INSTITUTE OF CHEMICAL SCIENCES AND ENGINEERING

NEWSLETTER 2012

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

NEWSLETTER 2012

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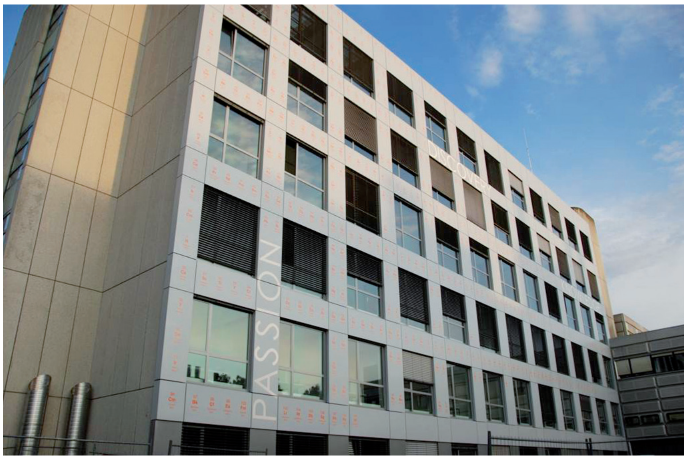
MESSAGE FROM

ISIC DIRECTOR PAUL DYSON



INSTITUTE OF CHEMICAL SCIENCES AND ENGINEERING CH BUILDING, EPFL, LAUSANNE

ISIC's Tech Transfer Record

69	active patent families*, of which
53	have running licenses or TT agreements
48	have active licenses, amendments or TT agreements
298	active research grants

*A patent family is the group of patent applications and patents from one specific invention.

Our sustained commitment to excellence has seen ISIC rise on the international stage. Toward the end of 2011, a Taiwanese ranking of scientific papers for world universities listed EPFL as the third most important academic research center in Europe for chemistry. Since ISIC is considerably smaller than competing departments the ranking represents a considerable achievement. Just as 2011 ended well, 2012 got off to a superb start with the announcement of the new EPFL campus in the Valais. A major theme of this new venture will include chemistry/chemical engineering and biotechnology, and consequently ISIC will be strongly involved in the development of this campus.

The news of the new campus came at a critical moment. These are turbulent times for chemical and associated industries and we are dedicated to training the next generation workforce that will help maintain a strong and healthy economy. The educational and research themes of the campus will be decisive in this sense and it will allow us to grow chemical engineering to levels far beyond those at any previous time in our history. Despite economic uncertainties, our students remain highly sought after, with many receiving job offers even before graduating.

ISIC has also benefited enormously from philanthropic donations during 2011/2012. Generous support from diverse sources has become increasingly important for us to provide excellence in both research and teaching. Further details of major funding successes are provided in this issue along with other leading developments from the last 12 months. As always, I hope you enjoy reading this newsletter. Your comments are welcome, sent either by e-mail to secretariat.isic@epfl.ch or by regular mail to me at the address below. Please visit our website for more detailed information and forthcoming events that might interest you, **http://isic.epfl.ch**.

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SIVULA TARGETS NEW ELECTRONIC DEVICES, SOLAR ENERGY CONVERSION WITH SOLUTION-PROCESSED MATERIALS

Kevin Sivula, head of ISIC's Laboratory for Molecular Engineering of Optoelectronic Nanomaterials, is developing solution -processed electronic materials to fabricate new devices that could help improve current methods of solar energy conversion and even create new opportunities. So don't just think about solar panels - think solar paint.

Traditional semiconductors are costly because they're made of crystalline materials such as silicon, which have to be very pure and processed using expensive techniques. While some researchers focus on reducing the price of these traditional crystalline materials, Sivula is exploring another direction: improving the electronic properties of inexpensive alternatives such as polymer or oxide semiconductors, which can be processed at low cost using solution-based methods. The resulting devices could be painted onto roofs for solar energy conversion, printed into magazines, or woven into fabrics.

"My approach is to take these other materials and tweak them to make the electronic properties better so that they're as useful as the high performance materials that we already have," said Sivula, who was appointed tenure track assistant professor in Chemical Engineering last year. "Take transition metal oxide materials for example—we know that they're stable and widely available and we can make them in a way that is commensurate with covering the Earth."

The problem with solution processable semiconductor materials is that they generally exhibit atomic ordering over a much smaller-length scale compared to their crystalline counterparts — nanometers versus millimeters. And because a semiconducting material's conducting electronic states, and therefore ability to transport electric charge, extend as far as the crystalline ordering, Sivula's approach means controlling the orientation of the materials on that nanolength scale.

While this could be done with expensive "top-down" approaches, he tries to control the morphology by manipulating the structure of the materials from the "bottom up." That is, by engineering the molecular structure of the materials, the group can control how a given material interacts with itself and with other materials. They thus not only control the morphology on the necessary scale, but also induce the ordering of the material through self-assembly. And this in turn allows them to direct optical and electronic properties such as light absorption, the semiconductor band gap, charge transfer and carrier transport.

There are a number of challenges. Polymer semiconductors, for instance, exhibit a trade-off between solubility and therefore processability on the one hand and semiconducting and electronic properties on the other: making such a polymer more crystalline makes it more effective at transporting charges, but also less soluble. Sivula targets a happy medium, but also tries to "trick" the system into being processable and soluble in liquid form, but to then self-organize into a crystalline, highly conductive material when cast out from an ink-jet printer, for example.

The techniques are scalable and economically feasible and will ideally lead to devices that are printable, flexible and able to cover large surfaces for prices in line with the cost of coal- or methane-based power. "It goes beyond just solar energy conversion," he said. "We have to look fundamentally at the electronic properties of these materials. They could also be used in light-emitting diodes, flexible displays or integrated into inks that can be printed out."

His approach has already proven successful in earlier work with former advisor Michael Grätzel. This project focused on hematite, the red-hued iron oxide that the ancient Romans associated with Mercury, the god of war. The mineral, inexpensive and stable, can be solution-processed into a thin film at low temperature and under the right conditions, it can split water into oxygen and hydrogen as it absorbs sunlight. The problem with this iron oxide is that it's not a very good semiconductor material.

Sivula developed an encapsulation strategy that controlled the nanostructure of these iron oxide-type materials when heated to a high temperature—something that had never before been demonstrated in the literature. This new approach helped Sivula and colleagues make a solar paint from oxide nanoparticles and a special combination of surfactants and porogens that reaches fairly high photoactivity.

"IT GOES BEYOND JUST SOLAR ENERGY CONVERSION. WE HAVE TO LOOK FUNDAMENTALLY AT THE ELECTRONIC PROPERTIES OF THESE MATERIALS. THEY COULD ALSO BE USED IN LIGHT-EMITTING DIODES, FLEXIBLE DISPLAYS OR INTEGRATED INTO INKS THAT CAN BE PRINTED OUT."

"Hematite has been looked at since the 1980s for this sort of application, but back then they said the material can't work because its semiconducting properties are so poor, that we'll never be able to make it better,'" Sivula said. "But in the past ten years, with the advent of nanotechnology, we have been able to say we can make it better if we can control the morphology on this nanometer-length scale."

