Institute of Chemical Sciences and Engineering

Ecole Polytechnique Fédérale de Lausanne

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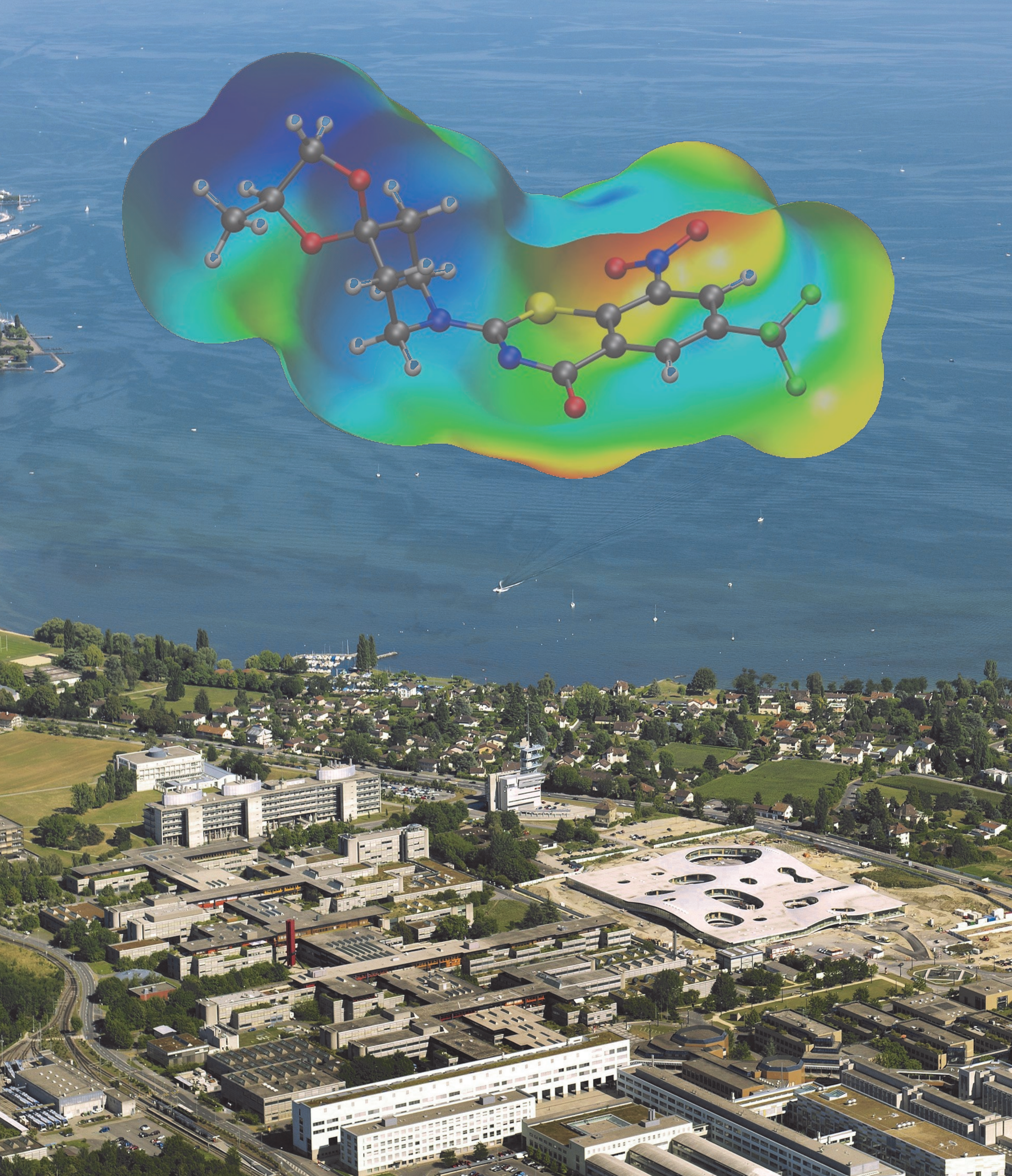

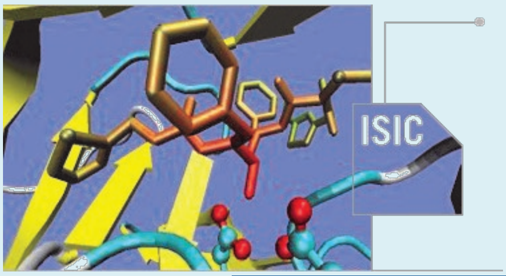

ISIC Newsletter
Issue 1

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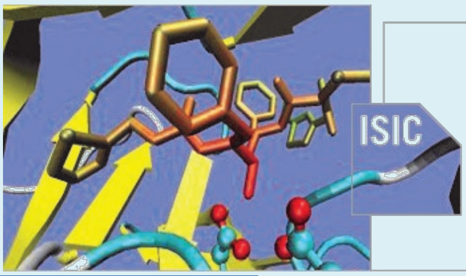
INSIDE THIS ISSUE

Front cover:
Photo of Lake Geneva and EPFL campus:
Alain Herzog, EPFL.

The surface map shows the electrostatic potential surface of a drug candidate for tuberculosis, BTZ (1,3-benzothiazin-4-one). The class of compounds, first synthesized by **Dr. Vadim Makarov** from the **Russian Academy of Science**, is being developed by the **New Medicines for Tuberculosis** consortium, which is funded by the European Commission and led by **Prof. Stewart Cole**, the director of the **Global Health Institute** at EPFL. The mechanism of action of the BTZs is currently being investigated by **Prof. Kai Johnsson** at ISIC. Tuberculosis, an infectious bacterial disease, is estimated to have infected about a third of the world's population and one in every ten of those will become sick with active TB in his or her lifetime, according to the World Health Organization. Graphic: LCMD, **Prof. Clémence Corminboeuf**

Back cover:
Graphic, provided by **Dr. MER Sandrine Gerber**, shows Golgi α-mannosidase II from Drosophila Melanogaster complexed by an inhibitor. Researchers in her group are studying α-mannosidase inhibitors as potential treatments for cancer in collaboration with the **University Hospital of Lausanne**. Derivatization of the group's lead inhibitor into more lipophilic esters led to promising inhibitory activity on glioblastoma and melanoma cell growth and further studies for the development of this new anti-cancer strategy are underway.



Message from Paul Dyson, ISIC's Director

Prof. Paul Dyson, Director ISIC

The chemical sciences are of vital importance in the modern world and the research undertaken in our Institute addresses many of the major challenges facing humanity. Research spans fundamental studies in theoretical chemistry and biochemistry to applications in devices and engineering. Fundamental research in our Institute led to the discovery of **dye sensitized solar cells**, and drugs and diagnostics developed within our Institute are now in widespread use. We continue to take a leading role in all aspects of chemistry including research at the interface of biology and physics as well as in sustainability and materials science.

