. Our group has the expertise to address these challenges." The lab uses molecularly engineered interface materials as charge-extraction layers of perovskite-based panels, but also to act as a shield for humidity and UV-induced degradation. This achievement could also be transferred to light-emitting diodes and field-effect transistors, photo-detectors, and lasers.

In the near future, Nazeeruddin's group will address issues of stability under heat and light-soaking conditions. Since the perovskite materials are salts and are sensitive to humidity, they will look at questions regarding the tolerance limit for humidity, and develop methods to overcome humidity-induced instability. One promising solution is already under investigation, in a collaborative project with Paul Dyson at EPFL is the development of functional additives.

"There is also a need for fundamental understanding in charge-transfer dynamics," says Nazeeruddin. "Applying this knowledge on the molecular engineering of contact materials can enhance the short-circuit current and open-circuit voltage of the perovskite solar cells."

The lab will also be addressing the mechanism of exciton generation in perovskites. Finally, Nazeeruddin considers dissociation and charge-migration dynamics are also key requirements for the intelligent design of perovskite materials.

"We have fantastic future at Sion," he says. "We would like to control perovskite crystal growth and morphology, and at the same time to understand the physics behind these interesting materials." This will be crucial for pushing device performance beyond the 24% mark, and propelling perovskite technology on a realistic market scale.

"The scientific and economic impact of perovskite solar cells will be enormous," he adds. "The technological advancements are likely to lead towards commercial exploitation, eventually contributing to global energy demands." The ultimate goal is grid-free supply of energy with a grid parity, which would make communities self-sufficient in terms of energy demands and consumption.

The joint venture between Sion and Abengoa promotes cross-pollination between researchers in academia and the private sector. The benefits of Nazeeruddin's research are not going unnoticed by the city's local economy. "In the coming months, with the help of our operational director Marc-André Berclaz, I plan to showcase our work to various small-medium enterprises who are interested in the energy sector."

The endeavor is a first step towards the broader development of Energypolis at Sion, as well as the wider Swiss Innovation Park, for which EPFL has partnered with the western Swiss cantons (Valais, Fribourg, Neuchâtel, and Geneva).

SION: WENDY QUEEN FIGHTS EMISSIONS



Having joined EPFL Valais Wallis in September 2015, Wendy Queen leads her group into the search for new materials for gas separation. “It is estimated that we spend 10-15% of the world’s energy on separation processes,” she says. “Meanwhile, atmospheric CO₂ levels

are rising at an alarming rate. All this makes new materials for energetically favorable gas separations essential – and it will offer a large payoff from an environmental and economic perspective”.

Queen received her PhD in inorganic chemistry in 2009 from Clemson University (South Carolina), with her research focusing on the synthesis and characterization of extended solids that contained low-dimensional magnetic metal oxide nanostructures. During that time, she synthesized a number of materials with unique magnetic properties, using high-temperature molten salt as a structure-directing agent for the formation of noncentrosymmetric frameworks, porous solids, and water-soluble metal-oxide clusters.

Her focus expanded during her postdoc. “While my PhD work involved the use of common synthetic and characterization techniques, I decided to use my postdoctoral training as an opportunity to gain expertise in more advanced forms of characterization.”

During her post-graduate research, Queen pursued a deeper understanding of the structure-derived function of inorganic materials, a theme that has come to characterize her entire scientific career. Supported by an NRC/NIST grant in 2009, she was able to build a research program on small-molecule interactions in nanoporous adsorbent materials. Using neutron and x-ray diffraction and inelastic and quasielastic scattering, coupled with standard adsorption measurements, her research helped her gain molecular-level insights into the adsorption behavior of a wide variety of porous adsorbents, e.g. activated carbons, porous organic cages, zeolites, and metal-organic frameworks.

The work provided the field with critical insight into the adsorption and gas separation behavior of some of the most well-studied frameworks in the field – as well as a number of key papers in journals like *Energy & Environmental Science*, *Chemical Science*, *Journal of the American Chemical Society*, and *Science*.

Following her postdoctoral fellowship, Queen joined the Molecular Foundry at Berkeley, which is a nanoscience research center funded by the US Department of Energy. There, she launched and co-directed a new user program focused on the synthesis and characterization of porous crystalline materials. The position allowed her to interact with government, academic, and industrial labs, and to work with them on a wide array of projects. These included CO₂ sensors for smart buildings and the development of composites such as water scavengers for the encapsulation of moisture-sensitive photovoltaics.

Published in a *Chemical Science* cover article, Queen’s work uncovered the molecular-level interactions of CO₂ binding in a prominent family of metal-organic frameworks whose adsorption properties can be readily tuned with metal-substitution. “This information was important for carbon capture, and we were able to compare it with the DFT calculations of our collaborators.” The theoretical results lined up perfectly with experimental determinations of intramolecular CO₂ angles, CO₂ binding geometries, and isosteric heats of CO₂ adsorption.

But it wasn’t all just data. “My experience at Lawrence Berkeley National Laboratory brought me to the realization that, in addition to understanding the structure-derived function of energy-related materials, one of my passions is mentoring young scientists.” This impetus was decisive in bringing Queen to EPFL Valais Wallis.

“THE LFIM AIMS TO CONTRIBUTE KNOWLEDGE TOWARDS SOLVING GLOBALLY IMPORTANT PROBLEMS, AND IN PARTICULAR THOSE RELATED TO THE REDUCTION OF CO₂ EMISSIONS AND REDUCING ENERGY CONSUMPTION.”