The biggest hurdle facing the group right now is increasing efficiency, Sivula says. To date, the state-of-the-art with solution-processed polymer cells is a solar conversion efficiency of 8 or 9%. Hematite-based devices can convert about 5% of the solar energy into chemical energy stored in hydrogen. The group is aiming for a device that has at least 10% efficiency overall. If they can in turn make this device cost about $80 per square meter and last for about 10 years, the cost of the fuel produced would be about $7 a kilogram, making it competitive with fossil fuels, Sivula said.

The challenge is to get the materials being studied to the levels of efficiency or stability needed, even as crystalline semiconductor technology becomes increasingly affordable. Sivula is nonetheless convinced that his approach will allow us to achieve cheaper energy conversion devices and electronics more quickly.

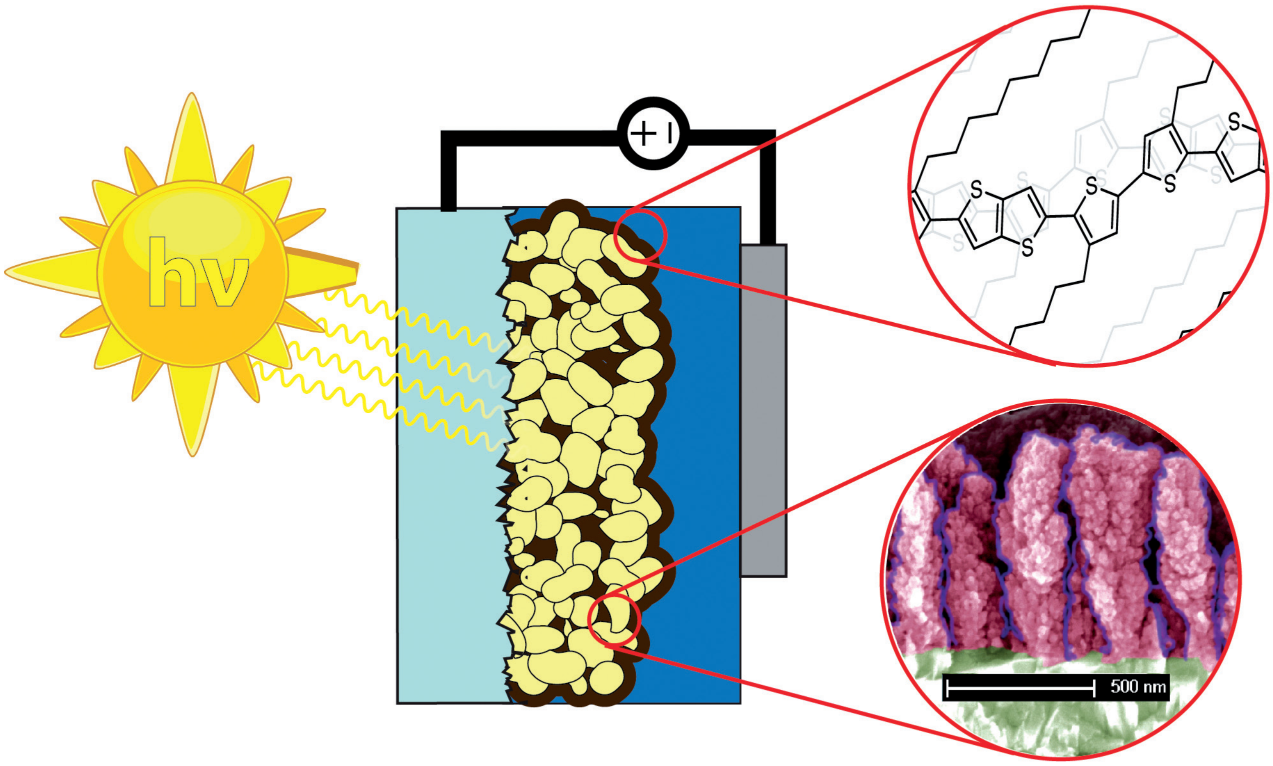
"The current cost of producing crystalline semiconductor devices using the required techniques is only reasonable due to the low cost of the fossil fuel-based energy used to create them," Sivula said. "To reach a sustainable situation, we need to drastically reduce the cost of the devices. This can be accomplished with solution-based methods, and we need this as soon as possible."

Future projects involve making new molecules with such bottom-up techniques, investigating how they organize and crystallize and processing them in ways that induce a given order with the goal of making them better semiconductor materials and increasing performance in the targeted devices. Indeed, researchers are just beginning to be able to control electronic material structures from a chemical standpoint, he said. While the immediate goal is the conversion of solar energy, it's possible that all electronic devices might someday be made with these sorts of materials.

"It would be great if, for instance, we could just print computer processors and high efficiency energy conversion devices with an ink jet printer," he said. "Right now, this is a fantasy, but maybe we're not so far off."

Biography

Born in the United States, Kevin Sivula studied at the University of Minnesota, where he obtained a Bachelor's degree in chemical engineering. He continued his studies in the field at the University of California, Berkeley, earning his doctorate in 2007. He then joined Professor Michael Grätzel's group at EPFL, where he developed nanostructured films with an iron oxide base for hydrogen production using solar energy. He won the 2011 Zeno Karl Schindler Prize, awarded by the EPFL Research Commission on behalf of the Zeno Karl Schindler Foundation. The award distinguishes postdoctoral work of particular excellence performed at EPFL, in the field of environmental sciences and/or sustainability. In 2011, he was appointed tenure track assistant professor in ISIC at EPFL, and he is now the head of the newly formed Laboratory for Molecular Engineering of optoelectronic nanomaterials (limno.epfl.ch). Sivula enjoys snowboarding and painting in his free time.



The general structure of a hybrid (organic/inorganic) solar energy conversion device. Two electrodes, one transparent (light blue) sandwich the active components of the device. The active materials employed are put into intimate contact through nanostructuring. The insets show the types of materials used. The top shows the chemical structure of thiophene-based semiconducting polymer and the bottom shows a nanostructured oxide semiconductor. Sivula's work focuses on controlling the structure and morphology of both of these classes of materials in order to enable facile processing and to enhance device performance.

DUBIKOVSKAYA LAB TARGETS KILLER DISEASES WITH NEW IMAGING TOOLS AND TECHNIQUES

A 2011 World Health Organization study found that non-communicable ailments including heart disease, stroke, diabetes and cancer now make up two-thirds of all deaths globally. Elena Dubikovskaya's research may improve our understanding and treatment of each of these conditions.

While researchers have learned a lot about such illnesses in recent years, knowledge is still hampered by a lack of tools that allow scientists to see important biological processes within the body. Dubikovskaya is trying to fill that gap with visualization procedures that combine synthetic chemistry, optical imaging and an understanding of cellular functions at the molecular level.

Take mitochondria. The organelles play an important role in a number of biological processes, including cell differentiation, cell cycle control, cell survival, neuronal protection and aging. Mitochondrial dysfunction, in turn, contributes to a wide range of diseases, including cancer, Alzheimer's disease and diabetes. As mitochondria dysfunctions are increasingly linked to a number of diseases, it gets more and more important to identify ways of characterizing them.

"A disease like diabetes affects metabolism, the immune system, the endocrine system, etc. and you can't just mimic this on a Petri dish," Dubikovskaya said. "There's nothing that works on the level of the whole organism to detect or quantify mitochondrial dysfunction, and we're trying to develop these tools."