> ***"All signs are positive, with continual growth in student numbers, research (gauged by publications, citations, funding, prizes, etc.) and also in tech-transfer."***

While our mission to strive for excellence in teaching and research has remained largely unchanged over the years, the institute has changed considerably, in terms of its structure, faculty and research priorities. Arguably the greatest change occurred in 2001 when the Institutes of Inorganic Chemistry and Organic Chemistry at the **University of Lausanne** formally merged with the Institutes of Physical Chemistry and Chemical Engineering at EPFL to form what is now known as the Institute of Chemical Sciences and Engineering (ISIC). The first director of ISIC, **Prof. Tom Rizzo**, who oversaw this transformation and built the management structure is now Dean of our Faculty, which also includes mathematics and physics. His successor, **Prof. Hubert Girault,** made further changes to cement a single and strong institute that has proved itself in various international evaluations. ISIC was in the excellence group of the first CHE Ranking of Excellent European Graduate Programmes in the Natural Sciences and Mathematics conducted in 2008. In the 2009 Academic Ranking of World Universities, compiled by **Shanghai Jiao Tong University,** ISIC was placed as number 7 in Europe, with all the higher ranked departments being considerably larger.

Photo: Alain Herzog

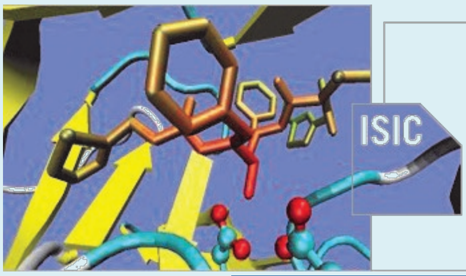
My role as Institute Director is not only to sustain our excellent position but to take us forward and upwards. All the signs are positive, with continual growth in student numbers, research (gauged by publications, citations, funding, prizes, etc.), and also in tech-transfer. Indeed, as you browse this newsletter you will see a range of on-going activities and some of our achievements. More information can be obtained from our website (http://isic.epfl.ch), which also provides details of events and up-to-date news on major accomplishments. Links to the Doctoral School in Chemistry and Chemical Engineering headed by **Prof. Pierre Vogel** and the Section of Chemistry and Chemical Engineering, responsible for our undergraduate teaching program, headed by **Prof. Jacques Moser** are provided at ISIC's homepage.

While every year is important to us, with new students starting, others leaving, 2011 is the year of chemistry and also marks 10 years since the amalgamation of chemical sciences at the University of Lausanne and EPFL to form our single united institute. We plan to host a number of events during this year aimed at potential students, our current students and collaborators and also events for our alumni. Indeed, we are grateful to all our collaborators, alumni and others who play a key role in helping ISIC successfully confront the challenges that lie ahead.

To conclude, I hope you enjoy reading this magazine. Your comments are welcome, either by e-mail to **secretariat.isic@epfl.ch** or by regular mail to me at the address given on the inside cover. If you would like to visit the institute or attend any events listed on our website, please do not hesitate to contact us.

Institute facts at a glance

- Number of Professors: 25
- Number of SNF Professors: 3
- Number of MER (senior scientists): 10
- Number of PhD students: 140 (enrolled in the Doctoral Program in Chemistry and Chemical Engineering)
- Research staff (post-docs, scientific collaborators): 138
- Number of master and bachelor students: 295 (enrolled in the Section of Chemistry and Chemical Engineering)
- Number of trainee apprentices: 24



Alumnus Jacques Membrez, Givaudan SA

__Jacques Membrez__ completed his undergraduate work in chemical engineering at EPFL in 1992 and finished his PhD with Professor __Albert Renken__ in 1996. He became a process development chemist at Givaudan SA in 1996 and was named Head of Process Development in 2003. Givaudan, with about 25 percent of the 18 billion Swiss franc global market, is the world's biggest maker of flavors and fragrances, producing ingredients for a wide range of products, including the prestigious perfumes of the most renowned fragrance houses. In his free time, Jacques Membrez observes stars and planets, reads books, watches movies and spends time with his friends and his three children.

How did you come to choose EPFL?

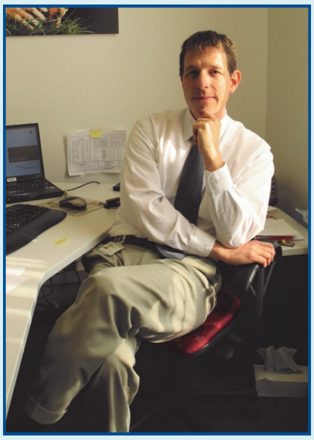
That's pretty simple. In Switzerland, if you want to have a world class education in chemical engineering, you have two choices. You either go to **Swiss Federal Institute of Technology** in Zurich (ETHZ) or EPFL in Lausanne. Because I'm quite good in German, I didn't really want to try out the Swiss-German speaking part for that purpose only. EPFL also had a very good reputation among the students where I got my matura. The secondary reason is that at that time, EPFL gave students a very special mix between fundamental chemistry and engineering, coming from the time of EPUL, EPFL's ancestor. That wasn't the case at ETH and this mix was (and perhaps still is) quite unique in the world. EPFL students get a really high-level education and mix of basic sciences, general chemistry, inorganic and organic chemistry and chemical engineering, with high level practical sessions in all those important fields. High-level practical teaching is crucial for future chemists and chemical engineers.

Did you always want to be a chemist?

No, I could have been a physicist. I'd always been rather fascinated by changes in matter, but I wanted to know what I was going to do with my education and I thought at the time that chemistry was less theoretical, which is partly true. I guess I could have been a doctor, also a lawyer. There were lots of choices. I loved science though. Between that and the reputation of EPFL, with many of my friends coming here, to a lovely city, it was a good set of reasons to start studying chemical engineering here.

What's your best memory from EPFL?

My best memories are from the labs, doing the practical work. There were many interesting experiments and the spirit between students was very good. This extended far beyond the practical work sessions. We went to the Satellite, had a good time with friends and had some very nice beer tasting sessions. It was a great mixture of practical science and friendship. Also, we had a radiochemistry lab. At that time, it was very rare to have this and it had a level of security comparable to a nuclear power station. I loved it, this was really fun. It was really something different from organic chemistry or plain engineering calculations. Radioactivity or radiochemicals can't be studied easily. I haven't used this at all in my industrial career but it's a good memory. You got to dress in special clothes, go through sets of doors, check your radioactivity level and do these strange manipulations behind thick walls. The Geiger counters clicking away....it was good.



Dr. Jacques Membrez

How have things changed at EPFL?

It has become vast, huge. It's sounds like a cliché, but when I joined EPFL it was a small town, then it grew into a big city. It takes 20 minutes to get a book back to another library, and this is really a big change. Also, I think we students at that time were probably more focused on academics than conscious about the reality of industry, or even much concerned about it. That was the outer world and, at the least the guys studying with me, we felt like we were living in the academy, not close to industry. We were pretty active in our studies, but when it came to extracurricular activities, with very little time left to relax, we preferred to rest and socialize rather than organize a seminar with industrial partners. Times have changed and students today are maybe more mature and aware of the reality of industry than we were.

What do you do at Givaudan?

As head of the chemical process development dept., I'm basically responsible for transferring new patented products, new technologies and new processes from research to production. Most of the details -- production methods, technologies used -- cannot be published. I'm based in Vernier, near Geneva, which is the largest production center of the Givaudan group and also the headquarters of the company. My departments consist of several laboratories and a state-of-the-art pilot plant. I employ both organic chemists and chemical engineers.