The Laboratory of Functional Inorganic Materials is housed within the new chemistry campus of EPFL-ISIC-Valais, in Sion. Heading the lab, Queen envisions her research in a two-pronged approach. First, to rationally design materials for targeted applications and control their crystallization, which is necessary to incorporate them into composites or to deposit them on surfaces. Second, to focus on assessing several aspects of nanoporous materials, including small molecule adsorption/separation and their conversion into other value-added chemicals.

Ultimately, Queen’s group aims to develop an internationally recognized and respected research program that can contribute knowledge towards solving globally important problems, and in particular those related to the reduction of CO₂ emissions and reducing energy consumption. But she also expects it to raise students’ awareness to the multi-level approaches that are required to solve large-scale, global problems, such as climate change. This, she believes, will help the next generation of scientist to realize the importance and relevance of their research carried out in an internationally competitive field.

“I think the new lab in Sion is unique in that it houses several research groups that are scientifically diverse, but share common missions in energy-related research such as carbon dioxide capture and utilization,” she says. “I expect that the exciting, collaborative atmosphere will promote high-impact science.”

THE NEW LAUSANNE CENTRE FOR ULTRAFAST SCIENCE



HIGH HARMONIC GENERATION SET-UP FOR THE PRODUCTION OF ULTRASHORT VACUUM ULTRAVIOLET (10-120 eV) PULSES. THE SET-UP HAS BEAMLINES FOR PHOTOELECTRON SPECTROSCOPY STUDIES IN THE LIQUID PHASE (CHERGUI-ISIC), THE GAS PHASE (DRABBELS-ISIC) AND FOR SINGLE CRYSTALS (GRIONI-IPHYS, CARBONE-IPHYS, CHERGUI-ISIC).

In 2015, the Lausanne Centre for Ultrafast Science (LACUS), under the directorship of Professor Majed Chergui (ISIC), was announced. The new centre brings together experimental and theoretical research groups from EPFL's Faculties of Basic Sciences, Engineering and Life Sciences.

Research in biological, chemical, and physical processes now demands the manipulation of various degrees of freedom on timescales below the timeframe of thermalization. This can only be done with ultrashort femtosecond pulses of electrons or light over a wide range of the electromagnetic spectrum.

"Such pulses offer high time-resolution that allows us to explore some of the fastest processes in nature," says Majed Chergui. "Meanwhile, the technology of ultrafast light sources expands the possibilities for applications in imaging and medical diagnosis. The broad spectral bandwidth of ultrashort laser pulses translates into data bandwidth in optical communications. Finally, the high-field strengths at moderate pulse energy enable precise cold ablation in medicine or of thermally sensitive materials."

Given the rising cost and complexity of ultrafast science and technology, collaboration in the field has become imperative. EPFL has the largest concentration of research teams working on ultrafast science and technology in Switzerland, and LACUS aims to foster sustainable synergy between groups, maintaining EPFL's leadership at the national and international level. The Centre is already collaborating with Swiss Light Source and SwissFEL at the Paul Scherrer Institute, but the centre will launch new collaborations in the near future. In particular, LACUS also aims to establish and reinforce links with partners in industry.

The aim of LACUS is to provide the scientific community with a technology platform featuring state-of-the-art electron and light sources, covering the entire electromagnetic spectrum. It also brings novel methods in measurement and characterization, aiming to improve and extend the application range of its technologies. Finally, LACUS will pool resources to create a research environment for students and researchers, engaging in teaching and outreach activities.

The mid-term vision is to create a Science of Light (SOL) centre that will group EPFL's ultrafast sciences with the nanosciences and biophotonics in a common new building. But for now, LACUS aims to make the latest ultrafast electron and laser technology accessible in the form of a platform to the broader EPFL research community.

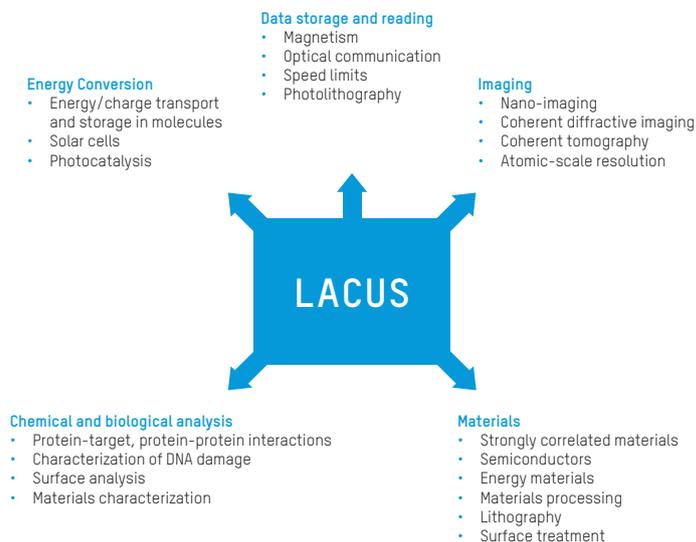
To do this, LACUS will offer a wide range of experimental parameters, including pulse duration, wavelengths, field strengths, repetition rates, and others. These sophisticated tools are needed to address the new classes of scientific and practical problems that arise as we delve deeper into the complexities of matter.

Specifically, LACUS will provide frontier electron and light sources of various pulse durations, ranging from the THz range to the vacuum ultraviolet and the soft X-ray range. This will also allow unusual combinations of tools, such as a THz pump/XUV probe or IR pump/XUV, photons with electron pulses, photons and scanning tunnelling microscopy (STM), and others. The sources will be supported and run mainly by groups from EPFL's faculty of Basic Sciences that are directly involved in developing and maintaining the various technologies.