"A DISEASE LIKE DIABETES AFFECTS METABOLISM, THE IMMUNE SYSTEM, THE ENDOCRINE SYSTEM, ETC., AND YOU CAN'T JUST MIMIC THIS ON A PETRI DISH."

One of her projects focuses on mitochondrial membrane potential. Perturbation of the potential—fundamental for the normal performance, differentiation and survival of cells—has been noted in nearly all cases where mitochondrial malfunction is linked to human disease. Although in most cases it's unclear whether changes in the mitochondrial membrane potential are a cause or an effect, changes in the potential directly reflect the life to death transition of the cell, Dubikovskaya said. Measurements of this potential should then provide important information about the molecular mechanisms controlling cell functions. Current fluorescent dye-based methods for measuring this membrane potential suffer from some drawbacks: none of them work in living organisms such as mice, the probes are highly toxic and tend to produce a lot of false negative and false positive results.

Dubikovskaya thinks a new method that combines novel chemical biology approaches with high sensitivity optical imaging tools and improved algorithms for data analysis will allow her lab to exploit the differences in mitochondrial membrane potential associated with various diseases to identify new ways of clinical interventions and drug development. This new chemical biology tool uses bioorthogonal "click" reactions, which are reactions whose components react selectively and rapidly with each other in the presence of all the chemical functionality found in living systems. When combined with high-sensitivity optical imaging, these methods should overcome the limitations of existing probes and also allow measurements in much more complicated biological settings, she said.

Dubikovskaya's lab, which currently consists of four post-docs and five PhD students, will initially focus on the application of the new method to examine the mitochondrial mechanisms of beta-cell dysfunction in diabetes. The onset of diabetes, which the WHO says will kill twice as many people by 2030 as it did in 2005, is provoked by the death of beta cells, which are responsible for generating insulin. The demise of the beta cells is, in turn, provoked by the death of their mitochondria, Dubikovskaya said.

"WE DON'T KNOW VERY MUCH ABOUT THIS PROCESS THOUGH BECAUSE WE DON'T HAVE TOOLS THAT CAN ASSESS WHEN THE MITOCHONDRIA IS HEALTHY OR DYING."

"We don't know very much about this process though because we don't have tools that can assess when the mitochondria is healthy or dying," she said. "We want to look at the biology and see what causes this important event. It's important to develop these tools for basic science, but hopefully there will be medical applications in the future."

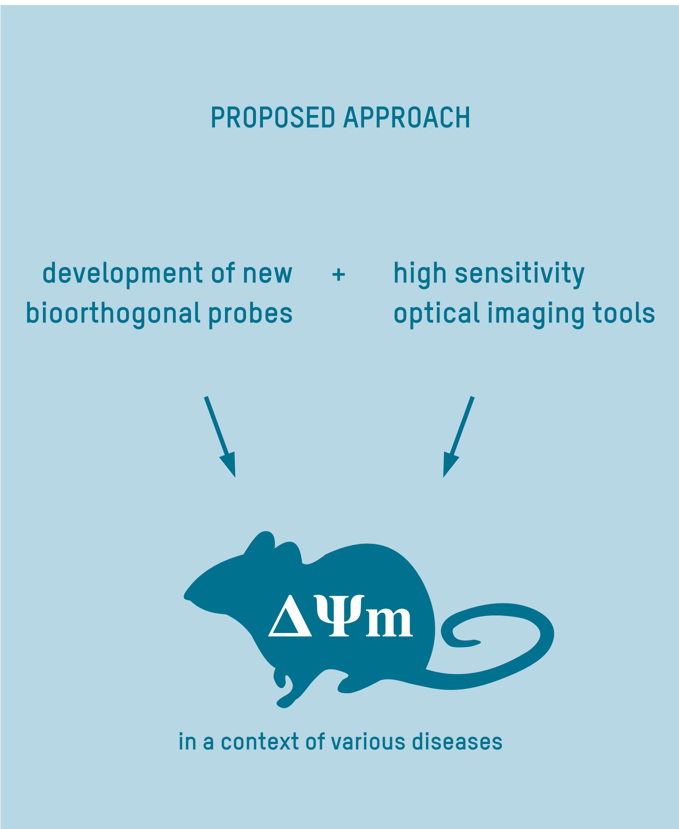
The group will also work on speeding the rates of and expanding the variety of the bioorthogonal click reactions to enable more widespread use to, in turn, answer important biological questions. After identifying new bioorthogonal reactions, Dubikovskaya plans to use them in several other biological applications, including biomolecular labeling and imaging of several other important cellular processes.

One specific application is the non-invasive imaging of insulin-receptor binding in live cells and animals. Insulin, a peptide hormone that plays an important role in regulating glucose, fat, and steroid metabolism in the body, is one of the only effective drugs for the treatment of diabetes. Its signaling system is central to regulating metabolism, reproduction, growth and development, survival and lifespan, as well as multiple central nervous system functions. While the creation of insulin analogs has improved our understanding of the relationship between structure and function, many questions about the biology of the insulin-receptor complex remain unanswered. The approach may also be used for the imaging of other cell surface small ligand-receptor interactions as well as development of new drug screens that can affect this important process.

Imaging is also a critical element of another project in Dubikovskaya's group—the development of probes for image-guided surgery in oncology. Surgery plays a central role in cancer treatment and complete removal of the cancerous cells is the single most important prognostic factor for disease-free survival in virtually all solid tumors. During operations, surgeons generally have to rely on sight, experience and tactile information to determine the spread of the tumor cells into surrounding tissues. As a result, incomplete microscopic resections may lead to cancer re-growth in 40-60% of cases for several types of cancer. The development of fluorescent probes that give doctors a clear view of cancer cells during surgery would make it easier to remove exactly what needs to be removed, and no more.

Dubikovskaya's group is working on the development of such a probe for use in several types of human cancer and plans to test it in the clinic soon within the framework of her collaboration with University of Groningen Medical Center.

Biography
Elena Dubikovskaya is now tenure track assistant professor of bio-organic chemistry at ISIC. She received her MS degree from University of Central Florida under the supervision of D. Howard Miles in the field of medicinal chemistry of natural products. She then continued her PhD studies in the field of medicinal chemistry and drug delivery in the group of Paul Wender at Stanford. After graduation with a PhD degree in 2008, she moved to the University of California at Berkeley where she did her postdoctoral studies in the field of chemical biology in the group of Carolyn Bertozzi.



SECTION OF

CHEMISTRY AND CHEMICAL ENGINEERING GAINING IN GLOBAL RENOWN

With all the international accolades going to ISIC's world-class research, it's easy to forget that the unit's scientists are, first and foremost, excellent teachers focused on the critical task of educating EPFL's undergraduate students. At the start of the last school year, the Section of Chemistry and Chemical Engineering welcomed more than 100 first-year students for the first time ever, with 10% even coming from distant countries such as Brazil, South Africa and China.

"People coming from so far to start their studies is something really new for us," said Jean-Luc Marendaz, vice-director of the section, which is headed by Prof. Jacques-E. Moser. "This is not surprising though as we provide one of the best educational environments and experiences in chemical sciences in the world."

