SCHOOL OF BASIC SCIENCES

FSB ANNUAL REPORT 2017

IPHYS ISIC MATH

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

DEAN'S FOREWORD

It is my pleasure to share with you the inaugural annual report for the School of Basic Sciences (FSB) at EPFL.

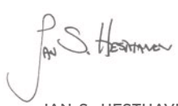
It has been a privilege for me to serve as Dean of FSB for almost a year. The diversity and enthusiasm I have witnessed throughout FSB has truly impressed and excited me. The School is endowed with an extraordinarily dedicated group of people - technicians, administrators, teachers, scientists and students - who, in close interaction with FSB Professors, all strive for excellence in all of EPFL's missions: research, education, and innovation. I am grateful for having been given the opportunity to be part of this community and to play a role in its continued success and growth.

This last year has been fantastic for the School of Basic Sciences. While FSB research groups have received more than 30 major international prizes and awards, we continue to successfully attract the most talented researchers worldwide. The School draws an increasing number of students both at the Bachelor and Master level (20% of EPFL), as well as at PhD level (25% of EPFL). Furthermore, thanks to the 12 Massive Open Online Courses (MOOCs) lead by FSB faculty, over 65,000 students worldwide attended our classes.

Innovation and technology transfer were fostered through the creation of one start-up company, while two others received InnoGrants to further mature ideas originating from our researchers. This all confirms the central role FSB plays at EPFL in achieving excellence across research, education and innovation.

I hope you will enjoy browsing through this annual report and experience the broad diversity of activities, the outstanding quality of research, and the commitment of the member of FSB to the success of the school and EPFL.

With the best wishes for a successful and rewarding 2018,



JAN S. HESTHAVEN
Dean of the School of Basic Sciences, EPFL

TABLE OF CONTENTS

FACULTY NEWS

IPHYS ISIC MATH

MATH

Emmanuel Abbé and Maria Colombo appointed at the Mathematics Institute

Emmanuel Abbe was appointed Full Professor of Mathematics (75% SB and 25% IC).

Emmanuel Abbe is regarded as one of the world's leading experts in data science, working at the interface of mathematics, information theory, statistics and theoretical computer science. His area of expertise is stochastic block model analysis, and his advances are important to a number of other subject areas, e.g. human biology, genomics, and the analysis of artificial neural networks. Abbe has also received several prestigious awards, including the Latsis Prize. He will join EPFL on August 1st, 2018.

Maria Colombo was appointed Tenure Track Assistant Professor of Mathematics.

Maria Colombo is a very talented young researcher who has already attracted international attention for a number of articles in prestigious academic journals. Her areas of research are the analysis of partial differential equations and variational calculus, which is concerned with functionals (e.g. integrals involving an unknown function and its derivatives). She has attracted particular interest for making significant advances in the regulation of the transport equation, which describes the behavior of particle systems in the presence of external force fields. She will join EPFL on August 1st, 2018.

IPHYS

Jamal S. Rahi named Tenure Track Assistant Professor of Biophysics

Sahand Jamal Rahi is an innovative scientist with a multidisciplinary approach who shows great potential. In particular, he studies the behavior of biological molecules such as DNA and proteins. His work uses findings from theoretical physics and statistics. One of his specialist areas is the calculation of the Casimir effect between metallic objects. At EPFL, Sahand Jamal Rahi will work closely with colleagues from the disciplines of physics, cell biology and molecular biology, and will contribute to the international positioning of the Institute in these subjects.

IPHYS - ISIC

Frédéric Courbin, Ivo Furno, and Ignacio Pagonabarraga named Adjunct Professors

Frédéric Courbin is an internationally acclaimed astrophysicist who specializes in gravitational lensing. He has exceptional scientific expertise and will in particular boost the visibility of EPFL and the Laboratory of Astrophysics through his analysis and interpretation of data relating to Euclid, the ESA's planned space telescope.

Ivo Furno is regarded as a world expert in the field of plasma physics. He focuses on how this field of physics can be applied in practice, such as in fusion reactors or industry. Ivo Furno contributes significantly to the Swiss Plasma Center and to EPFL by creating synergies within plasma physics as well as with the basic and engineering sciences.

Ignacio Pagonabarraga is an internationally recognized researcher and specialist in soft condensed matter. As Director of EPFL's Centre Européen de Calcul Atomique et Moléculaire (CECAM), which is based at EPFL, he makes important contributions in the field of computer-aided calculation. Ignacio Pagonabarraga is also very successful at attracting research funding from the European Union.

PRIZES AND AWARDS

ISIC

Xile Hu awarded the National Latsis Prize 2017

The National Latsis Prize is among the most important scientific distinctions in Switzerland, and includes a monetary award of CHF 100,000. It is awarded by the Swiss National Science Foundation (SNSF) on behalf of the International Latsis Foundation to recognize *"researchers up to the age of 40 for exceptional scientific work conducted in Switzerland."*

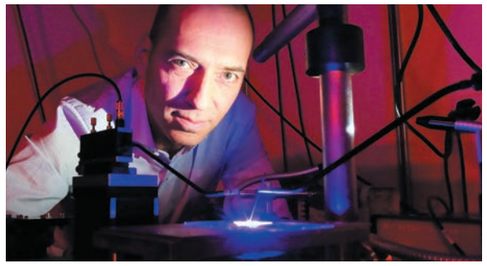
This is the 34th award of the Latsis National Prize, and was presented to **Xile Hu** by the SNSF on 11 January 2018, during a ceremony at Bern's Hôtel de ville.

Xile Hu is recognized *"for his impressive scientific career and his excellent research on the fundamental understanding of catalysis."* Catalysis is a branch of chemistry focused on substances that accelerate reactions or transform molecules. Xile Hu has distinguished himself by his pioneering research on the production of solar fuels, as well as on the synthesis of molecules with high added value.

"I have decided to not worry too much about the barriers between fields, as long as it works and gives interesting results," he says. "I try to always bring something new or unpredictable into my research, but that is not necessarily obvious. In science, we want things to happen in a logical way – so when we suggest something unprecedented or not deemed to be feasible, we can look a bit crazy."

IPHYS

Nicolas Grandjean wins the Quantum Devices Award



The Quantum Devices Award, awarded every year, honors pioneering contributions to the field of compound semiconductor devices and quantum nanostructure devices including physics and epitaxial growth. This prize was initiated by Fujitsu Quantum Devices Ltd. in 2000 and is now sponsored by the Japanese section of the International Symposium on Compound Semiconductors steering committee.

Nicolas Grandjean has been awarded the Quantum Devices Award for *"fundamental contributions to the physics and technology of III-nitride quantum structures"* during the Compound Semiconductor Week 2017 organized in Berlin. He has contributed to the understanding of the physics of GaN nanostructures, which are at the heart of blue LEDs. He is also acknowledged for the first demonstration of a polariton laser operating at room-temperature. Such a GaN-based device should require ten times less energy to operate than a conventional solid-state laser. This breakthrough could enable very low power lasers for use in optical data-storage systems.

MATH

Maryna Viazovska awarded several international prizes

In the spring of 2016, **Maryna Viazovska**, then postdoctoral assistant at Humbolt Universitaet Berlin stunned the mathematical community by posting on *ArXiv* the solution of the sphere-packing problem in dimension 8, and one week later, jointly with H. Cohn, N. Elkies, A. Kumar and D. Radchenko the solution of the problem in dimension 24.

The sphere-packing problem in dimension n asks for the best possible way to fill the n-dimensional space by n-dimensional spheres that are all in the same dimension. This is an age-old problem in geometry that goes back to Johannes Kepler, and studied amongst others by Lagrange and Gauss. Nowadays it has found numerous applications in information theory (error-correcting codes), physics, and material sciences, in particular in the study of crystals.