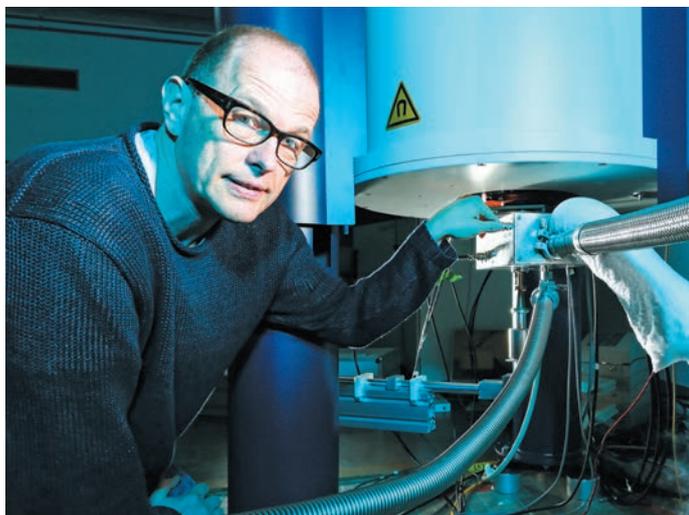
However, the groups will also collaborate with users from EPFL's faculties of Life Sciences and Engineering to cross-fertilize basic research with applications. For example, LACUS plans to develop the following technologies for use in the life and materials sciences:

- Optical Coherence Tomography (OCT) in the deep-UV
- XUV-CT in the water window:
- 2D UV spectroscopy for protein-target interactions
- Coherent lensless imaging in the XUV-soft X-ray range
- Fluorescence imaging
- Ultrafast and steady state electron techniques (diffraction, microscopy and spectroscopy)
- Photon-Induce Near-Field Electron Microscopy (PINEM)

"With the impressive diversity of techniques and methods we have within LACUS, we are in a leading position to address crucial fundamental questions," says Majed Chergui. "But we will also be able to apply these tools for practical purposes, such as imaging in medicine and biology, ultrashort laser pulse machining of materials, and others."



WAKING PROTEINS UP FROM DEEP SLEEP TO STUDY THEIR MOTIONS



FREEZE, SLEEP, WAKE UP, AND MOVE

A team of scientists at EPFL, IBS-Grenoble, and ENS-Lyon led by Lyndon Emsley and Martin Blackledge developed an innovative solution to the motion problem: freeze the proteins and then watch them “wake up” from deep sleep. By freezing proteins down to temperatures of -168°C , the researchers were able to completely stop all the motions of interest in the molecules. Then, they slowly raised the temperature to the point where the proteins could regain their natural motions, but at a much slower pace. This way, it was possible to look at each motion a protein makes individually and – more importantly – in sequence.

To do this they used a spectroscopic technique called nuclear magnetic resonance (NMR), which exploits the magnetic properties of certain atoms like hydrogen and carbon. NMR works by placing the sample of the protein inside a strong magnetic field, and observing how it responds to radio frequencies. This complex response allows them to determine the degree of motion of each atom in the protein, e.g. its backbone, a side-chain, or the surrounding water, etc.

Because the proteins in this study needed to be frozen down, the team had to adjust their NMR methodology to work with samples at very low temperatures, in order to “wake the proteins up” from sleep, while constantly spinning at a specific (“magic”) angle to the NMR’s magnetic field, to provide enough spectral resolution. Finally, every NMR experiment took days to perform. These complications were overcome by using a newly developed probe specifically designed to work with NMR at low temperatures.

In order to carry out their functions, proteins need to move. **Lyndon Emsley’s group** and their colleagues have developed a new technique to study motions in proteins with unprecedented accuracy. The method, which is based on NMR, freezes proteins down to immobility, then slowly heats them to “wake them up” and restart motions individually and in sequence, providing a slow-motion image of real conditions. The breakthrough method, which was developed at EPFL’s advanced NMR facility, is published in *Science*.

PROTEIN MOTION IS HIGHLY COMPLEX

Motion is part of a protein’s function, allowing it to adjust its 3D shape and interact with other molecules like biological molecules and synthetic drugs. Understanding how a protein moves is thus the key to developing drugs that can efficiently interact with it. These “functional” motions however are complex, and can be thought of as the mechanism of a watch, where motions between interlocking cogs and springs, at different timescales, result in the smooth movement of the hands.

In a protein the cogs and springs are the molecules that make it up: amino acids form its backbone each with side-chains of different molecules branching out on all sides in three dimensions. In addition, water molecules on the protein add further layers of complexity. But unlike a watch, whose individual movements are all well defined, each of the component motions in a protein are actually random. As a result, protein motion seems almost chaotic, and is notoriously difficult to study.

A HIERARCHY OF MOTION

Using their innovative approach, Emsley’s team found that the sequence of protein motions follows a specific hierarchy as temperature increases: first the protein’s solvent molecules, then the protein’s side-chains and water molecules, and finally the protein’s backbone. The sequence culminates with a functionally active protein at temperatures even as low as -53°C , well below physiological levels.