"PEOPLE COMING FROM SO FAR TO START THEIR STUDIES IS SOMETHING REALLY NEW FOR US. THIS IS NOT SURPRISING THOUGH AS WE PROVIDE ONE OF THE BEST EDUCATIONAL ENVIRONMENTS AND EXPERIENCES IN CHEMICAL SCIENCES IN THE WORLD."

The section is currently the largest school of chemistry in Switzerland in terms of yearly graduates. While the number of new students has steadily grown flat over the last three to four years, the department is this September expecting 120 new students in first year chemistry, a jump of 62%. There is a similar trend at the MSc level, with an overall increase of 70%. The programs in chemical engineering and biotechnology are particularly sought after, with a doubling of the number of students. Marendaz expects the long-term trend to show

...

a steady increase in the number of students in the section, with more or less equal numbers of men and women starting chemistry or chemical engineering degrees. The department received almost twice as many applications in 2012 as five years ago for the master's program, which is increasingly competitive: it has an acceptance rate of just 10% to 15% for foreign students.

"It's really competitive," Marendaz said. "We have very high requirements."

At the same time, the section is working hard to make facilities and courses even more attractive. One important element of this, Marendaz says, is asking for student evaluations. In an initial round, students are asked to give an overall rating of between zero and six (excellent) to the course and professor. Any courses that do not achieve a mark of four or above are examined through a more detailed questionnaire.

"THE VISIBILITY OF CHEMISTRY AT EPFL HAS CLEARLY BEEN ENHANCED OVER THE PAST YEARS."

"There are many possible reasons for lower scores – the documentation, the accompanying exercises, the speed of the course, for example – and it's important to identify them," Marendaz said. "Without the feedback from students it would have been impossible to identify these issues. This is something that both the section and the teachers take very seriously."

Most courses receive excellent evaluations, and more than a third of the section's courses receive ratings of five or above.

"Teaching is an important consideration, both in the hiring of new professors and even more so for promotion," Marendaz said. "A significant part of the dossier is related to teaching—he or she has to have proven skills in this métier to get a promotion."

Another innovation in recent years involves the introduction of an internship program for students in chemical engineering. The master's students spend four to six months in a company to get their first hands-on experience of the workplace. External teachers also play an important role, especially in the master's program in chemical engineering, where a significant proportion of the curriculum is taught by people working in industry.

"This gives students a chance to really see the direct link between their studies and their future jobs," Marendaz said.

The preparation serves the students well, with some 60% of the chemical engineering graduates immediately starting careers at companies including Novartis, Lonza, Syngenta, Firmenich, Givaudan, Nestle, BASF and Dow Chemical. Of the chemistry students, most go on to complete a PhD, with some 50% choosing to stay at EPFL.

"The visibility of chemistry at EPFL has clearly been enhanced over the past years," Marendaz said.

FEATURE ON CÉSAR PULGARIN

PULGARIN GROUP LOOKS OF RADICALS TO CLEANSE

Many people take vitamins to neutralize the oxidants circulating around in their bodies. Professor César Pulgarin, on the other hand, thinks of efficient ways to generate them.

The free radicals linked to cellular damage and disease in people can also be used to break down pollutants and kill bacteria. Pulgarin, professor titulaire in ISIC and head of the Advanced Oxidation Processes Group, aims to generate these radicals through photochemical, photo-catalytic, ultrasonic, electrochemical and chemical means, and then harness their destructive power to do good. Projects aimed at producing clean drinking water for isolated populations, purifying water used in agro-industrial activities and developing materials to help combat infections that spread in hospitals are just a few of the applications they're developing.

"The hydroxyl radical is a very, very powerful oxidative species," Pulgarin said. "It's responsible, in part, for the aging of all living organisms, but in the lab, we try to maximize their generation because they are so efficient for the degradation of pollutants and the inactivation of bacteria."

One important way this efficiency is being put to use is in the purification of drinking water. Significant proportions of the populations of developing countries—as much as 40 or 50%—lack access to safe water, particularly in countries where many of the people live in rural areas. The group is now looking at two main ways of addressing this problem.

The first method, aimed at very poor populations in remote areas, involves a system for purifying drinking water in standard PET bottles. The helio-photocatalytic process takes advantage both of the sunlight and the dissolved iron found in water, particularly in tropical countries. The process involves putting water into PET bottles, adding hydrogen peroxide—an inexpensive and widely available oxidant—and placing them in full sunlight, for example of the roofs of houses for a given amount of time. The group has obtained good results in South America and Africa and is continuing to study the water produced.

"THE HYDROXYL RADICAL IS A VERY, VERY POWERFUL OXIDATIVE SPECIES," PULGARIN SAID. "IT'S RESPONSIBLE, IN PART, FOR THE AGING OF ALL LIVING ORGANISMS."

"The water is safe from a microbiological point of view, but we have to continue this research to ensure that we don't generate harmful compounds during treatment, for example," he said.

The second technique also uses solar light and the bacteria-killing powers of the hydroxyl radical, but involves a bigger installation with a reactor and is rather meant for a small town or group of families with some education. Pulgarin has tested pilots in South American countries including Colombia, Argentina and Peru, and also in Morocco, Tunisia and Burkina Faso in Africa.

Another of Pulgarin's projects putting the photochemical generation of hydroxyl radicals to use involves the development of systems for cleansing toxic and/or non-biodegradable substances from water used in agro-industrial activities.

Pesticides are one example: a project in Colombia focuses on the water used to clean bottles of pesticides and the airplanes that spray

TO HARNESS DESTRUCTIVE POWER WATER, BEAT INFECTION

the toxic chemicals. The water itself contains toxic pesticide residues that are often improperly treated. A project funded by the Swiss Agency for Development and Cooperation supported the development of a system that couples advanced oxidation, solar photo-treatment with simple biological treatment. The water's impurities, exposed to hydroxyl radicals in a first step, are rendered non-toxic and biodegradable. The water can then be conducted to a simpler and much-less-expensive biological treatment step and finally recycled into use for cleaning. The process, which includes the tricky task of identifying exactly when the water has been rendered non-toxic and ready for biological processing, is being used in sugar cane production in Colombia, and also commercially in an industrial installation in the south of Spain.

"OUR ORIENTATION IS THE SOLUTION OF THE PROBLEM, BUT THE TOOLS USED FOR UNDERSTANDING THE PROCESS IS BASED ON RIGOROUS SCIENCE."

Hydroxyl radicals are also being readied to fight hospital-acquired infections. The problem is growing everywhere in the world, but particularly in places where the liberal use of antibiotics has encouraged the spread of bacteria such as Methicillin-resistant Staphylococcus aureus, or MRSA.

"The percentages of these kinds of acquired illness are progressively increasing," Pulgarin said. "Patients arrive at the hospital with one thing, but more and more of them are leaving it with something else, sometimes worse than what they had to start with."

The idea here, again based on the photochemical generation of the radicals, is to develop a polymer material capable of supporting a solid photocatalyst such as titanium dioxide or copper oxide sometimes doped with metals such as silver. The interaction of the catalyst with the light of the room produces hydroxyl radicals, which in turn fight the spread of infection by killing the bacteria.