How well did EPFL prepare you for this job?

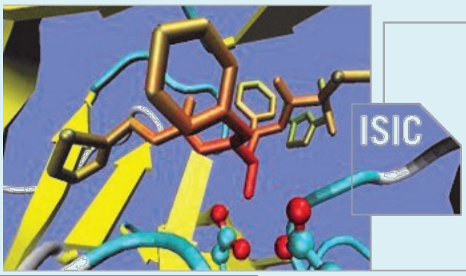
We had very good chemical and biochemical engineering professors like Albert Renken and **Urs von Stockar, Philippe Javet** and **Eric Plattner.** We really learned a lot from them. In other fields, we also had very good professors, but the list is too long to name them all. They educated a whole generation of chemical engineers and you can find their former students almost everywhere in Switzerland. It was really a generation of high level professors and the impact they've had on the industrial landscape is significant. When you came out of this school you were ready to face many, many problems, except one -- human conflicts. I'm not sure how it is now, but at that time you weren't prepared to manage people. And I think it's not a bad thing after all, because people management has, in my opinion, no place in chemistry schools, or only as options. This is something you can learn in postgraduate training and when you jump into industry. What do you do when you have someone coming into your office saying `I don't want to work with that guy anymore.'?

Tell me about a big challenge at work.

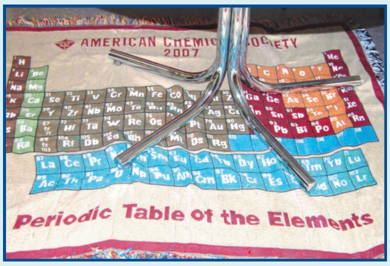
I had to turn a process from batch to continuous. This took a couple of years of my engineering life. This was quite challenging and also quite new for the company. I had to talk to other engineers, to mechanical engineers, electrical engineers and other chemists. This allowed me to get to know a lot more about the company and about my job and I really learned a lot with this big challenge. Everything I applied to this project was from the precious toolbox that I acquired at EPFL. When we finished the project my team and I went out and had a good time together in a nice restaurant.

What's your advice for chemistry students today?

Learn as much as you can, work hard, and stay humble. You may be ambitious, but if you're not humble, your life will be tough in the industry. There are a lot of people who don't have even 10 percent of the education you have but in certain fields they'll know much more than you anyway. If you stay humble, give the best of yourself, you can get the knowledge, make an exchange. This sort of thing always happens when you go in the chemistry workshop. There are very experienced workers and sometimes they'll tell you something's not going to work. You then have two options. You can either protect yourself behind your diplomas, or listen to the people and let them explain to you in their own words why it's not going to work. And in 50% of the cases, it's really not going to work because of practical, unexpected hard facts. You can learn a lot from experienced people, and if you don't try to do that you'll have difficult relationships with people, lose a lot of information and pleasure...and it just won't work!



Sandoz Chair Studies Electronic Structure



Clémence Corminboeuf's conference table sits on a rug depicting the periodic table. It was a gift, but she says she probably would have bought it herself.

Prof. Corminboeuf, now an assistant professor and head of ISIC's **Laboratory for Computational Molecular Design**, has been interested in science in general ever since she can remember and in chemistry since she first had it in school...but not in the kind of chemistry involving beakers of hydrochloric acid and Bunsen burners.

"I came to visit EPFL before I started university but they'd arranged a visit to a production site where there were 20-meter-high vats of chemicals," she said. "I prefer to understand things from the microscopic level and that was not my style. I wanted to be a fundamental chemist."

And now, after going to the **University of Geneva** instead, she's studying the theory of electronic structure.

The accurate design of chemical compounds with specific physical, chemical or biological properties is the main goal of many academic and industrial research areas. In pharmaceuticals, for instance,

> ***"Months of computer time for a single computation are not acceptable."***

research may suggest that a certain disease is linked to a given protein -- the histone deacetylase class of enzymes, for example, is thought to be crucial to cancer cell proliferation. With knowledge of both the electronic structure of the enzyme's active site and the catalytic mechanism, scientists may be able to create a molecule that can bind to and block production of the so-called HDAC enzymes, stopping tumor growth. Prof. Corminboeuf and her team are using quantum chemical approaches to eventually design and tune molecular properties.

"We want to design molecular systems with tailored properties, but we first aim to introduce accurate and innovative computational methods that allow us to do that," she said. Rewind 84 years. In 1926, **Erwin Schrödinger** introduced a fundamental equation that can be used to determine everything we need to know about electrons in molecules. There's a hitch with the equation though; it can only be solved precisely for atoms with one electron, such as hydrogen.

Prof. Clémence Corminboeuf, Head of the Laboratory for Computational Molecular Design

Since then, many approximate solutions have been proposed for larger systems. One such method, density functional theory, has been successfully used in quantum chemistry since the 1990s. The basic idea of DFT is to replace a complicated mathematical object, the N-electron wave function, by the electron density as a basic variable. This fundamental change of variable can be, in principle, done without loss of rigor as the electron density determines all the properties of a molecular system.

Prof. Corminboeuf first got interested in DFT while working on her master's thesis in Canada, and then completed her PhD under the joint supervision of professors at the University of Geneva and **Technische Universität Dresden.**

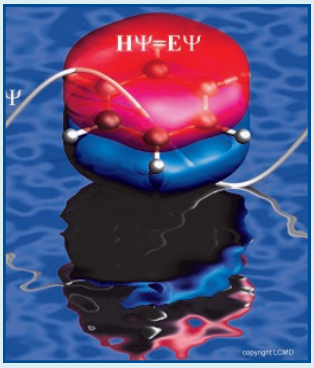
She had long known that she wanted an academic career though and, for Prof. Corminboeuf, this meant going even further away: in 2005, she went to **New York University**, where "about 100 friends wanted to come and visit," and then in 2006 she became a research associate at the **University of Georgia, in Athens** (USA), where "nobody came to see me." This was where she worked closely with **Paul Schleyer**, a pioneer in the field of computational chemistry and someone she still talks to regularly.

Despite the success of DFT in chemistry, the method still has some practical flaws, especially when used to model weak interactions. Prof. Corminboeuf is trying to refine and improve the performance of DFT and has had good success with a correction based on a simple chemical concept that reflects the molecular topology called branching.

"Chemists always use concepts like charge, branching, strain, chemical bond, etc., that lack a clear physical basis," she said. "Our laboratory uses and defines these concepts with the goal of leading to constructive developments."

The team isn't just tackling conceptual problems, but also practical problems such as decreasing the computer cost involved in the calculation of molecular properties.

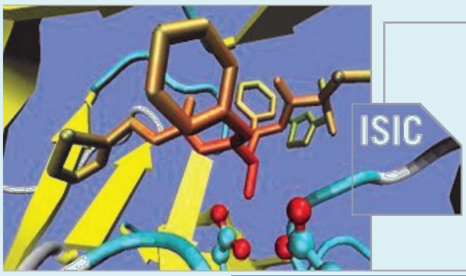
They use a machine that has about 300 nodes, each of which has two 3.0 GHz quad-core processors with 16GB of RAM memory. A standard desktop contains one node of this type, with only 4GB of RAM memory. The accurate computation of molecular properties for a system of 100-150 atoms requires several processors and 16 to 32GB of RAM at least - such computations aren't even possible on a standard desktop. Computations for such systems take a week or two on the lab's machines and that's still acceptable, she said. For larger systems, that is, those of a few hundred atoms, months of computer time would be necessary.