The cause for all this excitement is that this is an area where major advances are very sparse: the 2-dimensional case goes back to the 40's (due to László Fejes Tóth), while the 3-dimensional version (a.k.a "Kepler's conjecture") was solved in 1998 by T. Hales with a proof using numerical verification by computer involving more than 50,000 lines of code, in addition to intricate theoretical arguments.

Little was known about sphere-packing in other dimensions. The most recent major breakthrough occurred nearly 15 years ago with the work of H. Cohn and N. Elkies who identified the best sphere-packing in dimension 8 and 24. These involved remarkable and beautiful mathematical objects possessing an unusually large number of symmetries — the E8 and the Leech lattices (for dimensions 8 and 24 respectively) — and which appear in several areas of mathematics, such as number theory, group theory, and mathematical physics. Viazovska's proof that the E8 lattice (and subsequently the Leech lattice) was indeed responsible for the densest packing in dimensions 8 and 24 made a completely unexpected use of one of the most important areas of number theory: the theory of modular forms.

The elegance of the method and its potential were immediately recognized worldwide and in particular by the mathematicians of EPFL; she was immediately invited to give a colloquium lecture on her work that quickly evolved to an offer to join EPFL as Tenure Track Assistant Professor. She accepted in the fall of the same year, starting in the spring 2017, and has since produced further outstanding work.

As expected, international academic recognition quickly followed: in the spring of 2017 Viazovska's two *ArXiv* papers were published in the *Annals of Mathematics*, which is one of the most — if not the most — prestigious mathematical journals worldwide; She has been invited to give colloquium talks and lecture series in the most renowned universities (including Harvard and Princeton) and she is an invited speaker at the 2018 International Congress of Mathematicians to be held in Rio.

In 2016, Viazovska received the **Salem prize**, awarded to young mathematicians having done outstanding work in the area of harmonic analysis. She received the **Clay research award** in 2017 from the Clay Mathematics Institute, which is famous for setting up seven Millennium-prize problems whose solutions will be awarded $1 million each. The Clay research award recognizes the finest contemporary breakthroughs in all areas of mathematics and is given to mathematicians of any age and stage of career.

In 2017, Viazovska was awarded the **SASTRA Ramanujan prize**, named after the legendary indian mathematician Srinivasa Ramanujan (1887-1920). The prize is awarded to a young mathematician (under 32 years old — the age Ramanujan died) for outstanding work in Ramanujan's fields of research and is arguably the most prestigious prize worldwide awarded to a young number theorist: in Viazovska's case the prize was particularly well deserved as her work was described by several international leaders as "purely Ramanujanesque".

Viazovska's latest award came in November 2017, when she received one of the four **New Horizons in Mathematics Prizes**, awarded to junior researchers who have already produced important work in mathematics. The New Horizons prizes include $100,000 per winner, and are part of the prestigious Breakthrough Prizes. These are known as the "Oscars of Science" and are funded by Silicon Valley billionaires, entrepreneurs, and philanthropists, and are awarded annually at a glamorous ceremony celebrating top achievements in physics, life sciences and mathematics.

Through her work and awards, Maryna Viazovska stands on the same footing as several young outstanding mathematicians, many of which eventually received the Fields Medal, including Andrew Wiles, Laurent Lafforgue, Terence Tao, Elon Lindenstrauss, Stanislas Smirnov, Ngô Bao Châu, Manjul Bhargava, Maryam Mirzakhani and Peter Scholze; all of these are now considered leaders in their respective fields.

ISIC

Kevin Sivula wins Werner Prize 2017

The Werner Prize is awarded annually by the Swiss Chemical Society to promising young Swiss scientists or scientists working in Switzerland under 40 in order to recognize their outstanding independent chemical research.

Kevin Sivula, head of EPFL's Laboratory for Molecular Engineering of Optoelectronic Nanomaterials, has been recognized for his *"significant contributions to the advancement of materials and methods for photoelectrochemical energy conversion"*.

The Prize was awarded on 21 April 2017 during the SCS Spring Meeting in Berne. Sivula has been invited to give a 30-min lecture on his latest research. He shares the Prize with Professor Christoff Sparr from the University of Basel.

ISIC

Michael Grätzel wins 2017 Global Energy Prize

The Global Energy Prize has been awarded since 2003 by The Global Energy Association (Moscow), and with the support of three leading Russian energy companies: Gazprom, Surgutneftegas and the Federal Grid Company of Unified Energy System. It is presented annually in St Petersburg by the President of the Russian Federation, and winners receive an amount of 39 million rubles (~695,000 CHF).

So far, the award has been given to 34 scientists and researchers around the world who have demonstrated outstanding achievement in their respective fields. The particular focus of the Prize is research and technology in energy, and it highlights leading scientific work that pushes the boundaries of important research while also pursuing the interests of humanity.

Michael Grätzel, director of EPFL's Laboratory of Photonics and Interfaces, is being honored for *"transcendent merits in development of low cost and efficient solar cells, known as 'Grätzel cells'"*, for which Grätzel is world-famous. The cells aim at creating cost-efficient, large-scale engineering solutions for power generation, as they have proven to be much cheaper and easier to manufacture compared to other photovoltaic cells. Grätzel's lab has been consistently improving their stability and efficiency, while also carrying out research in energy- and electron-transfer reactions in mesoscopic systems in the context of solar electricity and fuels.

ISIC

Xile Hu wins the Tajima Prize

The Tajima Prize of the International Society of Electrochemistry (ISE) is given annually to electrochemists under 40 years old on the basis of their published work. The prize consists of a certificate and 1,000 CHF, and the winner is invited to give a 40-minute lecture at the Annual ISE Meeting of the following year, with ISE covering registration and banquet fees.

This year, the Prize has been award to **Xile Hu** for his research on catalysts composed of Earth-abundant elements for chemical transformations of relevance to synthesis, energy, and sustainability. In particular, Professor Hu has developed remarkable electrocatalytic materials for water splitting, which can be potentially utilized for storing renewable energy such as solar and wind.

The award will be presented to Xile Hu at the 2018 Annual ISE Meeting in Bologna, Italy.

ISIC

Anders Hagfeldt wins the Björkén Prize

UPPSALA UNIVERSITET

The Björkén Prize

The Björkén Prize is one of Uppsala University's major science prizes for outstanding scientific research or other work based on science that brings honor to Swedish research or contributes to the material improvement of the country. It has been awarded since 1902. The 2016 Prize went to Auli Niemi for her work on the geological storage of carbon dioxide and to **Anders Hagfeldt** for his work on solar cells.

MATH

Clément Hongler wins the 2017 University Latsis Award EPFL

Clément Hongler, an EPFL alumnus with a PhD in mathematics from the University of Geneva, holds the Chair of Statistical Field Theory at EPFL after having been a Ritt Assistant Professor at Columbia University. This year, he was awarded the University Latsis Award EPFL for his work on the mathematical and probabilistic aspects of statistical mechanics, and in particular for his resolution of several landmark problems regarding the Ising model at the critical temperature.

Two of the major scientific achievements of the 20th century are the developments of Quantum Field Theory and Statistical Mechanics. Quantum Field Theory describes high-energy physics, in particular elementary particles, by means of symmetry considerations. On the other hand, Statistical Mechanics aims to understand how global, macroscopic phenomena emerge from individual, microscopic behaviours.

These two fields began to converge in the second half of the 20th century, leading to Statistical Field Theory, one of the great successes of mathematical physics. However fascinating, the mathematical understanding of this picture has remained an open problem. A beautiful castle built on shaky foundations. This is where mathematicians are called in to help.

The Ising Model lies at the heart of Statistical Mechanics. It is archetypical in the study of phase transitions, that is, sharp changes in the global behaviour of a system. The model consists of atomic entities that tend to align on their neighbours. When the strength of this alignment crosses a critical threshold, we see the Ising phase transition: beyond this point, a global large-scale order arises. In the last hundred years, this model has seen a wide range of applications from magnetism to ecology to image processing and statistical inference.