"We have never really observed bacterial resistance to these hydroxyl radicals, they have not developed such a mechanism," Pulgarin said. "That's of course also the case for animal cells, otherwise we could live much longer. But in the case of bacteria, it's a good thing."

Such a material may be best suited for preventing bacteria development on surfaces such as hospital walls, Pulgarin said. The challenges with the project involve ensuring sufficient hydroxyl radical production with the limited light-intensity in some hospital areas and creating a durable material that is both affordable and safe for patients.

As complex as existing problems are, Pulgarin says he and colleagues will be challenged to come up with more and more sophisticated tools to eliminate micro-contaminants from water and the environment. While most chemicals were used at the level of production 50 years ago, today's individual households are generating more and more chemical pollutants— the average home contains about 60 different chemicals dedicated to a variety of uses, from cosmetics to weed control in the garden, and domestic activities are becoming "industrial," he said.

Many of these substances cannot be degraded by existing wastewater treatment systems and so end up unprocessed in areas such as lakes and rivers, where they pose a risk to the environment and potentially to people who consume the water. While the risk to the human drinking water supply in Switzerland appears limited because of stringent legislation governing the elimination of these micropollutants from potable water, it's likely that tougher laws will require that they are also prevented from entering any natural bodies of water at all. Pulgarin and his group have developed a cleansing system using hydroxyl radicals produced from a combination of iron salts, hydrogen peroxide and UV illumination. The system is set up to clean the water after biological treatment, but before it's released into natural bodies of water, and is now running as a pilot project in Lausanne.

"The risk for many animals in the natural system has already been demonstrated, but there's also a question of risk for humans," he said. "There isn't necessarily any evidence yet, but there are more and more suspicions. We have to be very cautious with these emerging pollutants."

Though the group's work is focused on solving applied environmental problems, the research underpinning their work is sophisticated and complex, following the rigorous rules of the many fields the work overlaps, Pulgarin said. For example, in the drinking water projects, the group is studying the complex mode of action of the photocatalytic process on bacteria components such as the membrane, DNA, etc.

"We try to contribute to the understanding of the action models," he said. "Our orientation is the solution of the problem, but the tools used for understanding the process is based on rigorous science."

Biography

César Pulgarin studied chemistry as an undergraduate at the University of Lausanne, received a Master's degree in environmental chemistry from the University of Geneva and a PhD in bio-inspired synthesis of natural substances from the University of Neuchâtel. Pulgarin has been working at EPFL since March 1989 and was named adjunct professor in 2011. He has published 170 papers in indexed international journals and books and presented 120 papers at international meetings. He is the world's most cited author in 1) TiO_2 photo-assisted bacterial inactivation in water and 2) Coupling of photochemical and biological processes for pollutant degradation. He has been involved in fifteen African, South American and European international research projects and has supervised 20 PhDs and post-docs, 120 master, diploma, seminar and training theses.

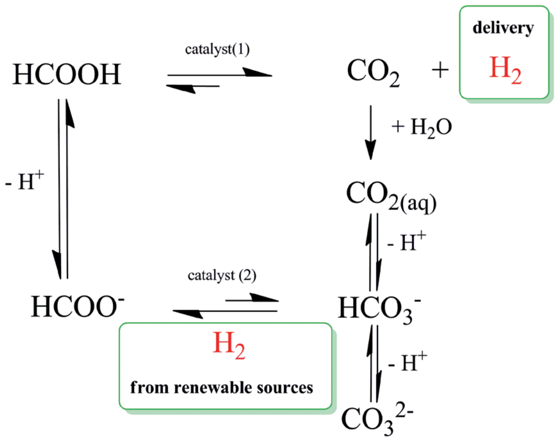
LAURENCZY AND COLLEAGUES DETAIL NOVEL METHOD OF FORMIC ACID-BASED HYDROGEN DELIVERY IN *SCIENCE* PAPER

Hydrogen may be set to play a key role in strategies for renewable energy. It can be used to store power generated from the wind and sun and also be used as a carrier for the clean production of electricity, heat and fuels.

Exploiting it isn't entirely straightforward though: generating hydrogen from renewable sources and storing it in a safe and reversible manner both remain challenging. Professor Gabor Laurenczy, professor titulaire in ISIC and head of the Group of Catalysis for Energy and the Environment, has figured out ways of addressing these problems.

The first step involves developing a system to transform hydrogen and carbon dioxide present in the atmosphere into formic acid with the help of a catalyst. Then, last year, Laurenczy and colleagues including researchers from the University of Rostock, Germany, published a paper in *Science* detailing a method of releasing hydrogen from formic acid with the help of a very active iron catalyst system.

"This catalyst is very cheap and very efficient," Laurenczy said. "You can store hydrogen in formic acid and then, when you need it, turn it back into hydrogen and carbon dioxide with the help of a catalyst. You can then use this hydrogen as an energy source, transforming the chemical energy to electricity very efficiently, or for other purposes."



The breakthrough described in the Science paper hinged on identifying a new iron-based catalyst that proved capable of efficiently liberating hydrogen at near-ambient conditions. Other methods of extracting hydrogen from formic acid rely on the use of precious metals such as ruthenium and iridium, or other catalyst systems that are active only in toxic solvents.

The results of the two bodies of research—safe storage and efficient and environmentally friendly release or of hydrogen —address many issues. Storing hydrogen in a liquid rather than as a flammable gas under high pressure means that it's much safer and can be contained in lighter, more compact vessels. Production of the hydrogen gas, now mainly achieved by processes such as stream reforming and coal gasification that are based on limited fossil resources such as natural gas, coal and oil, can be approached in a more sustainable manner.

The work has caught the attention of industrial partners who are working to develop products based on the system described. A Canadian company, Tekion, is set to introduce a small 100 watt charger that will produce electricity from formic acid via a PEM hydrogen fuel cell. The group is also working with Granit SA, a Lausanne-based company, about further development of an entire storage and delivery unit.

"We would like to develop the whole system of energy storage and delivery in a way that we don't need any network or grid, you would just put this unit somewhere next to a solar panel or wind energy source," he said. "You'd have the primary renewable energy source and at the same time reduce carbon dioxide into formic acid, which you could then use to produce electricity via hydrogen fuel cells."

The group, in collaboration with the University of Applied Sciences and Arts Western Switzerland in Yverdon and Granit Green Networks in Orbe, plans to test drive a formic acid-powered boat on Lake Neuchâtel this summer.