"Months of computer time for a single computation are not acceptable," she said.

Prof. Corminboeuf, whose one-year old daughter spent a lot of time in her mother's office during her first three months, says she does her best thinking at home while doing miscellaneous tasks. She's also lucky to have a chemist husband, she said.

"Sometimes you just wake up at 4 a.m. and need to discuss work," she said. "You're never off. That's difficult for people who aren't in the academic world to understand."



Prof. Xile Hu Tackles Problem of Sustainable Energy

Prof. Xile Hu, Head of the Laboratory for Inorganic Synthesis and Catalysis

Xile Hu chose a course of study that didn't land him his first "real job" until he was 29 years old: he understands the importance of long-term thinking.

That may make Prof. Hu, whose first position was admittedly the one he holds now -- assistant professor of chemistry and head of ISIC's Laboratory of Inorganic Synthesis and Catalysis -- well suited to tackling the problem of sustainable energy.

"The energy problem never stops," he said. "Demand is going to continue to increase because of population and economic growth; this isn't an issue that's going to go away. And a scientist likes to contribute what he can to solve a problem."

Prof. Hu, post-docs and PhD students in his lab are trying to develop catalysts that can be used to produce hydrogen gas from water. Hydrogen gas seems like a good energy carrier because it doesn't produce carbon dioxide when it's converted to electricity by fuel cells; what's needed is an economical way to extract it from water.

> *"When you're somewhat good at something, you start to like it."*

The most efficient, commercially available catalyst for the process is now based on platinum, a metal that sells for more than $1,600 an ounce. Platinum is also used as a catalyst in fuel cells, which use hydrogen gas and oxygen to generate electricity quietly, efficiently, and with heat and water as the only byproducts. Hu hopes his research might eventually lead to a catalyst based on iron rather than on the precious metal.

"Down the line, we're going to have a problem with platinum," Prof. Hu said. "It's among the least abundant elements, it's potentially toxic, especially on a large scale. Iron is abundantly available, relatively non-toxic compared to heavy metals. And it's dirt cheap."

Prof. Hu didn't set out to be a chemist. He wound up where he is now after deciding that of the more than 2,000 universities and colleges in China, there was only one he wanted to go to: **Peking University**, more than 1,600 kilometers from his home in the Fujian province of south-eastern China.

Prospective students had to select four potential majors and Hu's first choice was microelectronics. That was a popular field for the incoming class in 1996 though and a lot of the very best students wanted to study it. He got materials chemistry, his second choice.

Catalytic H_2 production (bubbles) from water

The initial classes were dull, Prof. Hu says, but he refused to change his major. "People were telling me `you don't get a job studying chemistry, you should go be a lawyer or something,' but I was stubborn," he said. "And at one point, when you're somewhat good at something, you start to like it."

Prof. Hu finished his undergraduate work and then made good on his next big decision: to go to the U.S. "I thought that if you want to get a really good education, you go to the U.S.," he said. "Of course, I didn't know about EPFL at the time."

He finished his PhD at the **University of California at San Diego** and followed it up with a post-doc at **Caltech** in Pasadena, California. That's when he first got interested in energy.

Prof. Hu's lab, which was started after he came to EPFL in 2007, is looking to nature for inspiration in developing the iron-based catalysts. Hydrogenases are the enzymes that nature uses to produce hydrogen. The curious thing about these proteins, Prof. Hu says, is that all of the three different classes now known have common features: an iron-containing active site - or region of the enzyme that binds to a substrate - that has sulfur, and unusual carbon monoxide and cyanide ligands.

The fact that all three enzyme classes share this trait is a sign of convergent evolution and suggests that they are key to efficient hydrogen gas production and activation, he said.

> *"There are many different challenges and we're just at the beginning of the race."*

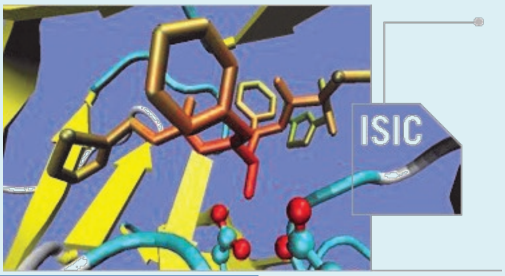
Besides developing practical hydrogen-producing catalysts, another of the lab's projects is to study and hopefully mimic the activity of the active site of a particular enzyme, known as Hmd, or the iron-sulfur cluster-free hydrogenase. No one has managed to mimic the site's activity so far, and doing so will allow a greater understanding of how the enzyme activates hydrogen, Prof. Hu says.

Much of the work is still in the early stages and it's too soon to talk about a "solution" to the problem, he said. "Even if I had a catalyst that was dirt cheap, that worked perfectly well, it still doesn't mean the whole system will work."

"Chemists, physicists, materials scientists and a lot of others are involved - we're just a part of the whole scientific community working on it. There are many different challenges and we're just at the beginning of the race."

Prof. Hu enjoys tackling the problems, though some still question his choice of profession. "My parents are visiting now," said Prof. Hu, who responded to an e-mail within 10 minutes after 9 p.m. on a Sunday night. "They keep asking me 'why are you always working'?"

Prof. Hu's office



Molecular Motion Observed As Never Before

Majed Chergui, head of ISIC's **Laboratory of Ultrafast Spectroscopy**, and his collaborators focus on the "real time" description and analysis of chemical reactions. They have developed a novel X-ray technique that allows the observation of molecular motion on a time scale never before achieved.

While conventional chemistry can describe the outcome of a given reaction, it does not describe how the reaction actually takes place. On the microscopic level -- that of the atoms and molecules involved -- a reaction results in a structural rearrangement of reactants, which then yields products.

Reactions require an initial input of energy. In nature and in chemical engineering, this input may come from chemical, thermal, or electrical energy, or from light. Chemical physicists prefer to use light, because its quantum nature means the amount of deposited energy per single molecule or atom can be chosen precisely.

Accurate knowledge about the electrons involved in the process allows scientists to monitor or even control the outcome of the light-triggered reaction. Light stimulates different quasi-simultaneous processes though and understanding the steps

> ***"Detailed descriptions of these reactions are fundamentally important to understanding nature in general, and man-made processes in particular."***

involved becomes complicated. What's more, molecules are usually found in many-body environments that include substances such as solvents or proteins. Interactions are complicated, and scientists have not been able to observe the atomic-scale dynamics behind them.

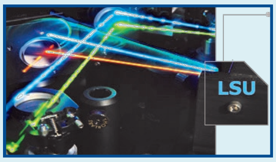
Detailed descriptions of these reactions are fundamentally important to understanding nature in general, and man-made processes in particular, Prof. Chergui says. The aim of his group is to "see" how molecular systems evolve in real-time; the idea is similar to **Etienne-Jules Marey's** use of a camera in the 19th century to shed light on the motion of a falling cat.