In the 1980s, physicists made spectacular predictions for the 2D Ising Model, based on ideas from Statistical Field Theory. These predictions had a deep influence on mathematical physics, but remained unproven until recently. Hongler's recent proofs of these conjectures is one of his key contributions. He connected microscopic symmetries and macroscopic ones: microscopic excitations enjoy relations that reveal beautiful symmetries emerging at large scale. Such techniques also allowed Hongler to explain the behaviour of random interfaces arising in the model, and have revealed new algebraic structures, solving classical problems and producing surprising new results.

The insights and technology that Clément Hongler has developed, which connect small and large scales, help deepen the mathematical understanding of both Quantum Field Theory and Statistical Mechanics. Exciting predictions, in particular relating exceptional-symmetry algebras with scattering experiments, now seem within reach of mathematical techniques. The impact on other sciences appears very promising since many applied disciplines use Ising-type models as a theoretical basis: the highly precise results obtained for such models promise to bring clear and simple answers to applied problems.

IPHYS

Edoardo Baldini wins 2017 Chorafas Prize

The Chorafas Prize is awarded each year by the Dimitris N. Chorafas Foundation *"for outstanding work in selected fields in the engineering sciences, medicine and the natural sciences."* The Foundation was instituted in 1992 by Dr Dimitris N. Chorafas (1926-2014), a Greek engineer, author, and philanthropist who was also its President from 1996 to 2014.

The Prize is given to a selection of graduating doctoral students in the natural ("hard") sciences from the Foundation's partner universities in Europe, North America, and Asia; the list includes EPFL, MIT, UCLA, and ETHZ among others. The evaluation of the PhD students aims to reward "research characterized by its high potential for practical application and by the special significance attached to its aftermath." The best doctoral students in each partner university are chosen and are awarded $5,000 each. **Edoardo Baldini** is a former PhD student co-supervised by Majed Chergui (ISIC) and Fabrizio Carbone (IPHYS). His thesis is titled: *"Nonequilibrium Dynamics of Collective Excitations in Strongly Interacting and Correlated Quantum Systems"*. Baldini received his PhD in December 2016 and is now a Postdoctoral Fellow at MIT.

IPHYS

Olivier Schneider awarded the Craie d'Or 2017

Physics students have decided to reward the teaching of quality that they get by voting every year, at the end of their bachelor curriculum, for the three best teachers of their bachelor years. The teacher taking first place receives the Craie d'Or, a trophy created for this occasion by Pierre Wets, Antonio Gentile and Nicolas Turin of the Physics Auditoriums. The Craie d'Or winner also becomes ineligible for two years.

On 2 June 2017, the 3rd-year students designated their best teachers for the first time. Their delegates, Quentin Talon and Tara Tosic, revealed the winners at the end of the poster session of Physics Lab III, in front of a full auditorium. The 2nd place was taken by Paolo De Los Rios (Analytical Mechanics, 2nd year) and the 3rd place was taken by Donna Testerman (Advanced Linear Algebra, 1st year).

The Craie d'Or was awarded to **Olivier Schneider** for his 3rd year course (nuclear and particle physics). Moved by the appreciation of the students, he first thanked them for creating the award and making him the first recipient. He added that he was accepting this trophy with humbleness, as he is aware that many of his colleagues also deserve it.

IPHYS - ISIC

Beat Fierz, Fabrizio Carbone, and Jérôme Waser awarded ERC Consolidator Grants

The European Research Council's (ERC) Consolidator Grants are given annually to researchers of any nationality with 7-12 years of research experience after completion of their PhD, as well as *"a scientific track record showing scientific talent and an excellent research proposal"*.

The Consolidator Grants, which generally provide funding for five years, are part of the ERC's commitment to support *"the highest quality research in Europe with competition-based financing"*, with the ultimate aim *"to establish and solidify European research as cutting-edge research."*

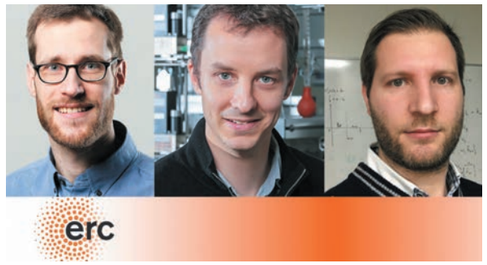
Beat Fierz directs the Laboratory of Biophysical Chemistry of Macromolecules. His research focuses on chromatin, the nucleoprotein complex organizing the genome. His lab uses a combination of molecular biology and computational simulations to study the underlying molecular mechanisms by which post-translational modifications and protein effectors work together to propagate signaling cascades that remodel the structure of the chromatin. "Our approach will yield fundamental insights into chromatin and DNA-damage response signaling, and can also be used in broader chemical and biomedical research," says Fierz.

Fabrizio Carbone directs the Laboratory for Ultrafast Microscopy and Electron Scattering. His research focuses on the study of ultrafast phenomena in solids and nanostructures. Specifically, his lab studies novel superconductors, charge-density waves, spin-density wave solids, and phase transitions in low-dimensional materials. "In this project, we aim to manipulate a handful of charges and spins using light pulses," says Carbone. "Such an ability will provide us with a unique tool for understanding the physics of quantum materials and exploiting their potential for advanced applications."

Jérôme Waser directs the Laboratory of Catalysis and Organic Synthesis. His research focuses on the discovery of new reactivity in organic chemistry, especially using catalysis. The lab uses high-energy molecules to perform chemical transformations, and develops non-conventional bond disconnections to synthesize chemical building blocks and bioactive molecules. "The project is called SeleCHEM," says Waser. "Our goal is to develop new methods for the functionalization of chemical bonds in challenging settings – specifically, we will focus on the functionalization of biomass-derived building blocks and biomolecules."

IPHYS - ISIC - MATH

Three SB scientists awarded ERC Starting Grants 2017



Ulrich Lorenz, Jeremy Luterbacher, and Alessandro Vichi

The ERC Starting Grants are given each year to researchers of any nationality and in any field of research with 2-7 years of experience since their PhD, with a promising scientific track record and an excellent research proposal. The application must be made from an EU or associated country, and each Starting Grant can be up to €1.5 million given over a period of five years.

The 2017 ERC Starting Grant Winners include three researchers at EPFL's School of Basic Sciences. The winners are:

Ulrich Lorenz - ISIC
PROJECT
Visualizing the Conformational Dynamics of Proteins by Time-Resolved Electron Microscopy.

Jeremy Luterbacher - ISIC
PROJECT
Nanostructured catalyst overcoats for renewable chemical production from biomass.

Alessandro Vichi - IPHYS
PROJECT
Charting the space of **C**onformal **F**ield **T**heories: a combined nu**M**erical and **A**nalytical a**P**proach' (CFT-MAP).

IPHYS

SNSF professorship awarded to Christophe Galland

The Swiss National Science Foundation (SNSF) has awarded a professorship to **Christophe Galland**, Ambizione fellow in the Laboratory of Photonics and Quantum Measurements, for his project *"Quantum dynamics of phonons in nanostructures and molecules"*.

The highly selective SNSF professorships are meant for young researchers who intend to pursue an academic career and wish to establish their own team to carry out a research project. The funding period is four years and may be extended by no more than two years.

Starting with a team of two PhD students, Christophe Galland will develop new optical techniques to probe the vibrational dynamics inside nanoscale systems such as molecules and nanomaterials.

Ultrashort laser pulses (<10-12 sec) will excite the vibrations via a process in which the vibrational energy increases by one level (one quantum of vibration) while a photon is simultaneously reemitted (one quantum of light). Real-time counting of these photons will enable the indirect measurement of the vibration at the quantum level.

This research aims at improving our understanding of ultrafast quantum phenomena naturally occurring at the molecular scale in processes like photosynthesis and vision. Moreover, the techniques developed in the project will contribute to the advancement of quantum technologies, in particular in the field of optical signal processing.