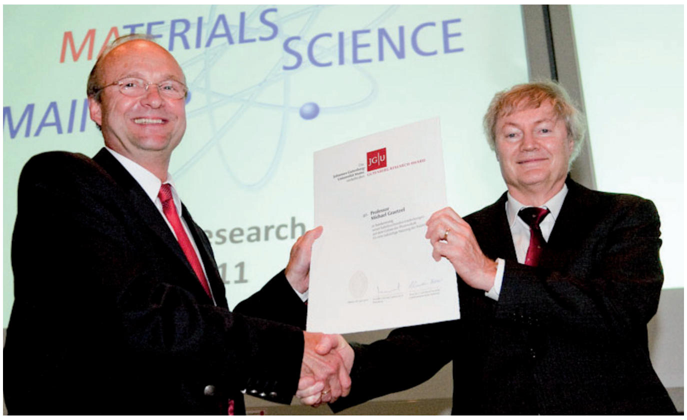
Efficient Dehydrogenation of Formic Acid Using an Iron Catalyst, Boddien, A.; Mellmann, D.; Gartner, F.; Jackstell, R.; Junge, H.; Dyson, P. J.; Laurenczy, G.; Ludwig, R.; Beller, M., *Science*, Vol. 333, num. 6050, p. 1733-1736

NICOLAI CRAMER AWARDED SCS'S 2012 WERNER PRIZE, THIRD IN A ROW FOR ISIC

Nicolai Cramer won the 2012 Werner Prize for his work on selectivity in carbon-hydrogen and carbon-carbon activations. The broad theme of Cramer's work is the design of efficient catalytic processes that operate through uncommon modes of activation and will result in a rapid increase in molecular complexity. His current focus is on the development of novel asymmetric metal-catalyzed reactions using rhodium-, palladium-, iridium-, and copper-complexes designed to selectively functionalize unactivated C-H and C-C bonds. Projects involve the development of new and robust ligand systems that fit the needs of these metals and the envisioned reaction mechanisms. Cramer and his group plan to eventually apply these methods in the synthesis of complex natural products with intriguing and potent pharmacological properties.

This is the third year in a row that an ISIC scientist has won the prize, which the Swiss Chemical Society awards to a promising young Swiss scientist or scientist working in Switzerland for outstanding independent chemical research. The prize was awarded to Xile Hu, head of the Laboratory of Inorganic Synthesis and Catalysis, in 2011 and to Sandrine Gerber, from the Laboratory of Synthesis and Natural Products, in 2010.

GRÄTZEL GROUP DOCUMENTS RECORD-BREAKING EFFICIENCY OF DYE-SENSITIZED SOLAR CELLS IN *SCIENCE*



A group of scientists in the Laboratory of Photonics and Interfaces, led by Michael Grätzel, and in collaboration with Taiwanese researchers, improved the efficiency of dye-sensitized solar cells to 12.3%, a performance that's comparable to that of thin film silicon-based solar panels on the market. The research was published in a November 2011 issue of *Science*.

The scientists achieved the feat by replacing the standard dye components of the cells – ruthenium and iodine – with porphyrin and cobalt. This changed the composition and color of the cells, allowing them in turn to increase the absorption of sunlight and obtain a higher cell voltage. The result is a higher efficiency for converting solar into electric power.

While traditional photovoltaic cells use silicon as both the source of electrons and the conductor of the charge carriers, the dye-sensitized solar cells, also known as Grätzel cells, separate these two tasks between dye molecules and a porous titanium oxide nanostructure. This is why the method is frequently referred to as "artificial photosynthesis": in plants, sunlight absorbed in the leaf by chlorophyll converts carbon dioxide and water into oxygen and glucose, providing energy. In Grätzel cells, chlorophyll is replaced by dye molecules and the leaf structure by the oxide nanostructure. The cells presented in the *Science* paper result in even closer imitation of the natural process—the new porphyrin having a structure closely related to that of chlorophyll and a green tint.

Dye-sensitized solar cells can be used to create flexible, transparent solar panels and represent a promising alternative for a number of applications. This new efficiency benchmark brings them within the efficiency range of thin film silicon cells. The theoretical maximum efficiency of dye sensitized solar cells is 31%, compared with 28% for traditional silicon-based devices.

Grätzel, who heads the Laboratory of Photonics and Interfaces, earlier this year won the Albert Einstein World Award of Science from the Interdisciplinary Committee of the World Cultural Council. The award is a prestigious acknowledgement from outstanding personalities of the scientific community from five continents. The committee awards the prize for "outstanding contributions to the welfare of mankind and the health of the planet," in this case for helping to solve one of the most important technical problems relating to energy and sustainability through the development of the Grätzel cell. The invention and development of these solar cells is leading to breakthroughs that will strongly increase our ability to consume renewable solar energy, the panel said. The 29th Award Ceremony took place at Aarhus University in Denmark in April.

Last year, Grätzel won the 2011 Gutenberg Research Award. The prize is awarded in recognition for excellence in scientific research. He also won the 2011 Federation of European Materials Science Societies' Materials Innovation Prize and the Wilhelm Exner Medal of the Austrian Trade Association. Grätzel has published more than 900 papers, two books and holds over 50 patents. Scientific American ranks him among the top 50 scientists worldwide.

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DYSON WINS CENTENNIAL LUIGI SACCONI MEDAL FOR HIS CONTRIBUTIONS TO ORGANOMETALLIC CHEMISTRY

ISIC Department Head Paul Dyson was awarded the Centennial Luigi Sacconi Medal for his contributions to organometallic chemistry, encompassing synthesis, catalysis and metal-based cancer drugs.

The Division of Inorganic Chemistry of the Italian Chemistry Society, together with the Fondazione Luigi Sacconi, awards the medal to a scientist who has obtained particularly significant results in inorganic chemistry. In December 2011, Dyson was awarded the beautiful hand-crafted gold medal at a ceremony in Rome at the Accademia dei Lincei, which was founded in 1603 by Federico Cesi and was the forerunner of the Pontifical Academy of Science. Dyson delivered the award lecture in Florence in January this year, describing his latest results on organometallic drugs that display antimetastatic activity. He explained the mechanistic studies undertaken to elucidate their mode of action at a molecular level as well as further studies into how their structure was refined to overcome certain types of resistance mechanisms. He also paid tribute to Luigi Sacconi, a prolific inorganic chemist who he greatly admires. Some of Sacconi's groundbreaking concepts have become part of the standard textbook material that Dyson teaches to EPFL chemistry students.

TSYBIN AWARDED ERC GRANT TO DEVELOP SUPER-RESOLUTION MASS SPECTROMETRY FOR HEALTH AND OTHER APPLICATIONS

Today's state-of-the-art mass spectrometers can acquire the high-resolution data needed for in-depth structural analysis of organic, inorganic and biological molecules — they just do it slowly. The European Research Council has awarded Prof. Yury Tsybin, head of the Biomolecular Mass Spectrometry Laboratory, a 1.5 million euro Starting Grant to speed things up and open new avenues in molecular structure analysis.

Faster acquisition of high-resolution data is essential in areas such as biology, where the dynamic range of the concentration of proteins, for example, is huge. A slow measurement will capture part of the protein population, but leave potentially useful information unrecorded. Quicker measurements would mean that the same amount of sample could yield deeper analysis and answers that researchers might not otherwise find.

"If you can do measurements faster, you may have both a technical advantage and an analytical advantage," Tsybin said. "The technical advantages mean your instrument runs faster, you can analyze more samples in a day and the sample consumption is lower. The analytical advantage gives you new information about your sample, for example, the identification of new proteins in terms of more correct, unambiguous information."

Tsybin's group is using Fourier transform mass spectrometry, or FTMS, as a basis technique because of its superior performance. This approach involves recording the frequency of periodic ion rotation in strong magnetic fields or periodic ion oscillation in electrostatic fields and then performing a Fourier transform on the recorded time-domain induced current signal to get the frequency domain spectrum. The final mass spectrum is received from the frequency domain spectrum using the known relation between ion frequency and m/z value. The resolving power of the FT signal processing-based method can be described as resolving power per turn/oscillation multiplied by the number of turns/oscillations. The Fourier transformation element requires sinusoidal signals though — this is the limiting factor to obtaining high resolution quickly. Speeding up the process will mean increasing the resolving power per turn/oscillation or per unit of time. But how?