There were two main obstacles to the main work of Prof. Chergui's group. The first was the problem of which time-dependent properties can actually be measured. Structural changes can be visualized by the exact positions of the involved nuclei and the atomic structure of a given molecular system by a measurement of the relative distances and angles between its constituents.

Prof. Majed Chergui, Head of the Laboratory for Ultrafast Spectroscopy

This information is not directly available with optical spectroscopy though, and scientists need theoretical input relating observables -- linked to absorption and emission spectra -- to nuclear positions, and thus to molecular structure. The problem is, this input, given by quantum chemical calculations and molecular dynamics simulations, results in an unambiguous translation of optical spectra into structure only in a few rare cases.

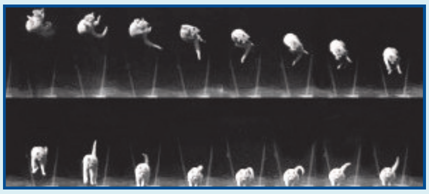
As an alternative, Prof. Chergui's group decided to use structural techniques based on X-rays to measure inter-nuclear changes. Because X-rays both have short wavelengths, inter-nuclear separation can be measured directly with <100 femtometer spatial resolution. While this method is almost as old as optical spectroscopy, its use in ultrafast snapshots of atomic structure is entirely new.



The second difficulty is related to the time scale. Photochemical reactions lead to an ultrafast structural change. While the timescales vary as a function of the process, a typical value can be assessed by comparing it to the vibrational period of bound atoms. A half-oscillation typically spans values of a few femtoseconds to several hundred femtoseconds (1 fs = 10^{-15}, or one quadrillionth, of a second. That is, an fs is to a second what a second is to about 31.7 million years). During this time, the nuclei involved move only a few percent of their initial relative distance. If researchers can record snapshots of the atomic positions as fast as half a vibrational period, they can put a sequence of snapshots together to produce a "molecular movie" of the evolving reaction and obtain a nearly complete understanding about chemical reactivity.

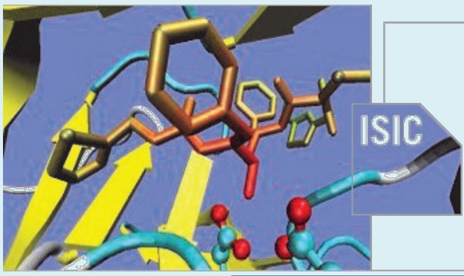
Though lasers that permit such shutter speeds exist, no existing optical methods were able to capture the molecular structure. To overcome this limitation, Prof. Chergui's team combined lasers delivering femtosecond pulses of ultraviolet-visible light with a source of femtosecond X-ray pulses, in a technique now known as ultrafast X-Ray Absorption Spectroscopy.

Prof. Chergui and colleagues at the **Paul Scherrer Institute** in Villigen, Switzerland published a paper on their work in the journal ***Science*** in February 2009. It is available at www.sciencemag.org. The group's scientists, including **Fabrizio Carbone**, who published an article in *Science* in July 2009 on earlier work done using high-speed electron microscopy to investigate graphite reactions, are planning experiments on a wide range of molecular systems on surfaces or as thin films. Their research may lead to applications in magnetic data storage or solar energy.



Etienne-Jules Marey's falling cat

Born in 1956 in Casablanca, Prof. Chergui grew up in Algeria and Lebanon. He obtained his BSc in Physics and Mathematics from **King's College**, London in 1977, then his MSc in Atomic and Molecular Physics (1978) and his PhD (1981) from the **Université Paris-Sud**. He completed his habilitation in 1986 at the **Université Paris-Nord**. He joined the French National Center for Scientific Research as staff scientist in 1982 and moved in 1987 to the **Freie Universität Berlin**. He was appointed full professor of Condensed Matter Physics at the **University of Lausanne** in 1993 and became Professor of Physics and Chemistry at EPFL in 2003.



diagnoSwiss Enables Testing in Emerging Markets

diagnoSwiss, founded in 1999 as a spin-off from the ISIC's Laboratory of Physical and Analytical Electrochemistry, headed by **Prof. Hubert Girault**, is making bioanalysis equipment that can be used in pharmaceutical research, industrial control, food safety or bioterrorism. The products are based on microfluidic technologies and allow for fast, inexpensive protein analysis.

The company, which started off by developing a method of separating proteins and peptides according to their isoelectric point, has combined disposable microchips and electrochemical detection to develop diagnostic platforms that are especially well suited to fast analysis of low volumes of material.

Enzyme-linked immunosorbent assay, or ELISA, tests are used to detect substances such as hormones, bacterial antigens and antibodies in blood or urine, and also in pharmaceutical research and food safety.

They may involve, for example, attaching an antigen to a solid surface and washing a sample over it to see if it contains antibodies to the sample. In this case, another antibody that detects the first is linked to an enzyme, and, finally, a substance that the enzyme can convert to some detectable signal is added. In fluorescence ELISA, for example, antigen/antibody combinations are made to shine so that the amount of antigen in the sample can be inferred through the magnitude of the fluorescence.

> ***"The idea is to bring computerized testing at a price that's appropriate for developing countries."***

diagnoSwiss's chips, which are compatible with conventional robotics and reagents, are thin polymer laminates incorporating an array of micro-channels with integrated gold microelectrodes. While the diagnoSwiss chips can be used for any micro-analytical application, they're being principally used for ELISA tests.

The biochemicals used in the diagnoSwiss tests are the same as those used in conventional assays, but the enzyme "reports" the amount of sample by electrochemical means. Instead of measuring the amount through fluorescence, it's determined by the current resulting from, for example, an oxidation reaction of the enzyme product. The output results are plotted as intensity-concentration isotherms similar to any other system based on optics, and so is familiar to biochemists.

Electrochemistry is well suited for microsystems because its sensitivity doesn't suffer from the low number of molecules in the small volume of the microchannels, Chairman Girault said. diagnoSwiss' chips speed up bioanalytics and reduce lab costs.

Prof. Hubert Girault, diagnoSwiss chairman

"Because the system is based on nanovolumes, the detection is very fast, on the order of a few minutes," Prof. Girault said. "Results from classical ELISA tests take about an hour."

The diagnoSwiss chips have been developed for protein analysis in human in-vitro diagnostics. Most of the test kits that the company now provides are related to fertility and pregnancy, although a wider selection of products is planned.

One of the company's markets is the so-called BRIC countries -- Brazil, Russia, India, China -- and nations in the Middle East and Africa

"The idea is to bring computerized testing at a price that's appropriate for developing countries," Girault said. "We can't compete against the big companies, who offer completely automated, robotic systems. Our instruments are specifically for medical centers with a couple of medical doctors and a few nurses."

diagnoSwiss revenue has been generated through Business to Business deals such as licensing and services with larger players; for instance, diagnoSwiss has pursed a business development program for a French diagnostics company **bioMérieux.** The intellectual property linked to the protein separation has since been licensed to **Agilent Technologies**, who used it to develop the OFF-GEL electrophoresis fractionator. This product is now sold worldwide and extensively used in proteomic laboratories.