ISIC

EPFL-LCOM receives funding for eye research from Lions Club La Côte

The Lions Club La Côte is part of Lions Club International, the world's largest association of philanthropic clubs, with 1.36 million members in over 200 countries. Founded in 1967, the Lions Club La Côte has donated about one million swiss francs to charities for 50 years, focusing on the fight against blindness – a signature cause of Lions Club International – and other areas to support those in most need.

On the occasion of the 50th anniversary, this year the Lions Club La Côte has raised 150,000 CHF for the fight against retinoblastoma, a rare genetic cancer of the eye that affects children under four years of age.

The Lions Club La Côte donate the money to promote three causes:

- A retinoblastoma awareness campaign among healthcare professionals and the creation of a Swiss association of parents of children with retinoblastoma.
- A "support fund" for the rapid management of children with retinoblastoma.
- A research project that aims to develop an innovative treatment for retinoblastoma that will be less toxic to children and offers them better quality of life.

The research will be carried out in a collaboration between Francis Munier, a retinoblastoma specialist at the Hôpital ophthalmique Jules-Gonin, and **Paul Dyson**, head of EPFL's Laboratory of Organometallic and Medicinal Chemistry (LCOM). The research will build on a revolutionary treatment method developed by Munier, which involves injecting chemotherapy drugs directly into the eye to more efficiently target resistant tumors. The technique, currently used worldwide, is a last-resort strategy to save the eye of a child with retinoblastoma, and it reinforces the existing therapeutic arsenal while pushing the limits of more conservative treatments.

IPHYS - ISIC - MATH

Best PhD thesis awards 2017

CHEMISTRY AND CHEMICAL ENGINEERING

Norman Pellet
FOR HIS THESIS
"Investigations on hybrid organic-inorganic perovskites for high performance solar cells"
THESIS DIRECTORS
Professors Michael Grätzel and Joachim Maier.

MATHEMATICS

Pham Van Thang
FOR HIS THESIS
"Erdös Distinct Distances Problem and Extensions over Finite Spaces"
THESIS DIRECTORS
Professor János Pach, Chair of Combinatorial logics, MATH.

PHYSICS

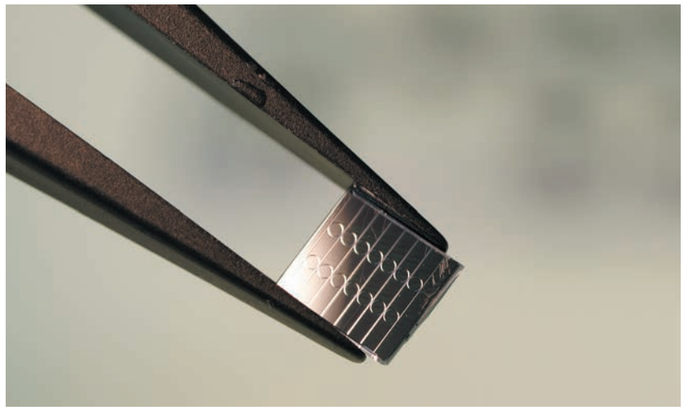
Fabio Riva
FOR HIS THESIS
"Verification and Validation Procedures with Applications to Plasma-Edge Turbulence Simulations"
THESIS DIRECTORS
Professor Paolo Ricci, Swiss Plasma Center (SPC).

RESEARCH HIGHLIGHTS

IPHYS ISIC MATH

IPHYS

Optical communication using solitons on a photonic chip



Optical microresonators made from silicon nitride on a chip for soliton based communications

©LPQM, EPFL

Optical solitons are special wave packages that propagate without changing their shape. They are ubiquitous in nature, and occur in Plasma Physics, water waves to biological systems. While solitons also exist in optical fibers, discovered at Bell labs in the 80s, their technological use so far has been limited. While researchers studied their use for optical communication, eventually the approach was abandoned. Now, a collaboration of a research group at Karlsruhe Institute of Technology's (KIT) Institute of Photonics and Quantum Electronics (IPQ) and Institute of Microstructure Technology (IMT) with EPFL's Laboratory of Photonics and Quantum Measurements (LPQM) have shown that solitons may experience a comeback: Instead of using a train of soliton pulses in an optical fiber, they generated continuously circulating optical solitons in compact silicon nitride optical microresonators. These continuously circulating solitons lead to broadband optical frequency combs. Two such superimposed frequency combs enabled massive parallel data transmission on 179 wavelength channels at a data rate of more than 50 terabits per second – a record for frequency combs. The work is published in *Nature*.

Optical frequency combs, for which John Hall and Theodor W. Hänsch were awarded the Nobel Prize in Physics in 2005, consist of a multitude of neighboring spectral lines, which are aligned on a regular equidistant grid. Traditionally, frequency combs serve as high-precision optical references for measuring frequencies. The invention of so-called Kerr frequency combs, which are characterized by large optical bandwidths and by line spacings that are optimal for communications, make frequency combs equally well suited for data transmission. Each individual spectral line can be used for transmitting a data signal.

In their experiment, the researchers from KIT and EPFL used optical silicon nitride micro-resonators on a photonic chip that can easily be integrated into compact communication systems. For the communications demonstration, two interleaved frequency combs were used to transmit data on 179 individual optical carriers, which completely cover the optical telecommunication C and L bands and allow a transmission of data rate of 55 terabits per second over a distance of 75 kilometers.

"This is equivalent to more than five billion phone calls or more than two million HD TV channels; it is the highest data rate ever reached using a frequency comb source in chip format," explains Christian Koos, professor at KIT's IPQ and IMT and recipient of a Starting Independent Researcher Grant of the European Research Council (ERC) for his research on optical frequency combs. The components have the potential to drastically reduce the energy consumption of the light source in communication systems.

The basis of the researchers' work are solitons generated in low-loss optical silicon nitride micro-resonators. In these, an optical soliton state was generated for the first time by **Tobias Kippenberg**'s lab at EPFL in 2014.

"The soliton forms through nonlinear processes occurring due to the high intensity of the light field in the micro-resonator" explains Kippenberg. The microresonator is only pumped through a continuous-wave laser from which, by means of the soliton, hundreds of new equidistant laser lines are generated. The silicon nitride integrated photonic chips are grown and fabricated in the Center for MicroNanotechnology (CMi) at EPFL.

Meanwhile, a startup from LPQM, LiGenTec SA, is also offering access to these photonic integrated circuits to interested academic and industrial research laboratories.

The work shows that microresonator soliton frequency comb sources can considerably increase the performance of wavelength division multiplexing (WDM) techniques in optical communications. WDM allows to transmit ultra-high data rates by using a multitude of independent data channels on a single optical waveguide. To this end, the information is encoded on laser light of different wavelengths.

For coherent communications, microresonator soliton frequency comb sources can be used not only at the transmitter, but also at the receiver side of WDM systems. The comb sources dramatically increase scalability of the respective systems and enable highly parallel coherent data transmission with light. According to Christian Koos, this is an important step towards highly efficient chip-scale transceivers for future petabit networks.

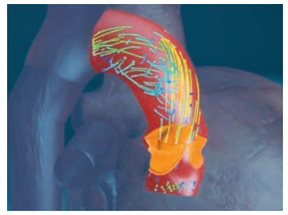
This work was supported by the European Research Council (Starting Grant 'EnTeraPIC'), the European Union (project BigPipes), the Alfried Krupp von Bohlen und Halbach Foundation, the Karlsruhe School of Optics & Photonics (KSOP), and the Helmholtz International Research School for Teratronics (HIRST), the Erasmus Mundus Doctorate Program Europhotonics, the Deutsche Forschungsgemeinschaft (DFG), the European Space Agency, the US Air Force (Office of Scientific Research), the Swiss National Science Foundation (SNF), and the Defense Advanced Research Program Agency (DARPA) via the program Quantum Assisted Sensing and Readout(QuASAR).