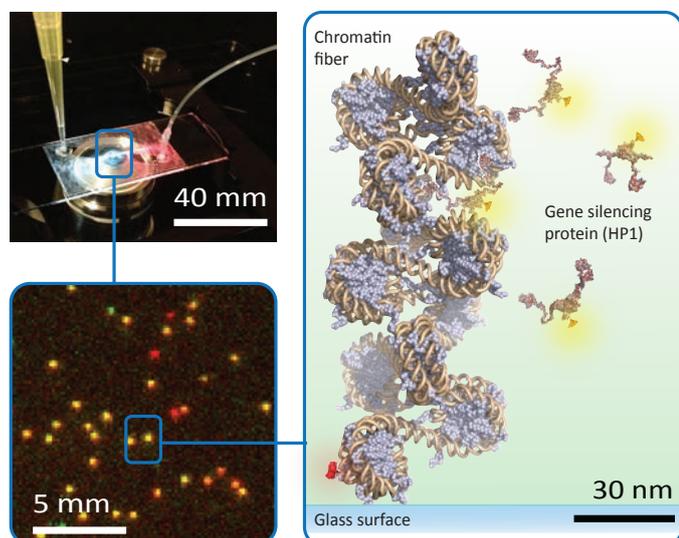
“Our work shows that we can use variable-temperature solid-state NMR to gain unique and novel insights into the role of protein dynamics in biology,” says Lyndon Emsley. The team is now interested in using this method to find out just how universal this hierarchy of motions is, and what might cause variations between different molecules.

This work is a collaboration of EPFL’s Laboratory of Magnetic Resonance with ENS-Lyon and the CEA/CNRS at University of Grenoble Alpes.

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FASTER, NOT STRONGER: HOW A PROTEIN REGULATES GENE EXPRESSION



SINGLE-MOLECULE FLUORESCENCE IMAGING DIRECTLY SHOWS DYNAMIC INTERACTIONS OF GENE SILENCING PROTEINS, SUCH AS HP1, WITH CHROMATIN FIBERS, CARRYING POST-TRANSLATIONAL MODIFICATIONS

By measuring the motion of single molecules, **Beat Fierz's group** discovered how specialized proteins control gene expression by binding and compacting discrete parts of DNA inside the cell. The findings have significant implications for genetics and cancer research.

Inside the cell, DNA is tightly coiled and packed with several proteins into a structure called “chromatin”, which allows DNA to fit in the cell while also preventing genes from being expressed at the wrong time. Guided by a chemical “barcode”, specialized effector proteins can bind chromatin and either unwind it or compact further to activate or silence genes. This system has enormous implications for biology and medicine, e.g. cancer research. However, the efficiency of effector-chromatin interactions have been elusive, especially given the weak binding between the two. Tracking these interactions one molecule at a time, Beat Fierz's group at ISIC showed for the first time how a major effector protein speeds up its search for chromatin binding sites pairing up with others of its kind. The elegant molecular mechanism is published in *Nature Communications*.

PACKAGING DNA

Every human cell contains an astonishing 1.8 meters of DNA. In order to fit, DNA is tightly wrapped around spool-shaped proteins, the histones, which package it down to 0.09 millimeters – a 20,000-fold reduction in length. The histone-DNA complex is called chromatin. Through it, the cell can regulate which genes are active at any given time by unwinding that part of packed DNA. Conversely, the cell can “repress” genes by forming compact and dense chromatin fibers. All this is done by “effector” proteins, which attach to chromatin and change their 3D structure to either open or compact DNA containing the gene of interest.

This mechanism is explored by a host of biological and medical fields, e.g. genetics and cancer research, as it is the key to regulating genes in a cell. However, there are gaps in our understanding of how such a crucial system remains efficient, given that the binding between effectors and histones is too weak. Several theories have been proposed, but the problem has persisted.

FASTER, NOT STRONGER

The lab of Beat Fierz at ISIC showed that a major effector protein increases its efficiency not by binding chromatin more strongly, but rather by binding and re-binding it faster. The protein, called HP1 α , dissociates from chromatin relatively easily, something that is common across proteins that interact with DNA. To make up for this “loose binding”, HP1 α speeds up its binding rate, but also gets together in pairs to maximize its binding sites.

The scientists used single-molecule measurements, a highly sensitive experimental method. The technique, never used in this context before, allowed the researchers to observe individual HP1 α proteins interact with chromatin in real time. The team also synthesized chromatin fibers that contained the appropriate chemical identifiers, and they used this system to explore HP1 α binding under different conditions and experimental parameters.

Along with the increase in binding rate, the scientists also found that when HP1 α connects to other HP1 α proteins to make dimers, it increases its binding sites so that it can maximize its interaction with chromatin. It is important to remember here that interactions inside the cell are not static; molecules connect and disconnect constantly, often competing for the same site. By increasing its binding speed and multiplying its binding site, HP1 α has a better chance of binding chromatin for longer and thus regulating gene expression.

Given the importance of this mechanism to cell proliferation and growth, it holds particular significance in cancer research, and potentially other diseases caused by problematic gene regulation. Fierz's group is now working on extending their single-molecule methodology to study more complex processes, in particular how damaged DNA is repaired. “We want to observe complex biology as it happens, and understand it on a quantitative level,” he says. “Our chemical methods give us complete control over protein-chromatin dynamics, and the current study sets the stage for such unprecedented insights.”

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REFERENCE

Kilic S, Bachmann AL, Bryan LC, Fierz B. Multivalency governs HP1 α association dynamics with the silent chromatin state. *Nature Communications* 18 June 2015. DOI: 10.1038/ncomms8313

A NEW METHOD FOR CHEAPER SOLAR-ENERGY STORAGE



A TUNGSTEN DISELENIDE THIN-FILM

Building on a unique idea, [Kevin Sivula's team](#) at ISIC developed a cost-effective new method for converting and storing solar energy into hydrogen.