Tsybin's answer lies in increasing the information flow density in the time-domain signal by modifying ion motion and detection principles and replacing or complementing the Fourier transform with another method of signal processing. The group is considering a number of alternative approaches to processing but has, for now, focused on the filter diagonalization method, or FDM, a recently developed super-resolution signal processing algorithm.

The technique had been used in quantum mechanics and nuclear magnetic resonance spectroscopy, but never applied to the generation of experimental mass spectra before Tsybin and colleagues tried it out. They published the first paper on this application in *Analytical Chemistry* (reference below) earlier this year.

"The results were very encouraging and we got very good feedback from the paper," Tsybin said. "We really believe there is potential here."

"WE EXPECT THAT EVEN IF TODAY OUR APPROACH OF MASS SPECTRA GENERATION BY SUPER-RESOLUTION SIGNAL PROCESSING TAKES HOURS AND DAYS, IN SEVERAL YEARS WE WILL REACH THE LEVEL OF SECONDS AND MILLISECONDS."

The approach nonetheless has its critics. One objection, Tsybin says, is that super-resolution methods won't work in routine experiments due to parameters such as the signal to noise ratio and a lack of sensitivity. Another criticism is that the calculations require too much computing power. While fast Fourier transforms can be performed on modern smartphones, for example, the FDM now requires powerful workstations and clusters of computers working together. Tsybin nonetheless believes that it will be feasible to perform FDM mass spectrometry in routine labs in the near future.

"Computers develop very fast and if you depend on them you can improve your method every year," he said. "We expect that even if today our approach of mass spectra generation by super-resolution signal processing takes hours and days, in several years we will reach the level of seconds and milliseconds for data processing with super-resolution mass spectrometry."

The group's next papers will focus on use of the new method in the field of proteomics and petroleomics, with the aim of finding out whether it truly allows for improved protein and hydrocarbon identification in extremely complex biological and environmental samples. The techniques being developed will gradually be applied in a wide range of applications linked more generally to life sciences and energy. The method development in this direction may even eventually be applied to differentiate positional isomers of small molecules by mass, "the ultimate goal of the whole field of mass spectrometry in terms of resolution," Tsybin said. "That effectively means actually weighing chemical bonds," he said. "That's something that normally catches peoples' attention."

Filter Diagonalization Method-Based Mass Spectrometry for Molecular and Macromolecular Structure Analysis, Kozhinov, A. N. and Tsybin, Y. O., *Analytical Chemistry*, Vol. 84, num. 6, pp. 2850-2856, 2012.

ISIC LAB'S INNOVATIONS REVOLUTIONIZE USE OF DYNAMIC NUCLEAR POLARIZATION

Dynamic nuclear polarization, or DNP, started off as a curiosity. The technique, which involves transferring magnetization from electron spins to nuclear spins, was initially a largely academic idea, "understanding for the sake of understanding," when first developed in the 1950s and 1960s, said Prof. Geoffrey Bodenhausen, head of ISIC's Laboratory of Biomolecular Magnetic Resonance. In 2009, when instrumentation company Bruker Biospin introduced a machine combining DNP with solid state nuclear magnetic resonance — an innovation that seems to have been ahead of its time — it sold a single unit.

It also lent one to EPFL though. And that's when things took off.

"We started using DNP in all sorts of applications that no one had anticipated," Bodenhausen said. "Since then, they've been selling like hotcakes."

Modern versions of the technique emerged thanks to pioneering work by Massachusetts Institute of Technology Prof. Robert Griffin, who had the idea of combining DNP techniques with solid state NMR. In 1997, he devised a method of spinning a sample at very high speeds, at a very low temperature of about -200 degrees Celsius, while irradiating it at the same time with powerful microwaves to enhance the NMR sensitivity of solid materials. Then, in 2003, Prof. Jan Henrik Ardenkjær-Larsen at the Denmark Technical University (DTU) devised a way of coupling DNP with solution state NMR by freezing small molecules at very low temperatures and then heating them quickly in an almost explosive transition that nonetheless maintains their nuclear polarization—the technique resulted in an increase in the signal-to-noise of more than 10,000 times in this type of NMR.

"These two development led to many attempts to copy them, improve on them, and go beyond what they did," Bodenhausen said.

EPFL's main contribution to the body of research was work done with colleagues from ENS Lyon on surface problems, working towards improved characterization of heterogeneous catalysts, Bodenhausen said. While a number of processes take place at surfaces, i.e., interfaces between liquids and solids, very little detail is known about them because of the lack of appropriate analytical tools.

For real-life, rugged and inhomogeneous surfaces, "microscopes are useless, X-rays are useless, neutrons are useless, almost everything is useless," he said. "There was a great need to get some sort of evidence about what's going on at surfaces."

EPFL researchers started looking at organic molecules grafted by chemical bonds onto to silica surfaces. Normally, one can't see these molecules by NMR, but the use of DNP made it possible to boost the signal of the molecules by a factor of about 50, so that one could actually see what was going on. The work, which continues today, has had a tremendous impact on the field, Bodenhausen said.

Scientists around the world continue to develop both DNP approaches. That said, EPFL is unique in that researchers here work side by side in the lab developing the two approaches. It was natural then that EPFL was selected to host the Third International Symposium on DNP last year. The conference, which was sponsored by a number of companies including Agilent Technologies, Sigma-Aldrich and Bruker Biospin, brought together leading experts in the field for several days of talks and posters.

Some of the work featured was that of Sami Jannin, a lecturer and researcher. Jannin, working at EPFL on solution state DNP NMR techniques, achieved much higher levels of polarization with a technique that involved transferring magnetization from the electrons to the protons and then, in a second step, to the nuclei rather than directly from the electrons to the nuclei of interest. This two-step method turns out to be about five times faster than current approaches and results in a signal that's three to four times as intense. The two-step method, in addition to providing such significant enhancements, is also more forgiving on the chemistry: the expensive radicals used in the one-step approach can be replaced by much cheaper ones that are readily available.

"When you achieve such dramatic steps forward, you open up new areas of chemistry," Jannin said. "You can use lower concentrations and look at more expensive samples. There are many things that can happen in the coming years."

Please see the website http://sdnpi.epfl.ch/meetings.html for additional information about the conference.

IN MEMORIAM PROFESSOR ERVIN KOVÁTS 1927-2012

In 1955, Ervin Kováts, then a post-doctoral student in Nobel laureate Leopold Ružicka's ETH Zurich lab, was asked to investigate the composition of essential oils using state-of-the-art techniques, including gas chromatography, a newly introduced approach. His ingenious use of the new technique led to contributions of fundamental significance, including his retention index system and the internationally designated Kováts retention indices. These indices revolutionized gas chromatography, allowing results to be compared and reproduced between labs across the world. In the years that followed, his research interests spanned various topics including gas chromatography and organic chemistry. He became full professor of technical chemistry at EPFL in 1967, a position he held until his retirement in 1994. Hungarian-born Kováts was awarded many honors, including the 1977 Tswett Medal, the Award of the Academy of Sciences of the U.S.S.R., the 1986 Martin Award by the Chromatographic Society, the Memorial Medals of the Technical University of Budapest (1986) and the University of Helsinki (1987), and the 2004 Halász Medal Award. The passing away of Prof. Kováts marks the end of an era for ISIC and the loss of a friend and colleague – however his name will remain known throughout the world in analytical chemistry labs where his indices are used daily.