REFERENCE

Pablo Marin-Palomo, Juned N. Kemal, Maxim Karpov, Arne Kordts, Joerg Pfeifle, Martin H. P. Pfeiffer, Philipp Trocha, Stefan Wolf, Victor Brasch, Miles H. Anderson, Ralf Rosenberger, Kovendhan Vijayan, Wolfgang Freude, Tobias J. Kippenberg, Christian Koos. Microresonator solitons for massively parallel coherent optical communications. *Nature* 08 June 2017. DOI: 10.1038/nature22387

MATH

Your own virtual heart for non-invasive heart diagnostics



One day, a virtual version of your own heart pumping may help doctors diagnose heart disease and determine the best treatment for you, without the need of surgical intervention or other invasive clinical practices. EPFL mathematician **Alfio Quarteroni**'s goal is precisely this as he builds mathematical tools to simulate heart function with increasing accuracy and that can be personalized to your heart based on medical scans. He recently added the behavior of a patient-specific aortic valve to his overall functioning heart model. The results are published on June 7th in *Biomechanics and Modeling in Mechanobiology*.

A PERSONALIZED VIRTUAL HEART FOR PREVENTING CARDIOVASCULAR DISEASE

The human heart is an extraordinarily complex organ that pumps an estimated 180 million liters of blood, which would fill more than seven Olympic-sized swimming pools in one's lifetime, thereby ensuring that oxygenated blood reaches the entire body. Cardiovascular problems may lead to malfunction, disease, or death. Heart disease causes 40% of deaths in the EU and costs an estimated 196 billion a year, yet 80% of acquired heart diseases and stroke episodes are preventable.

Quarteroni aims to help prevent or treat cardiovascular disease by providing a personalized virtual heart to patients, essentially a detailed mathematical description of a patient's heart and how it functions – or malfunctions.

Every person's heart is unique. Correctly modeling the intricacies of each individual heart therefore requires a customizable mathematical description of both its geometry and its dynamics. But doing so in a mathematically sound way is no easy task; it requires large amounts of patient-specific data and computational power to solve complex equations. Thanks to increasingly powerful computers, building a realistic virtual heart is becoming a reality.

HOW TO BUILD A VIRTUAL AORTIC VALVE

In constructing a virtual heart that is complete and functional, the aortic valve cannot be neglected. Quarteroni and his team recently added to their heart model the way blood flows from inside the heart into the aorta, taking into account the complex shapes and properties of the aorta's physiological membranes: the valve leaflets.

"A mathematical description of the aortic valve and its interaction with blood flow exists in the literature, but not at this level of detail for a specific patient," says Quarteroni.

From MRI scans of a patient, they reconstructed the shape of the aorta, which they represented using a 3D computational mesh. Using mathematical tools to characterize the mechanics of the valve, they described the movement of three triangular-shaped leaflets that make up the aortic valve. To determine how blood flows inside of the atria, the heart's cavities, they next approximated and numerically solved the mathematical equations (Navier-Stokes) that describe viscous fluid dynamics, adapting them for a patient-specific geometry. Even with this preliminary work, it is a relatively easy task to personalize the model to another patient by using a new set of MRI scans.

As the director of iHeart, an EU-funded project, Quarteroni's long-term vision is to build patient-specific virtual models of the entire cardiovascular system, including the heart, all of the body's blood vessels, and of the approximately five liters of blood flowing through the body.

"If successful, iHeart will help clinicians to tackle important questions efficiently, both in diagnostics and treatment, with a tremendous impact for society," says Quarteroni. "It will provide a unique, unprecedented research environment for exploring the heart with an immensely powerful and non–invasive mathematical microscope, making it possible to simulate cardiovascular disease, like carotid stenosis and aneuryisms that can affect the heart, the abdomen, the brain and other parts the body."

Quarteroni believes that a personalized virtual heart model may become clinically available in less than a decade. Earlier prototypes of the virtual model may be developed and tested sooner, possibly within a five-year horizon. This will require significant investment in the development of robust mathematical and numerical tools to simulate heart function that is tailored to a specific patient.

ISIC

A uranium-based compound improves manufacturing of nitrogen products

Nitrogen is abundantly available in nature and forms the basis for many valuable products, both natural and artificial. This requires a reaction known as "nitrogen fixation", whereby molecular nitrogen is split into two atoms of nitrogen that can then be connected to other elements like carbon or hydrogen. But performing nitrogen fixation to make ammonia on an industrial scale requires harsh conditions with very high temperature and pressure. EPFL scientists have now developed a uranium-based compound that allows nitrogen fixation to take place in ambient conditions. The work, published in *Nature*, forms a basis for the development of more efficient catalysts, while it highlights new concepts that can be expanded to metals beyond uranium.

Despite being widely used, ammonia is not that easy to make. The main method for producing ammonia on an industrial level today is the Haber-Bosch process, which uses an iron-based catalyst and temperatures around 450°C and pressure of 300 bar — almost 300 times the pressure at sea level.

The reason is that molecular nitrogen — as found in the air — does not react very easily with other elements. This makes nitrogen fixation a considerable challenge. Meanwhile, numerous microorganisms have adapted to perform nitrogen fixation under normal conditions and within the fragile confines of a cell. They do this by using enzymes whose biochemistry has inspired chemists for applications in industry.

The lab of **Marinella Mazzanti** at ISIC synthesized a complex containing two uranium(III) ions and three potassium centers, held together by a nitride group and a flexible metalloligand framework. This system can bind nitrogen and split it in two in ambient, mild conditions by adding hydrogen and/or protons or carbon monoxide to the resulting nitrogen complex. As a result, the molecular nitrogen is cleaved, and bonds naturally with hydrogen and carbon.

The study proves that a molecular uranium complex can transform molecular nitrogen into value-added compounds without the need for the harsh conditions of the Haber-Bosch process. It also opens the door for the synthesis of nitrogen compounds beyond ammonia, and forms the basis for developing catalytic processes for the production of nitrogen-containing organic molecules from molecular nitrogen.

FUNDING

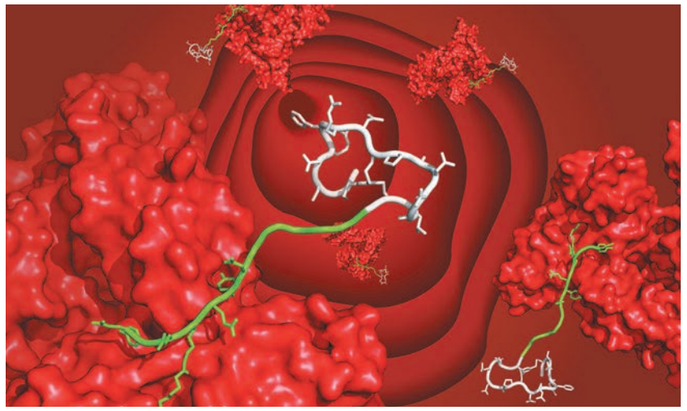
- **Swiss National Science Foundation**
- **EPFL**

REFERENCE

Marta Falcone, Lucile Chatelain, Rosario Scopelliti, Ivica Zivkovic, Marinella Mazzanti. Nitrogen Reduction and Functionalization by a Multimetallic Uranium Nitride Complex. *Nature* 20 July 2017. **DOI: 10.1038/nature23279**

ISIC

A new ligand extends the half-life of peptides from minutes to days



A bicyclic peptide (white) bound to serum albumin (red) through the newly developed ligand (green), floating in the bloodstream.
© C. Heinis/EPFL

Peptides are biological molecules, made up of short sequences of amino acids. Because they are easy to synthesize, show low toxicity and high efficiency, peptides such as insulin and other hormones can be used as drugs. But peptides are quickly cleared by the kidneys, which means that we can only use peptide drugs that act within minutes. This problem can be overcome by connecting peptides to ligands that bind blood-serum proteins such as albumin, allowing the peptide to linger in the bloodstream longer. EPFL scientists have now developed such a ligand, which is easy to synthesize and has a high affinity for human albumin. Published in *Nature Communications*, the new ligand could potentially extend the half-life of peptides from minutes to several days.