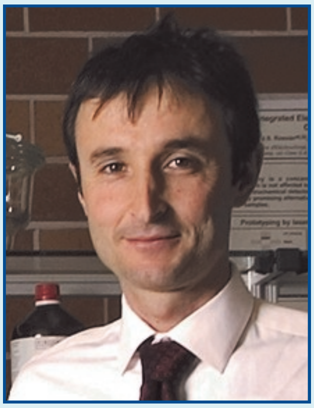
> ***"Don't believe too much of what you learn in business classes, be realistic, and rely mainly on common sense."***

diagnoSwiss has employed a mean of 10 collaborators during the last 10 years with fluctuations due to business opportunities and the outsourcing of non-strategic activities, Prof. Girault said.

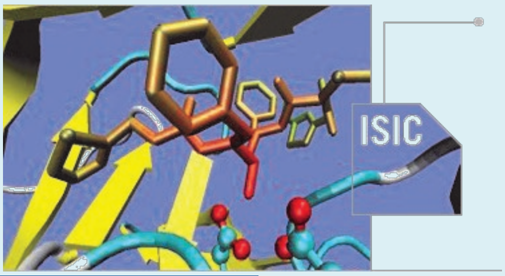
"It's impossible for a small company in the medical market to carry all the certification burden," he said.

Prof. Girault would like to see more start-ups coming out of EPFL. "Entrepreneurship is an important aspect and students shouldn't be afraid to start their own companies," he said. "I know that working in a big company is a lot more comfortable than starting your own, but maybe we need to look a little bit towards the U.S. and China, where there's more willingness to accept risk."

People looking to start their own business should try to define a unique product that's superior in some way to existing products, Prof. Girault said. "And don't believe too much of what you learn in business classes, be realistic and rely mainly on common sense."



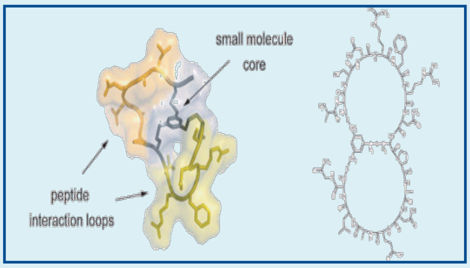
Dr. Joel Rossier, diagnoSwiss co-founder



SNSF Grants ISIC Three Professorships in Three Years

Heinis Gets SNF Grant to Study Small-Molecular-Weight Antibodies

Prof. Christian Heinis, head of ISIC's Laboratory of Therapeutic Proteins and Peptides, received in 2009 a **Swiss National Science Fund** professorship for his proposal on "Small-molecular-weight antibody-mimicking structures for therapeutic applications." Antibodies -- proteins that can detect and destroy elements foreign to the body such as bacteria and viruses -- have proven to be powerful drugs for the treatment of serious medical conditions such as cancer. Monoclonal antibodies, which are those made from single cell lines, are now the most widely used form of cancer immunotherapy. While they've proven to be effective, there are disadvantages associated with them: large molecular mass means they have to be injected, they don't penetrate into tissue well and they're very expensive to make. Prof. Heinis and his group are creating small molecules, which don't have those disadvantages, to mimic the therapeutic activity of antibodies. The initial focus is on inhibitors of plasma kallikrein and urokinase-type plasminogen activator. The enzymatic activities of these proteases are linked to hereditary angioedema, a disorder of the immune system, and cancer. Prof. Heinis will test the stability, pharmacokinetics and therapeutic effect of the antibody mimics in living organisms and the project may yield compounds that can be developed into treatments for patients. The funding of about 1.55 million Swiss francs runs for four years from September 2009. Prof. Heinis studied biochemistry at the **Swiss Federal Institute of Technology in Zurich (ETHZ)** where he also did a PhD in the research group of **Prof. Dr. Dario Neri**. He was a postdoctoral fellow in the group of **Prof. Dr. Kai Johnsson** at EPFL and in the group of **Sir Gregory Winter** at the **Laboratory of Molecular Biology** (LMB) in Cambridge, UK. In 2008 he was appointed Assistant Professor with tenure track for Bioorganic Chemistry at EPFL.



Structure of a human plasma kallikrein inhibitor active in human plasma

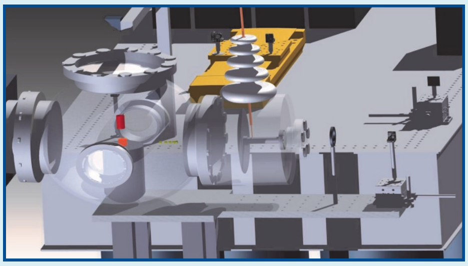
Prof. Fabrizio Carbone, who recently heard he'd been awarded an SNSF professorship

Prof. Christian Heinis, Head of the Laboratory of Therapeutic Proteins and Peptides

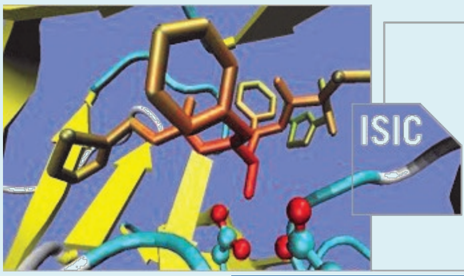
Prof. Andreas Osterwalder won a Swiss National Science Foundation Professorship in 2008

Carbone Gets SNF Grant to Develop Ultrafast Electron Diffraction Machine

Fabrizio Carbone, a scientist in ISIC's Laboratory of Ultrafast Spectroscopy, won an Swiss National Science Fund professorship in 2010 to develop an ultrafast electron diffraction machine. In the world of the infinitesimally small, matter has a dual nature and can be described both in terms of particles or waves. For this reason, electrons undergo diffraction and interference phenomena typical of light waves. Very high resolution images of crystals can be obtained through electron diffraction, and thanks to their much larger ability to interact with matter, compared to photons of similar wavelength (X-rays), they allow the study of atomically thin samples and light elements. Recently, the technology for generating ultrashort (femtosecond) electron pulses has been developed; these can be used to record ultrafast snapshots of a material structure after a convenient excitation. The motion of ions during the melting of one-atom thick ice on surfaces has been observed by ultrafast electron diffraction, as well as the transformation from graphite to diamond induced by intense infrared laser pulses, and the reconstructions of self-assembled films, very interesting for future molecular electronics. Carbone is helping to develop a state of the art ultrafast electron diffraction machine, capable of resolving atomic motions with a spatial resolution of a fraction of an hydrogen atom diameter and a temporal resolution capable of resolving atomic vibrations. Carbone completed his master's degree at the **University of Pavia** in 2001 and then worked as a research scientist in the advanced photonics research lab at **Pirelli & C. SpA** in Milan before completing a PhD at the **University of Geneva** in 2007. In April 2009, Carbone completed a post-doc in physical chemistry in the group of the 1999 winner of the Nobel Prize in Chemistry, **Prof. Ahmed Zewail**, at **California Institute of Technology** in April 2009.