Storing solar energy as hydrogen is a promising way for developing comprehensive renewable energy systems. To accomplish this, traditional solar panels can be used to generate an electrical current that splits water molecules into oxygen and hydrogen, the latter being considered a form of solar fuel. However, the cost of producing efficient solar panels makes water-splitting technologies too expensive to commercialize. Kevin Sivula's team at ISIC developed a simple, unconventional method to fabricate high-quality, efficient solar panels for direct solar hydrogen production with low cost. The work is published in *Nature Communications*.

Many different materials have been considered for use in direct solar-to-hydrogen conversion technologies but "2-D materials" have recently been identified as promising candidates. In general these materials—which famously include graphene—have extraordinary electronic properties. However, harvesting usable amounts of solar energy requires large areas of solar panels, and it is notoriously difficult and expensive to fabricate thin films of 2-D materials at such a scale and maintain good performance.

Kevin Sivula and his colleagues at ISIC addressed this problem with an innovative and cheap method that uses the boundary between two non-mixing liquids. The researchers focused on one of the best 2-D materials for solar water splitting, called "tungsten diselenide". Past studies have shown that this material has a great efficiency for converting solar energy directly into hydrogen fuel while also being highly stable.

Before making a thin film of it, the scientists first had to achieve an even dispersion of the material. To do this, they mixed the tungsten diselenide powder with a liquid solvent using sonic vibrations to "exfoliate" it into thin, 2-D flakes, and then added special chemicals to stabilize the mix. Developed by Sivula's lab (2014), this technique produces an even dispersion of the flakes that is similar to an ink or a paint.

The researchers then used an out-of-the-box innovation to produce high-quality thin films: they injected the tungsten diselenide ink at the boundary between two liquids that do not mix. Exploiting this oil-and-water effect, they used the interface of the two liquids as a "rolling pin" that forced the 2-D flakes to form an even and high-quality thin film with minimal clumping and restacking. The liquids were then carefully removed and the thin film was transferred to a flexible plastic support, which is much less expensive than a traditional solar panel.

"THE DEVELOPMENT OF A SIMPLE TECHNIQUE TO DEPOSIT THIN FILMS OF SEMICONDUCTING 2-DIMENSIONAL MATERIALS WAS THE KEY ENGINEERING BREAKTHROUGH IN THIS WORK, AND IS A STEP TOWARDS ECONOMICALLY-VIABLE SOLAR-TO-FUEL ENERGY CONVERSION."

The thin film produced like this was tested and found to be superior in efficiency to films made with the same material but using other comparable methods. At this proof-of-concept stage, the direct solar-to-hydrogen conversion efficiency was around 1%—already a vast improvement over thin films prepared by other methods, and with considerable potential for higher efficiencies in the future.

More importantly, this liquid-liquid method can be scaled up on a commercial level. "It is suitable for rapid and large-area roll-to-roll processing," says Kevin Sivula. "Considering the stability of these materials and the comparative ease of our deposition method, this represents an important advance towards economical solar-to-fuel energy conversion."

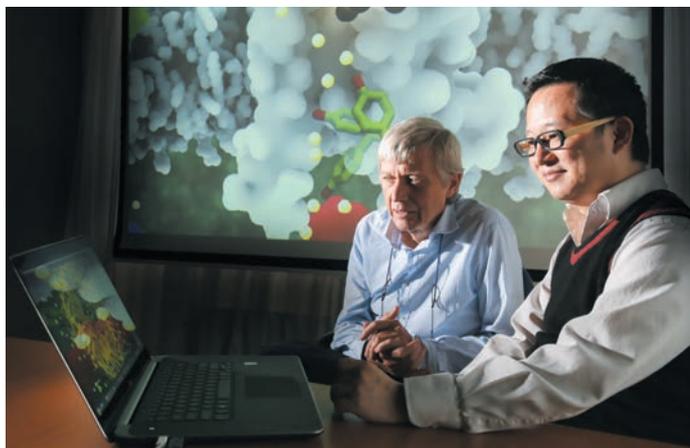
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This work was funded by the Swiss Competence Centers for Energy Research (SCCER Heat and Electricity Storage) and the European Commission's Framework Project 7 (FP7) through a Marie-Curie Intra-European Fellowship (COCHALPEC).

REFERENCE

Yu X, Prévot MS, Guijarro N, Sivula K. Self-assembled 2D WSe₂ thin films for photoelectrochemical hydrogen production. *Nature Communications* 01 July 2015. DOI: 10.1038/ncomms8596

TRACING WATER CHANNELS IN CELL-SURFACE RECEPTORS



HORST VOGEL AND SHUGUANG YUAN

G-protein-coupled receptors (GPCRs) mediate most of our physiological responses to external stimuli and are involved in many diseases. [Horst Vogel's group](#) used computer modeling to uncover central steps of GPCR signal transduction. Their findings could help in developing new medicines targeting this important class of cell surface receptors.

G protein-coupled receptors (GPCRs) are the largest class of cell surface receptors in our cells, involved in signal transmission across the cell membrane. One of the biggest questions is how a signal recognized at the extracellular side of a GPCR induces a sequence of conformational changes in the protein and finally evokes an intracellular response. Horst Vogel's group at ISIC used computer modeling to reveal in molecular detail the structural transitions that happen inside GPCRs during the signal transduction process. They discovered that a central step in the trans-membrane signaling process is the formation of a continuous water pathway inside the G protein coupled receptors. The work, published in *Nature Communications*, proposes that future therapeutic compounds might be selected based on their ability to interfere with the receptors' internal water channels.

GPCRS AMPLIFY EXTRACELLULAR SIGNALS TO FINALLY EVOKE INTRACELLULAR RESPONSES

GPCRs are membrane proteins on the cell's surface. There are approximately 800 different GPCR types, each of which can detect and bind specific molecules on the cell's surface, which are called 'ligands'. Upon binding a ligand, the GPCR transmits a signal across the cell's membrane where specialized, so-called G proteins work to amplify the signal using a cascade of biochemical reactions that evoke cellular responses.