Peptides combine a number of attractive features for drugs: low toxicity and immune reactions, high affinity and efficacy for their targets, and accessible chemical synthesis. The only problem is "renal clearance": peptides are generally cleared by the kidneys within a few minutes of entering the patient's blood. For example, one of the most common peptides, insulin, has a bloodstream half-life of only 4-6 minutes. Another hormone, oxytocin — given intravenously to induce or accelerate labor — has a half-life of 10-15 minutes.

Such short timeframes imposed by renal clearance severely limit the therapeutic potential of these potentially ideal drugs. One promising way to increase the half-life of peptides is to "piggy-back" them onto blood-serum proteins, such as albumin, which is the most abundant protein in the blood serum and has a half-life of nineteen days. This however, requires an intermediate ligand molecule that can be attached to the peptide during synthesis, and also have a high affinity and selectivity for human albumin.

The lab of **Christian Heinis** at ISIC has now developed such a ligand, which has a high affinity for human albumin and — more importantly — is easy to synthesize and attach to a peptide. The ligand is made by fusing a fatty acid with another peptide. The resulting molecule is referred to as a "chimera" and combines the best of two worlds from the field of albumin ligands.

Previous efforts built ligands based on either fatty acids or peptides, and have tried them on insulin. But whereas fatty acids somewhat extended the half-life of insulin, they generally didn't bind albumin very strongly. On the other hand, peptide-based ligands bind albumin well, but showed low solubility, meaning it didn't distribute insulin in the blood very well.

The new ligand literarily brings together the advantages of both fatty acids and peptides. The researchers searched for an amino acid sequence that would complement the fatty acid's weak binding of albumin. Using an elegant "iterative" synthesis and screening method they discovered a peptide sequence that increases the binding of the fatty acid twenty-seven times. The final chimera ligand binds human albumin with high affinity (K_d = 39 nM), is highly soluble, and can be appended to peptide drugs using standard synthesizing techniques.

The researchers demonstrated *in vivo* that the ligand prolongs the half-life of several bioactive peptides more than 25-fold. They then appended the ligand to an actual peptide developed to treat pathogenic thrombosis, which has a notoriously impractical short half-life. The ligand was shown to extend the effectiveness of the peptide by several hours, inhibiting the disease in rabbits.

"We expect that the tag presented in our work will interest a larger research and business audience because it is applicable to virtually any peptide moiety, including small proteins," says Heinis. "The ligand can be appended to any peptide during solid-phase peptide synthesis on standard synthesizers, making it easily accessible for academic and industry labs."

The innovative technology can potentially also be applied to modulate the pharmacokinetic properties of bicyclic peptides developed by Bicyclic Therapeutics, a startup co-founded by Christian Heinis and Sir Greg Winter (MRC LMB Cambridge, UK) in 2009, and of which EPFL is a shareholder. On June 1 this year, Bicycle Therapeutics received a series B investment of 52 million US dollars. The company's focus is the bicyclic peptide (Bicycle®) product platform, which combines properties of several therapeutic entities in a single modality: exhibiting the affinity and selective pharmacology associated with antibodies; the distribution kinetics of small molecules, allowing rapid tumor penetration; and the "tuneable" pharmacokinetic half-life and renal clearance of peptides.

FUNDING
Swiss National Science Foundation

REFERENCE
Alessandro Zorzi, Simon J. Middendorp, Jonas Wilbs, Kaycie Deyle, Christian Heinis. **Acylated heptapeptide binds albumin with high affinity and application as tag furnishes long-acting peptides.** *Nature Communications* **8**, 16092. DOI: 10.1038/ncomms16092 (17 July 2017).

IPHYS

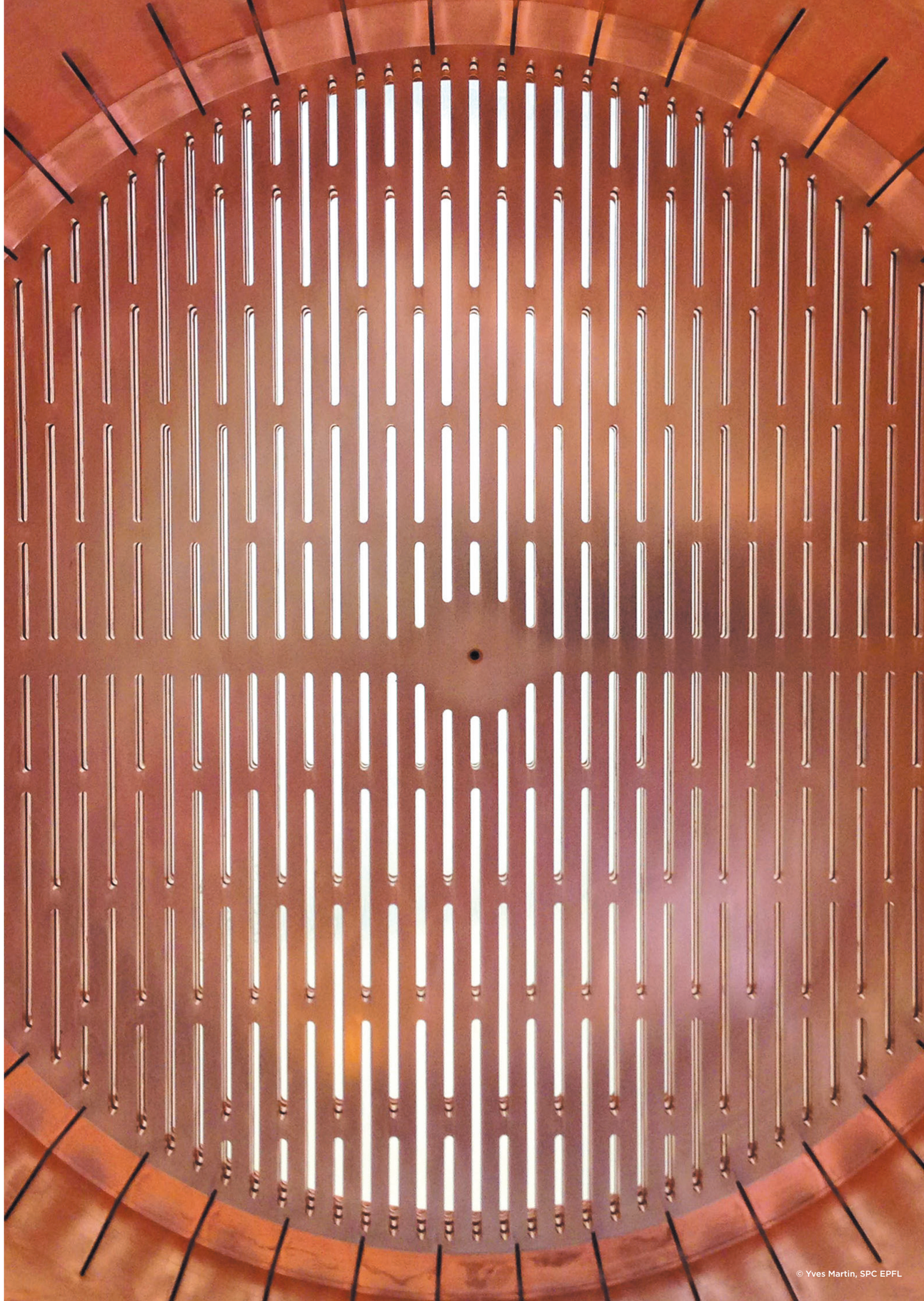
EPFL invention places second in UAE sustainable water competition

A prototype of the awarded non-electric gravitational solar-thermal water purification panel, which filters and sterilizes contaminated water using sunlight.
© Endre Horváth/EPFL

The Mohammed bin Rashid Al Maktoum Global Water Award is overseen by the United Arab Emirates' Water Aid Foundation (Suqia), launched by His Highness Sheikh Mohammed bin Rashid Al Maktoum, Vice President and Prime Minister of UAE and Ruler of Dubai. Suqia oversees the award under the umbrella of the Mohammed Bin Rashid Al Maktoum Global Initiatives (MBRGI). The Award aims to encourage leading corporations, research centers, institutions and innovators from across the world to compete to find sustainable and innovative solar-energy solutions to the problem of water scarcity across the world. The Award itself is valued at $1,000,000. The competition includes three categories: Innovative Projects (Small and Large projects), Innovative Research and Development (National and International institutions), and Innovative Youth.