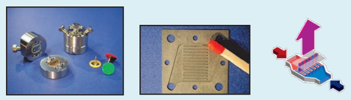
Electrons travel towards the sample as the exciting laser pulse approaches



Prof. Lioubov Kiwi Gets About 2.4 Million Francs in EU Funds

Prof. Lioubov Kiwi

Prof. Lioubov Kiwi, an adjunct professor and the head of ISIC's **Group of Catalytic Reaction Engineering**, won funding of about 2.4 million francs from the European Union's **Seventh Framework Program** within the PILLS, MONACAT, COPIRIDE and POLYCAT projects. The PILLS (**P**rocess **I**ntensification methodologies applied to **L**iquid-**L**iquid **S**ystems in structured equipment) project alone brings funding of about one million francs for EPFL. The aim of PILLS, which runs for 36 months until the end of 2011, is to develop and validate a design methodology and criteria for carrying out two-phase liquid-liquid reactions in connection with the development of a new generation of flexible, high-performance process equipment for continuous manufacturing. This should allow operators to improve the sustainability of chemical production, to diminish environmental impact and to increase safety. Prof. Kiwi and colleagues are developing a generic approach that can be applied to different industrial systems, showing wide applicability in the chemical industry. Two case studies are considered: the production of nitrobenzene, which is used to make aniline, a chemical that is in turn used to make products ranging from dyes to rigid polyurethane, and the cyclization of β-ionone, a fine chemical mainly used to make fragrances. EPFL's partners, including **Givaudan SA**, the world's biggest maker of flavors and fragrances, come from six countries. The team consists of a knowledge transfer company, two small and medium enterprises (SME), two equipment manufacturers and three potential end-users of this equipment. An e-learning course and practical training on the equipment will also be implemented during the project. Two other projects (MONACAT, COPIRIDE) also started in 2009. POLYCAT is scheduled to start on September 1, 2010. All of the projects are linked to the GGRC's main research topics of process intensification using micro-structured catalysts and reactors. Prof. Kiwi received her PhD degree in physical chemistry from the **Lomonosov Moscow State University** in 1982. She worked as a researcher and lecturer as Docent at **Novosibirsk State University's** Department of Physical Chemistry until 1993 when she came to EPFL for a sabbatical. She has been working in EPFL's Laboratory of Chemical Reaction Engineering since 1994. Dr. Kiwi was named adjunct professor at EPFL in December 2008.



Micro-mixers and -reactors for carrying out fluid-fluid and homogeneous reactions

ISIC Services—From Chemical Storage to Free NMR Tools

General Services provide administrative, technical and analytical support for the Institute's research and teaching activities; ISIC takes considerable pride in investing in the most state-of-the art instruments and in providing fast, high-quality analysis. Analytical facilities include high field nuclear magnetic resonance spectroscopy, high resolution mass spectrometry, X-Ray and elemental analysis.

The unit's services specialists can analyze samples themselves, or train researchers to perform measurements directly on the open-access instruments. New scientific equipment is made or modified in the mechanical and electronic workshops, which also provide support for the automation of data acquisition and processing. These facilities are also open to users outside EPFL.

Dr. Luc Patiny is the head of Chemical Information at ISIC. While day to day work involves maintaining and building up ISIC's chemical data storage, Patiny has also developed a worldwide shared database and set of NMR tools that's available to everyone.

> ***"We can tell we're doing a good job because of the number of people coming back."***

The department started storing information on a central database in 2005 to try to systematically save data being generated in the labs. "There are plenty of experiments done and a lot of data being generated, but unless you make a special effort, it'll be lost in ten years," Dr. Patiny said. "It's the same as on your hard disk. Unless you've carefully annotated something, it's `there somewhere' at best. We want to have easy access to our data in 20, 30 years."

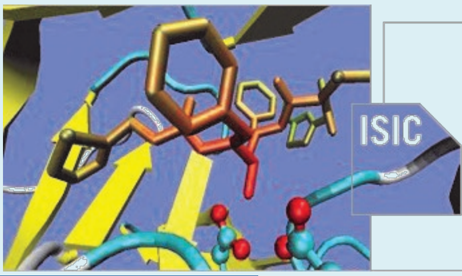
Research groups in the department saved more than 10,000 NMR spectra to the database in 2009. More information is available on **http://cheminformatics.epfl.ch.**

The publicly available website **www.nmrdb.org,** introduced about a year ago, is now being used by more than 1,000 chemists around the world every day. About 50 percent of the chemists using the tool are from the U.S., but scientists from China, India and Korea also use it. One of the more used feature on this website is the 1H NMR spectra prediction tool.

"There are other predictors but we really focus on the user interface and making it easy to use," Dr. Patiny said. "It's the 80/20 rule. It takes 20 percent of the time to make 80 percent of the functionality. It takes about 80 percent of the time to make it user friendly. And we can tell we're doing a good job because of the number of the people coming onto the website and the number of people coming back."

Dr. Patiny's site offers a number of NMR tools for free. For example, the NMR Predictor allows researchers to draw a chemical compound and generate the predicted spectrum. This in turn allows the researcher to easily compare his or her data with experimental results. The algorithm, developed by the chemist **Joao Aires de Sousa** at the **New University of Lisbon**, is very accurate compared with experimental NMR data, Dr. Patiny said. "It's as good as most of the commercially available packages," he said. "There's one that we know is more accurate, but it also costs several thousand francs."

Another tool, the NMR Resurrector allows scientists to transform NMR data as commonly communicated in scientific papers into a graphic that's easier to interpret. The website is available at **www.nmrdb.org**. To find out more about ISIC services, see: **http://isic2.epfl.ch/page69272.html**.



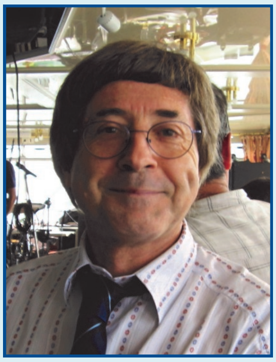
Awards, Prizes, Meetings

Selection of awards and prizes 2009-2010


Prof. Michael Grätzel

Balzan Prize : **Prof. Michael Grätzel** (Laboratory of Photonics and Interfaces) received the one-million Swiss franc Balzan Prize 2009 in recognition of his many contributions to the science of new materials, and in particular for his invention and development of a new type of photovoltaic solar cell, the Dye Sensitized Cell, commonly known as the Grätzel Cell. Grätzel's recent achievements paved the way for a revolution in the use of solar energy to produce hydrogen, thus providing a way to transform and store solar energy in the form of a very flexible fuel. These findings should have important applications in the production of sustainable energy.

Terrae Rarae: **Prof. Jean-Claude Bünzli** (Laboratory of Lanthanide Supramolecular Chemistry) has been awarded the Terrae Rarae 2009 Award during the 7th International Conference of Elements in Köln. This prize rewards Bünzli's seminal work in the domain of lanthanide based complex molecular and supramolecular assemblies with luminescent properties.


Prof. Jean-Claude Bünzli

EPFL Doctorate Award: **Dr. Agnieszka Kapalka-Cieciwa** (Group of Electrochemical Engineering) has been awarded the EPFL Doctorate Prize 2009 for her PhD thesis entitled "Reactivity of electrogenerated free hydroxyl radicals and activation of dioxygen on boron-doped diamond Electrodes." The work of Kapalka-Cieciwa has demonstrated the possibility to enhance non-faradaic electrooxidation processes which opens the way for designing a less energy consuming degradation of organic pollutants on boron -doped diamond anodes.