VENTURE CAPITAL FUNDS HEINIS' WORK ON CONSTRAINED CYCLIC PEPTIDES THROUGH BICYCLE THERAPEUTICS SPIN OFF

Biotechnology company Bicycle Therapeutics is benefitting from research done by Prof. Christian Heinis, now head of ISIC's Laboratory of Therapeutic Proteins and Peptides, during his post-doc with Sir Greg Winter at the Medical Research Council's Laboratory of Molecular Biology (LMB) in Cambridge, UK.

Antibodies have proven to be good targeted therapies for ailments such as cancer and autoimmune diseases because genetic selection can be applied to create both diversity and specificity. They are, however, limited by their large and complex structures, the fact that they have to be injected into the body and do not easily penetrate tissue. Medicines made from small molecules generally do not have these disadvantages, but are more difficult to tailor for many disease targets.

Bicycle Therapeutics, spun off from LMB in 2009, is developing a new class of therapeutic agent that combines the selectivity and specificity of the biologic therapies with some advantages of small molecule medicines.

The work is based on Heinis's research in Cambridge, where he came up with and developed a bicyclic peptide technology method for generating chimeric peptide-small molecule macrocycles with tailored binding specificities. The technique involves using phage selection to identify and optimize chemically constrained cyclic peptides that have both high target-specificity and binding affinities stable to unfolding and protease action. The identified peptides can then be recreated as synthetic peptides with an organochemical scaffold, which can in turn be considered mini-antibodies with covalent organic cores. These features should allow the class of molecule to overcome weaknesses of previous generations of peptide-based therapeutics.

"They're completely non-toxic and very specific, not binding to other proteins," Heinis said. "Now we need to see whether they have sufficient therapeutic activity. We'll do this with different diseases and different targets."

The company is managed by Chief Executive Officer Rolf Günther and Chief Scientific Officer John Tite. Heinis acts as a scientific advisor to the company. The Technology Transfer Office of EPFL has signed a license agreement with Bicycle Therapeutics to benefit from potential commercial success.

"It is a great pleasure to be involved in the spin off and to help translate a technology into commercial products," Heinis said. "At the same time, I am happy being a scientist in an academic laboratory, having the freedom to try risky projects and to work on new innovations."

Please see www.bicycletherapeutics.com for more information.

WASER AWARDED PRIX SCHÄFLI FOR WORK ON NOVEL REACTIONS IN ORGANIC CHEMISTRY

The Swiss Academy of Sciences awarded Jérôme Waser the 2011 Prix Schläfli for work done in the field of new reactions in fundamental organic chemistry. Using methods based on catalysts and the development of non-conventional reagents, the academy said Waser has opened new pathways for the formation of novel carbon-carbon bonds and the synthesis of heterocycles. The fundamental work is essential for future applications including synthesis of medicines, development of organic materials and the preparation of colorants for solar cells, the academy said. Waser's approach to discovering new reactions is based on two steps: the synthesis of energy-loaded molecules followed by the formation of new bonds controlled by a catalyst. The energy stored in the first step of the process allows for reactivity that's the inverse of what's found in nature and the new approach has led to two major fields of study. The first involves the use of the cyclic tension of cyclopropanes in the synthesis of heterocycles, which are found in many pharmaceutical products. The method has already been applied to the synthesis of natural alkaloids that may play an important role in the development of new bioactive substances. The second field deals with very reactive acetylene bonds. Using the hypervalent iodine reagent TIPS-EBX (TrIsoPropylSilyl Ethynyl BenziodoXolone) and gold or palladium catalysts, Waser's group was able to introduce acetylenes into electron-rich molecules important in organic chemistry such as olefins and heterocycles. These new methods are expected to find widespread use in the generation of bioactive compounds and organic materials.

ISIC ALUMNUS ALAIN FUCHS AWARDED EPFL ALUMNI AWARD FOR EXCEPTIONAL CAREER PATH

Alain Fuchs, CEO of France's National Center for Scientific Research, or CNRS, was presented with the 2011 EPFL Alumni Award for his exceptional career path. Fuchs, who graduated from EPFL in 1975, was named head of the most important French government-funded scientific research organization in 2010.

Fuchs studied chemical engineering at EPFL and went on to get his PhD in physical chemistry at the Université de Paris-Sud, Orsay, France in 1983. He was a post-doctoral research associate at the University of Edinburgh and did research at universities including Imperial College London, Technische Universität Berlin, University of Edinburgh, North Carolina State University and University of California Los Angeles. He was research director at CNRS from 1991 to 1997 and was director of the Laboratoire de Chimie Physique des Matériaux Amorphes, Université de Paris-Sud from 1997 until 1999.
In that year, he founded and became director of the Physical Chemistry Laboratory at Université Paris-Sud. He was named head of the Ecole Nationale Supérieure de Chimie de Paris (ENSCP, Chimie ParisTech), and professor at Université Pierre et Marie Curie in 2006.

Fuchs, born in Lausanne in 1953, is one of the major French actors of theoretical calculations related to the theory, modeling and molecular simulations of fluids confined in various types of porous materials (zeolites, metal-organic frameworks, surface force devices, etc.) of practical importance in chemistry in general, and in material sciences, adsorption and catalysis in particular. He is a fellow of the Royal Society of Chemistry, a Chevalier des Palmes Académiques (1996) and a Chevalier de la Légion d'Honneur

Interview with Prof. Alain Fuchs

How did your experiences as a student at EPFL prepare you for your current job?
As a student at EPFL, in the chemistry department, I learned a lot in chemistry and chemical engineering and all the related topics that are needed to become an efficient young scientist. But, above all, I learned how to grasp scientific ideas and techniques and extend them in an effective and useful manner, thanks to intensive practical classes. As a student at EPFL I developed a critical attitude towards my own work and to whatever the teachers had to offer as an answer to any of my questions. This opens up the route to any type of job, including my current one!

What's your best memory of your time as a student at EPFL?
We worked hard, of course, but in the friendly Lausanne way of life. From "trois décis de blanc" to "pédalo sur le lac à Vidy". And what a thrill it was to attend the Montreux jazz festival in July, once exams were over.

What is your impression of EPFL from recent visits? How have things changed since you studied there?
Things have change quite a bit from 1975, when I received my EPFL diploma from Prof. Cosandey at the Avenue de Cour location. EPFL has now become a truly elite, globally recognized research university and the Ecublens campus and facilities are truly amazing. But this doesn't happen in one day. When I visit EPFL today, I still feel the sort of winning spirit that prevailed in the early days.

What advice do you have for chemistry students?
You are very lucky to be here! Commit yourself to each and every activity that EPFL is able to offer. Specifically for the chemistry students, let me simply remind you that chemistry provides a bridge between molecules of inanimate matter and the highly complex molecular architectures which makes living organisms (quoted from J.-M. Lehn). The place to be in the coming decade is where chemistry meets information science and technology.

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