As these processes are of central importance for the proper function of our cells, even slight malfunctions of these processes can result in severe diseases. This makes GPCRs of utmost importance as targets for modern drug development, while a large proportion of current clinical drugs target various GPCRs. Therefore, understanding how GPCRs function at a molecular level can lead to the development of novel, powerful drugs for the treatment of diseases including cancer, diabetes, neurological disorders, inflammations, immunological disorders and cardiovascular disorders.

The 3D structures of a few GPCRs have already been solved by X-ray crystallography. However, this approach generates only static structures, which are not suited to uncover the structural changes that occur within the GPCRs during the signal transduction process.

MODELING GPCRS

The team of Horst Vogel has now used a method known as 'molecular dynamics computer simulations' to model prototypical GPCRs. The team succeeded in simulating the time course of transitions in the 3D structure of the GPCRs during the process of signal transduction across the cell membrane.

Vogel's team revealed in detail the important molecular steps of how a GPCR transmits a signal across the cell membrane. After binding a ligand on the extracellular side, the GPCR undergoes a couple of 3D changes. These then allow water molecules to enter the interior of the GPCR, reaching a 'water barrier' of amino acids.

After further structural changes, this barrier opens a gate and finally allows the formation of a continuous water channel extending from the ligand-binding site to the intracellular region of the receptor. The consecutive structural changes within the receptor, combined with the water channel are essential for the activation of G proteins on the intracellular side of the GPCR. Once activated, the G proteins can then amplify the signal.

"The discovery of these internal water channels can pave the way for novel approaches in drug development," says Horst Vogel. "By searching for compounds which bind to GPCRs and modulate their water channels, it might be possible to find more efficient therapeutic compounds."

This work includes a collaboration of EPFL's Laboratory of Physical Chemistry and Membranes with the University of Warsaw (Poland) and Case Western Reserve University (USA).

REFERENCE

[Yuan S, Filipek S, Palczewski K, Vogel H. Activation of G-protein-coupled receptors correlates with the formation of a continuous internal water pathway. *Nature Communications* 09 September 2014. DOI: 10.1038/ncomms5733](#)

PROFESSORS NICOLAI CRAMER AND CHRISTIAN HEINIS WIN SNSF CONSOLIDATOR GRANTS

Professor Nicolai Cramer was awarded a Consolidator Grant by the SNSF in the context of the so-called “Temporary Backup Schemes” for the European Research Council (ERC) grants. This transitional measure of the SNSF offers the awardee an adequate substitute for ERC grants.

Advances in organic chemistry are of importance for modern society and synthesizing tailored molecules in high purity is critical for many industries. In addition, important production requirements of sustainability and timeliness have been raised. Of particular relevance is the efficient production of enantiopure compounds due to their unique properties. In principle, the catalytic direct and enantioselective functionalization of carbon-hydrogen (C-H) bond is ideally suited for this task.

The possible range of substrates is immense and new synthetic disconnections could become possible allowing for a more efficient usage of our dwindling resources. However, especially enantioselective C-H activations remain longstanding challenges for catalysis research. In this respect, cyclopentadienyl (Cp) type ligands are an outstanding ligand class particularly useful for C-H functionalizations. However, the extreme scarcity of chiral versions of this ligand is one of the most critical limiting factors in the development of asymmetric C-H bond activations. The global objective for this project is the creation of novel Cp-ligand platforms and catalysts thereof enabling for broadly applicable enantioselective C-H functionalizations for a streamlined economic access to relevant arrays of synthetic molecules.

Recently, Cramer’s lab reported a breakthrough on chiral Cp ligand with a shield and bulk design. These ligands will be used with several transition-metals covering a range of noble metals as well as cost-effective base-metals possessing many intriguing reactivities and catalyze a multitude of different valuable reactions. For each of the different metal-catalyst, flagship reactions fulfilling the criteria of product importance and lack of alternative preparation methods are selected. Rendering them enantioselective would have transformative potential and close important gaps in contemporary catalysis. We aim

also expanding our available ligand sets by building a ligand toolbox based on a highly modular assembly line.

Duration of the project: 60 months

Total Amount: CHF 1,999,975

Professor Christian Heinis was awarded a Consolidator Grant by the SNSF in the context of the so-called “Temporary Backup Schemes” for the European Research Council (ERC) grants. This transitional measure of the SNSF offers the awardee an adequate substitute for an ERC grant.

Bioconjugation is required for the development and/or manufacturing of many therapeutics, e.g. pegylated proteins or antibody-drug conjugates. Heinis’s lab uses bioconjugation reactions for the directed evolution of antagonists based on bicyclic peptides.

But a limitation of available bioconjugation reactions is the lack of site-selectivity. Existing conjugation reactions typically modify multiple amino acids of a single type in a protein or peptide (e.g. multiple lysines or multiple cysteines). For example, several pegylated protein drugs and all clinically approved antibody-drug conjugates are randomly modified at multiple cysteine or lysine positions.

The aim of this project is to develop an entirely new, site-selective bioconjugation strategy and its application for the generation of peptide and protein therapeutics. The principle of the method is that only sites in a protein or peptide are chemically modified if a combination of two specific amino acids is present (e.g. lysine and cysteine).

Heinis proposes to apply this novel chemical conjugation strategy to three bioconjugation challenges in drug development: i) generation of proteolytically stable, orally available peptide drugs, ii) generation of antibody-drug conjugates with defined drug-to-antibody ratio, and iii) development of homogeneously pegylated therapeutic proteins.