Dimitris N. Chorafas Award: **Dr. Mélanie Abonnenc** (Laboratory of Analytical and Physical Electrochemistry) received the *award* in 2009 for her outstanding PhD thesis dedicated to the development of miniaturized analytical systems for mass spectrometry based protein studies.


Prof. Karl Gademann

Ruzicka Prize: **Prof. Karl Gademann**, head of the Laboratory of Chemical Synthesis at EPFL until January 2010, was rewarded for his achievements in the field of the chemistry of natural substances in 2009. The prize, named after the Nobel Laureate, **Leopold Ruzicka**, has been awarded to outstanding young scientists in chemistry since 1957. Gademann is now at the **University of Basel.**

Kuwait Prize: **Prof. Majed Chergui**, head of the Laboratory of Ultrafast Spectroscopy, won the Kuwait Prize, an annual award of about $100,000 granted by the Kuwait Foundation for the Advancement of Sciences to support scientific research in 2009. Prof. Chergui also won a 2010 **Humboldt Research Award**, granted in recognition of the achievements of a researcher whose fundamental discoveries, new theories, and insights have had a significant impact on his or her own discipline and who is expected to continue producing cutting-edge achievements in the future. The award is valued at 60,000 Euros.

Werner Prize: **Dr. MER Sandrine Gerber** (Laboratory of Glycochemistry and Asymmetric Synthesis) has been awarded the Werner Prize 2010 in recognition of her outstanding contribution to the design and synthesis of bioactive molecules and potential drug candidates. The award ceremony took place during the Spring Meeting of the Swiss Chemical Society in Bern.

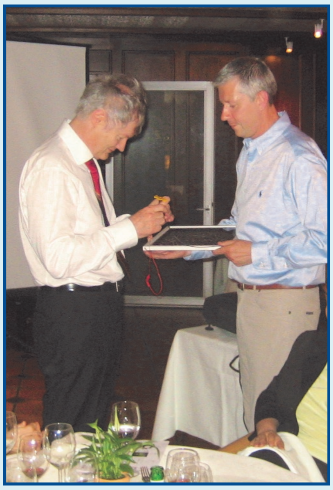

Dr. MER Sandrine Gerber

Fall Meeting of the Swiss Chemical Society: EPFL hosted the 2009 meeting on September 4, chaired by **Dr. MER Sandrine Gerber** and organized by ISIC. With 439 scientific contributions, in the form of oral communications and poster presentations in the field of analytical, medicinal, organic, inorganic, physical and computational chemistry as well as in polymer science, this annual meeting offers a unique platform for chemical research in Switzerland. More than 800 scientists from young researchers to professors and industrial participants met at this occasion. A special mini-symposium of inorganic chemistry was organized in honor of **Prof. Jean-Claude Bünzli** on the occasion of his 65th birthday.

Innovation workshop with ***Lonza Group AG:*** Thirteen scientists from Lonza's Life Sciences Ingredients research group and a member of the research and development team at Lonza Exclusive Synthesis went to visit ISIC labs on June 16, 2009. Researchers made presentations on and discussed a total of about 30 topics, including alternative means of synthesis and the development of new classes of products. The collaboration, which Lonza says will help it stay at the cutting edge of science and improve its market position, will continue in the form of masters, PhD and post-doc projects, and Lonza scientists' involvement in EPFL research.

Other Events, News

Prof. Thomas Rizzo (left), professor of chemistry and Dean of Basic Sciences with **Prof. Ahmed Zewail,** who was granted an honorary doctorate from EPFL at the Magistrale on Oct. 3. Zewail was awarded the 1999 Nobel Prize in Chemistry for his studies of the transition states of chemical reactions using femtosecond spectroscopy.



Prof. Michael Grätzel (left) and **Prof. Paul Dyson** connect a Grätzel solar cell to a fan donated by **Solaronix SA,** a company founded by one of Grätzel's former students. The fan was presented to the winner (**Prof. Kay Severin**, head of ISIC's Laboratory of Supramolecular Chemistry) of a friendly competition held at a party at the Fleur du Lac in Morges to celebrate Grätzel's 65th birthday. Grätzel was presented with a jeroboam of champagne.

Emeritus Prof. Hans Dahn. On October 23, 2009, EPFL hosted a mini-symposium in chemistry as a tribute to celebrate Dahn's 90th birthday. This celebration, sponsored by several Swiss companies including **Lonza**, **Ciba Holding AG, Givaudan SA, Novartis AG and Roche Holding AG,** brought together more than 100 scientists, from former colleagues of Dahn to young EPFL chemistry students. Lectures were given by three of his former PhD students and the symposium concluded with Dahn's speech entitled "Comment je suis tombé dans l'oxygène," relating his scientific career. Professor Dahn founded the **Institute of Organic Chemistry** of the University of Lausanne in the 1960s and made an important contribution to national and international recognition of Lausanne's chemistry institutes. After his retirement in 1989, Dahn continued to be very active in the Institute of Organic Chemistry, in particular through his many scientific publications.

Photo: Alain Herzog, EPFL

Upcoming seminars:

- Thursday, June 17, 2010, 5.30 pm
  Prof. Jean-Marie Lehn Nobel prize laureate (chemistry, 1987), Laboratoire de Chimie Supramoléculaire, ISIS, Strasbourg, France
  "Perspectives in Chemistry-Supra-Adaptive"

- Friday, September 17, 2010
  Prof. Kendall N. Houk, Department of Chemistry and Biochemistry, University of California, Los Angeles, California, USA

- Tuesday, September 21, 2010
  Prof. Peter G. Schultz
  Scripps Research Institute, La Jolla, California, USA

ISIC's research leaders

First row: Prof. Christos Comninellis, Prof. Jiri Vanicek, Prof. Jérome Waser, Prof. Jacques-E. Moser, Prof. Kay Severin, Prof. Melody Swartz[1], Prof. Pierre Vogel, Prof. Christian Heinis

Second row: Prof. Harm-Anton Klok[2], Prof. Hubert Van den Bergh[2], Prof. Geoffrey Bodenhausen, Prof. Horst Vogel, Prof. Fabrizio Carbone, Prof. Jeffrey Hubbell[1], Prof. Majed Chergui, Dr. MER Rudolf Hovius

Third row: Prof. Lothar Helm, Prof. Jean-Claude Bünzli, Dr. MER Anne-Sophie Chauvin, Prof. Kai Johnsson[1], Dr. MER Oleg Boyarkine, Dr. MER Sandrine Gerber, Dr. Georges Wagnières, Dr. MER Marcel Drabbels

Fourth row: Prof. Rainer Beck, Prof. Andreas Osterwalder, Prof. Lioubov Kiwi, Prof. Xile Hu, Prof. Ursula Roethlisberger, Prof. Michael Grätzel, Dr. MER Christine Wandrey[1], Dr. MER Thierry Meyer, Dr. MER Gabor Laurenczy

Fifth row: Prof. Paul Dyson, Prof. Vassily Hatzimanikatis, Dr. MER César Pulgarin, Prof. Clémence Corminboeuf, Prof. Yury Tsybin, Prof. Hubert Girault, Prof. Florian Wurm[1], Prof. Thomas Rizzo[3]

(1) Also on the faculty of EPFL School of Life Sciences
(2) Also on the faculty of EPFL School of Engineering
(3) Dean of Basic Sciences

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