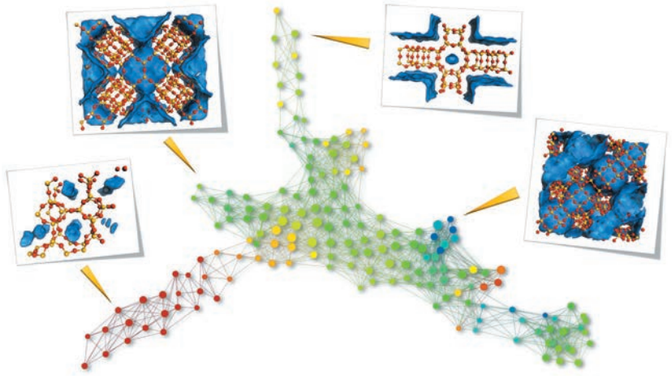
A patent-pending gravitational solar-thermal water purification panel developed by **László Forró**'s lab at EPFL came second in the Innovative Research and Development category. The device uses sunlight to filter and sterilize contaminated water. The technology is based on an innovative nanoporous photocatalytic aerogel composite membrane, which, upon solar irradiation, renders contaminated water safe by removing and inactivating infectious disease-causing biological agents such as bacteria, viruses, protozoa, and worms. The system does not require electricity or chemical agents, while lab tests predict that a 1-m^2 panel can filter 70 liters of drinking water in 5 hours. This amount is equal to the average daily water intake of a small community.

"This award would help us finalize the validation process of our cost-effective and sustainable water-purifying solution by independent certified laboratories and receive endorsements from third parties to distribute it in remote communities," says **Endre Horváth**, who leads the project. "We are honored and delighted to be winners today and to receive this award, and we are confident of the exposure it will grant us. This technology has the potential to provide a step forward for infrastructure improvements aimed at addressing health improvement under extreme poverty."


© Yves Martin, SPC EPFL

ISIC - MATH

A new tool for discovering nanoporous materials



Topological differences of top-performing materials for methane storage. Topological data analysis reveals the similarity between structures; each node represents a family of similar materials, while a network between two nodes indicates that they share at least one material. The further apart the nodes are, the more dissimilar the materials. The pictures show examples of nanoporous materials at the edges, and represent the topologically most different materials (red = Si, yellow = O, blue area = Pores).

Materials classified as "nanoporous" have structures (or "frameworks") with pores up to 100 nm in diameter. These include diverse materials used in different fields from gas separation, catalysis, and even medicine (e.g. activated charcoal). The performance of nanoporous materials depends on both their chemical composition and the shape of their pores, but the latter is very difficult to quantify. So far, chemists rely on visual inspection to see whether two materials have similar pores. EPFL scientists, in the framework of NCCR-MARVEL, have now developed an innovative mathematical method that allows a computer to quantify similarity of pore structures. The method makes it possible to search databases with hundreds of thousands of nanoporous materials to discover new materials with the right pore structure. The work is published in *Nature Communications*.

THE SEARCH FOR NANOPOROUS MATERIALS

Nanoporous materials comprise a broad category and can differ widely in their chemical makeup. What unites them is the presence of nano-sized pores in their three-dimensional structure, which endows them with catalytic and absorption properties. These pores can range between 0.2-1000 nanometers, and their size and shape (their "geometry") can have a decisive effect on the material's properties. In fact, pore shape is as important a predictor of performance as chemical composition.

Today, computers can generate large databases of potential materials and determine — before having to synthesize them — which materials would perform best for a given application. But their chemistry is so versatile that the number of possible new materials is almost unlimited, while we do not have a method for quantifying and comparing similarity between pore geometries. All this means that finding the best nanoporous material for any given application is challenging.

MATH TO THE RESCUE

A new method developed in a collaboration of the labs of **Berend Smit** and **Kathryn Hess Bellwald** at EPFL uses a technique from applied mathematics called "persistent homology". This technique can quantify the geometric similarity of pore structures by adopting the mathematical tools that are commonly used by Facebook and others to find similar faces in uploaded photos.

The persistent homology method produces "fingerprints", represented by barcodes, that characterize the pore shapes of each material in the database. These fingerprints are then compared to compute how similar the pore shapes of two materials are. This means that this approach can be used to screen databases and identify materials with similar pore structures.

The EPFL scientists show that the new method is effective at identifying materials with similar pore geometries. One class of nanoporous materials that would benefit from this innovation are the zeolites and the metal-organic frameworks (MOFs), whose applications range from gas separation and storage to catalysis.

The scientists used methane storage — an important aspect of renewable energy — as a case study. The new method showed that it is possible to find nanoporous materials that perform as well as known top-performing materials by searching databases for similar pore shapes.

Conversely, the study shows that the pore shapes of the top-performing materials can be sorted into topologically distinct classes, and that materials from each class require a different optimization strategy.

"We have a database of over three million nanoporous materials, so finding similar structures through visual inspection is out of the question," says Berend Smit. "In fact, going through the literature, we found that authors often don't realize when a new MOF has the same pore structure as another one. So we really need a computational method. However, while humans are intuitively good at recognizing shapes as the same or different, we needed to work with the math department at EPFL to develop a formalism that can teach this skill to a computer."

"In the field of algebraic topology, mathematicians have formulated the theory of persistence homology in any dimension," says Kathryn Hess. "Previous applications used only the first two of these dimensions, so it's exciting that chemical engineers at EPFL have discovered a significant application that requires the third dimension as well."

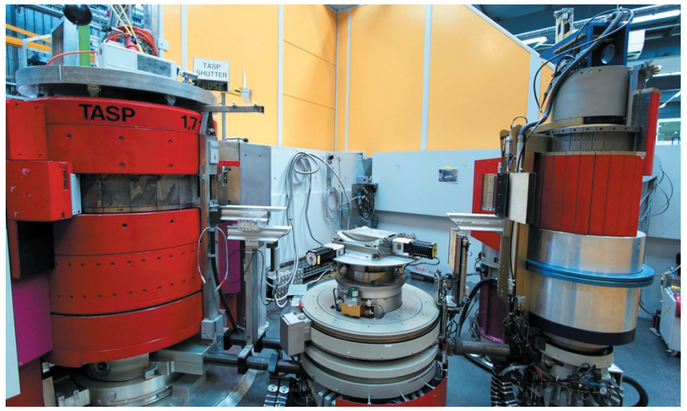
This work was a collaboration between EPFL, INRIA (France) and UC Berkeley. It was funded by the US Department of Energy, the National Center of Competence in Research (NCCR) 'Materials' Revolution: Computational Design and Discovery of Novel Materials (MARVEL)' the Deutsche Forschungsgemeinschaft (DFG), the European Research Council (ERC; Horizon 2020; GUDHI).