Duration of the project: 60 months

Total amount: CHF 1,650,718

PROMOTIONS IN 2015: TITULAR PROFESSORS



Sandrine Gerber leads the Group for Functionalized Biomaterials at EPFL, which focuses on the development of new chemical entities for bio-applications. The Group is mainly interested in the design, synthesis and evaluation of functionalized nanomaterials and biomaterials for therapeutic applications such as bone implants, imaging probes and cells transplantation devices.

Gerber was appointed Titular Professor in organic chemistry in December 2014, and is currently deputy to the director of ISIC, and a member of the Board of Directors of the Swiss Chemical Society. She studied chemistry at the Ecole Nationale Supérieure de Chimie de Paris in France, where she obtained a diploma of chemical engineer in 1993. The same year she obtained a DEA (Master degree) of organic chemistry at the University Pierre et Marie Curie (Paris VI, France).

From 1993 to 1996 she did a PhD in organic chemistry under the supervision of Prof. Jean-Pierre Genêt at the Ecole Nationale Supérieure de Chimie de Paris. In 1996, she moved to University of Lausanne for a post-doctoral stay under the supervision of Prof. Pierre Vogel. In 1998, she was appointed Maître-Assistante at the Institute of Organic Chemistry in the University of Lausanne.

In 2003, she qualified to direct research at the University Pierre et Marie Curie (Paris VI, France). The same year, she was appointed scientific adjunct at EPFL, and became senior scientist (Maître d’Enseignement et de Recherche) in 2006.

THE MARTIGNY REDOX FLOW BATTERY DEMONSTRATOR



The pilot hydrogen storage and production facility in Martigny (Valais) is a prototype for the future of renewable energy storage.

Operating since 2014, the facility at Martigny uses a redox battery system to store renewably sourced energy. The project is the fruit of a collaboration between Hubert Girault's Laboratory of Physical and Analytical Electrochemistry at EPFL, the District of Martigny, the Centre de recherches énergétiques et municipales (CREM) and the public-works institution Sinergy.

The facility is described as a "redox-flow battery demonstrator", as its main aim is to demonstrate the potential of these electrochemical storage systems to function as buffers for intermittent energy sourced from renewable sources, e.g. solar, wind etc. The idea is that, as we are progressively weaning ourselves off fossil fuels, the demand for renewable energy will rise to levels that are unsustainable with today's "real-time" harvesting systems: a passing cloud can stop solar energy output and wind can prove inconsistent; such interruptions to clean energy supply could be devastating in the near future.

The solution is to efficiently store energy in order to buffer its production and consumption. Redox-flow batteries like the one installed in the Martigny demonstrator are a promising way forward. The centerpiece in this installation is a redox-flow battery based on a vanadium solution.

Redox flow batteries (RFBs) are basically rechargeable electrochemical systems. Unlike conventional batteries, RFBs do not contain solid active materials, but rather two solutions of concentrated ions that can accept or donate electrons.

The RFB at Martigny uses two electrolyte solutions containing vanadium ions, one negatively charged and the other positively. The two solutions are separated by an ion-selective membrane, which separates the two liquids. When electrons move from one side of the battery to the other, an equal positive charge in the form of protons also move in the opposite direction to maintain the overall electroneutrality of the RFB.

When electrical voltage is applied to the RFB, e.g. coming from a wind turbine system, the negative electrode delivers electrons to the negative solution (catholyte) and extracts electrons from the positive solution (anolyte). The solutions then return to their respective storage tanks where they remain in a charged state until needed to provide current. The battery is then discharged by passing the charged solutions through the cell once more, releasing energy back into the electrical grid.

In this way, the Martigny demonstrator can provide a buffer for intermittent energy, providing constant power without interruptions. However, this particular pilot facility is unique from other installations, in that it is also able to store energy as hydrogen. The hydrogen is produced by indirect electrolysis, or a "hydrogen evolution reaction", outside of the main battery cells. The reaction takes place in a separate catalytic reactor that works in sync with the RFB system to convert excess electricity into hydrogen. Inside the reactor, one of the battery's electrolyte solutions interacts with a solid Mo_2C catalyst, resulting in the release of hydrogen, which can then be stored for later use in fuel cell vehicles, as a fuel for consumer applications, or as a reactant for many industrial processes. In this way, the excess energy from renewable sources never goes to waste.



Prof. Md. K. Nazeeruddin directs the Group for Molecular Engineering of Functional Materials at EPFL's satellite campus at Sion (EPFL Valais Wallis). His current research at EPFL focuses on Dye Sensitized Solar Cells, Perovskite Solar Cells, CO_2 reduction, hydrogen production, and light-emitting diodes.

He has published more than 509 peer-reviewed papers, ten book chapters, and he is inventor/co-inventor of over 50 patents.

Nazeeruddin received M.Sc. and Ph. D. in inorganic chemistry from Osmania University, Hyderabad, India. He joined as a Lecturer in Deccan College of Engineering and Technology, Osmania University in 1986, and subsequently, moved to Central Salt and Marine Chemicals Research Institute, Bhavnagar, as a Research Associate. He was awarded the Government of India's fellowship in 1987 to study abroad. After a year-long postdoctoral position with Professor Michael Grätzel at EPFL, he joined the same institute as a Senior Scientist. In 2014, EPFL awarded him the title of Titular Professor.

MICHAEL GRÄTZEL WAS AWARDED THE KING FAISAL INTERNATIONAL PRIZE IN SCIENCE



Professor **Michael Grätzel** won the 2015 King Faisal International Prize in Science, recognizing his work in developing photo-electrochemical systems for solar energy conversion.

The King Faisal International Prize is sponsored by the King

Faisal Foundation in Saudi Arabia. Every year, the award is presented to “dedicated men and women whose contributions make a positive difference” in five different categories: Service to Islam, Islamic studies, Arabic Language and Literature, Science, and Medicine.

Professor Michael Grätzel (EPFL) was awarded the Science Prize for 2015, whose topic was “Chemistry”. Grätzel is known for his world-famous

“Grätzel cells”, dye-sensitized solar cells that have revolutionized solar energy conversion technology. Grätzel cells are also simple and relatively inexpensive to manufacture, and feature unique flexibility and transparency.

The Prize included a handwritten Diwani calligraphy certificate summarizing the laureate’s work, a commemorative 24-carat, custom-made 200-gram gold medal, and a cash endowment of \$200,000.

In its press release, the King Faisal Foundation states: “*Professor Grätzel’s work has had and will continue to have a major impact on the practical realization of solar-energy conversion.*”

The award announcement took place in a ceremony in Riyadh, on February 3, 2015. Michael Grätzel shared the Science Prize with Professor Omar Mwanne Yaghi from the University of California, Berkeley.

MAJED CHERGUI WON THE EDWARD STERN PRIZE



Majed Chergui was awarded the Outstanding Achievement Award (Edward Stern Prize) from the International X-Ray Absorption Society (IXAS).

IXAS is an international scientific organization that represents scientists working on the field of structural analysis of molecules, materials and proteins using inner shell excitations induced by X-rays (or electrons). It was officially founded in 1994 following several informal X-ray Absorption Fine Structure (XAFS) conferences in the growing field of X-ray absorption spectroscopy.

The Edward Stern Prize represents the highest honor given by the Society. Winners are recommended by the IXAS Awards Committee and approved by the IXAS Executive Committee. The IXAS Awards Committee

invites nominations from both experimental and theoretical studies of XAFS. The Prize is awarded every third year on the occasion of the XAFS conference to two scientists for lifetime achievements.

Majed Chergui is Professor of Physics and Chemistry at ISIC, where he pursues a variety of ultrafast UV and X-ray spectroscopic studies on chemical and biological systems. Since 2013, he has been founding Editor-in-chief of the journal Structural Dynamics, published by the American Institute of Physics (AIP) and the American Crystallographic Association (ACA). He is also the director of the new Lausanne Centre for Ultrafast Spectroscopy at EPFL (LACUS).

With the Edward Stern Prize, the IXAS committee recognized Majed Chergui “*for his pioneering work in the field of time-resolved X-ray absorption spectroscopy.*”

XILE HU RECEIVED THE 2015 EFCATS YOUNG RESEARCHER AWARD



Xile Hu was awarded the 2015 European Federation of Catalysis Societies (EFCATS) Young Researchers Award, recognizing his work in catalysis for water-splitting reactions and organic synthesis.

The Award is given

every two years to a researcher under the age of 40. It is sponsored by BASF, the largest chemical manufacturer in the world, and is administered by the European Federation of Catalysis Societies (EFCATS). The Award “*recognizes individual contributions in the field of catalysis, with an emphasis on theoretical or experimental discovery and understanding of new catalysts and catalytic processes, synthesis and catalytic function of novel inorganic solids and complexes, mechanisms of reactions, deactivation phenomena.*”

The recipient of the 2015 Award was Xile Hu, Professor at EPFL’s Laboratory of Inorganic Synthesis and Catalysis in ISIC. With it, EFCATS

recognized Hu’s original contributions in the development of cost-effective inorganic catalysts for water splitting reactions and well-defined organometallic catalysts for organic synthesis.

Hu’s research group at ISIC combines methods in heterogeneous, homogeneous, and enzyme catalysis to develop a fundamental understanding of catalysis and develop novel catalysts with superior properties to those in current use. Highlights include:

- Discovering a new class of efficient hydrogen-evolution catalysts (amorphous molybdenum sulfides) and using them to achieve benchmark performance in sunlight-driven hydrogen production.
- Pioneering the use of single-layered metal oxides as exceptional oxygen evolution catalysts.
- Developing nickel- and iron-coordination complexes with widespread application in cross-coupling reactions.
- Merging coordination chemistry with chemical biology to obtain molecular-level mechanistic insights of the [Fe]-hydrogenase enzyme.

The Award was presented at the Europacat XII conference (Kazan, Russia, August 2015).

OTHER ISIC AWARDS FOR 2015



Michael Grätzel awarded the Merite Vaudois

04.03.15 — Michael Grätzel has won the 2015 Merite cantonal Vaudois.

Michael Grätzel wins 2016 SCS Paracelsus Prize

09.12.15 — Michael Grätzel has won the Swiss Chemical Society's Paracelsus Prize for 2016.



Two EPFL professors win 2015 Royal Society of Chemistry awards

05.05.15 — Professors Paul Dyson and Lyndon Emsley have won the 2015 Royal Society of Chemistry Bioinorganic Chemistry Award and Bourke Award respectively.



Majed Chergui elected EPS Fellow

02.06.15 — Professor Majed Chergui has been elected a Fellow of the European Physical Society.

Majed Chergui elected APS Fellow

07.10.15 — Majed Chergui has been elected a Fellow of the American Physical Society.



Ursula Röthlisberger elected member of the IAQMS

02.07.15 — Professor Ursula Röthlisberger was elected to become member of the International Academy of Quantum Molecular Sciences (IAQMS).

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