REFERENCE

Yongjin Lee, Senja D. Barthel, Paweł Dłotko, S. Mohamad Moosavi, Kathryn Hess, Berend Smit. **Quantifying similarity of pore-geometry in nanoporous materials.** *Nature Communications* 23 May 2017. **DOI: 10.1038/ncomms15396**

IPHYS

First observation: new type of entanglement in a 2D quantum material



The neutron spectrometer used in this study

Many physical phenomena can be modeled with relatively simple math. But, in the quantum world there are a vast number of intriguing phenomena that emerge from the interactions of multiple particles — "many bodies" — which are notoriously difficult to model and simulate, even with powerful computers. Examples of quantum many body states with no classical analogue include superconductivity, superfluids, Bose-Einstein condensation, quark-gluon plasmas etc. As a result, many "quantum many-body" models remain theoretical, with little experimental backing. Now, scientists from EPFL and the Paul Scherrer Institut (PSI) have realized experimentally a new quantum many body state in a material representing a famous theoretical model called the "Shastry-Sutherland" model. The work is published in *Nature Physics*.

While there are several one-dimensional many-body models that can be solved exactly, there are but a handful in two-dimensions (and even fewer in three). Such models can be used as lighthouses, guiding and calibrating the development of new theoretical methods.

The Shastry-Sutherland model is one of the few 2D models that have an exact theoretical solution, which represents the quantum pairwise entanglement of magnetic moments in a square lattice structure. When conceived, the Shastry-Sutherland model seemed an abstract theoretical construct, but remarkably it was discovered that this model is realized experimentally in the material $Sr_2Cu(BO_3)_2$.

Mohamed Zayed in the lab of **Henrik Rønnow** at EPFL and Christian Ruegg at PSI discovered that pressure could be used to tune the material away from the Shastry-Sutherland phase in such a manner that a so-called quantum phase transition to a completely new quantum many body state was reached.

Unlike classical phase transitions such as ice (solid) melting into liquid water and then evaporating as a gas, quantum phase transitions describe changes in quantum phases at absolute zero temperature (−273.15°C). They occur because of quantum fluctuations that are themselves triggered by changes in physical parameters — in this case pressure.

The researchers were able to identify the new quantum state using neutron spectroscopy, which is a very powerful technique to investigate magnetic properties of quantum materials and technological materials alike. Combining of neutron spectroscopy and high pressures is very challenging, and this experiment is among the first to do so for a complex quantum state.

In the Shastry-Sutherland model, the atomic magnets — arising from the spins of the atom's electrons — are quantum-entangled in pairs of two. The researchers found that in the new quantum phase the atomic magnets appear quantum-entangled in sets of four – so-called plaquette singlets. "This is a new type of quantum phase transition, and while there have been a number of theoretical studies on it, it has never been investigated experimentally," says Rønnow. "Our system may allow further investigations of this state and the nature of the transition into the state."

The need for high pressure limits what is experimentally feasible at the moment. However, Rønnow and Ruegg are building a new neutron spectrometer (CAMEA) at the Paul Scherrer Institute, which will be ready at the end of 2018, as well as another one at the European Spallation Source in Sweden, which will become operational in 2023. The 4-spin state in strontium copper borate will be among the first experiments for these new machines. As a next step, experiments combining pressure and magnetic fields may give access to yet undiscovered phases in quantum materials.

"Quantum many-body physics remains a challenge where theory has only scratched the surface of how to deal with it," says Rønnow. "Better methods to tackle quantum many-body phenomena would have implications from materials science to quantum information technology."

This work was carried out in collaboration with the Paul Scherrer Institut, the Carnegie Mellon University in Qatar, the University of Geneva, University College London, the Centro Brasileiro de Pesquisas Fisicas, the University of Innsbruck, the University of Cambridge, Nanyang Technological University, Université Pierre et Marie Curie, the Russian Academy of Sciences, the Institut Laue-Langevin, and the Forschungszentrum Julich GmbH.

FUNDING

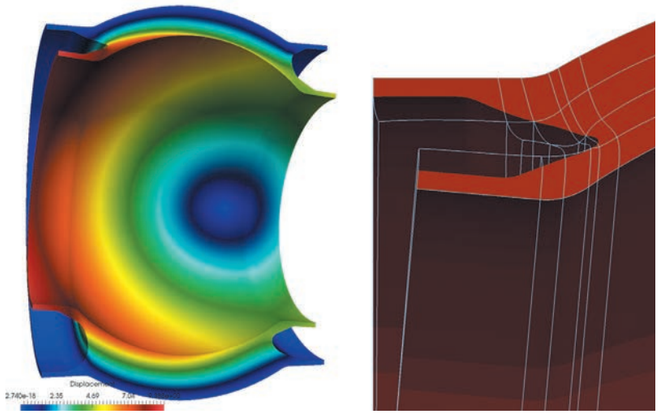
- **Swiss National Science Foundation**
- **Royal Society (UK)**
- **EPSRC (UK)**
- **Science Without Borders program of CNPq/MCTI-Brazil**
- **National Research Foundation (NRF) of Singapore.**

REFERENCE

M.E. Zayed, Ch. Rüegg, J. Larrea J., A.M. Läuchli, C. Panagopoulos, S.S. Saxena, M. Ellerby, D.F. McMorrow, Th. Strässle, S. Klotz, G. Hamel, R.A. Sadykov, V. Pomjakushin, M. Boehm, M. Jiménez-Ruiz, A. Schneidewind, E. Pomjakushina, M. Stingaciu, K. Conder, H.M. Rønnow. **4-spin Plaquette Singlet State in the Shastry-Sutherland compound $SrCu_2(BO_3)_2$.** *Nature Physics* 17 July 2017. DOI: 10.1038/nphys4190

MATH

CHANGE: the challenges for (adaptive) PDE solvers: the interplay of analysis and geometry



Non linear simulation of a rubber spherical bushing, geometry designed by Hutchinson Research Center

Industrial design and manufacturing relies in virtual prototyping for the development of new products. Before constructing a physical prototype of the product, a virtual model is generated. It consists of a detailed representation of the product, including its shape but also the physical properties of its parts, within a computer.

The virtual prototype is made alive in the simulation: the behavior of the object under real (e.g., the wind resistance of a car, or its deformation during a crash) conditions needs to be understood and "simulated" via a computer. In reality, what we teach to computers are not "real" physical models, but the equations governing such models or their simplification: here is where the mathematics of partial differential equations (PDEs, the family most models belong to) enters into play.

The paradigm used by **Annalisa Buffa** is to see the simulation of PDEs as a brick within an optimization loop, where, at each step, the geometrical entities are created, described and manipulated with a geometry processor, often through Computer-Aided Design systems (CAD), and then used as input in Computer-Aided Engineering systems (CAE) where they are handled and processed for the simulation (often referred to as analysis).

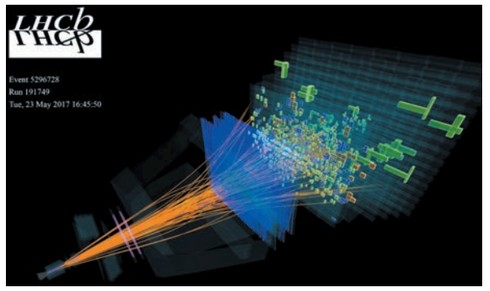
By bringing together skills from numerical analysis, geometry processing and scientific computing, this project has the ambition to propose a new paradigm for the numerical simulation, that integrates the different aspects of a workflow starting from geometric description and then moves up to quantification of errors. The final goal is to significantly increase the efficiency and quality of numerical simulation and to consequently play a major role in its spreading as a basic tool for innovation across industry and in sciences such as biology, chemistry and medicine.

"In my view, thanks to CHANGE, mathematical models that unify and embrace all aspects of the design process will be available in less than a decade, with their numerical counterparts and computer codes able to implement such mathematical models in robust and efficient way," says Annalisa Buffa. "The target community for the exploitation of our results is the one tackling non-linear mechanical problems such as virtual prototyping of tires or joints, the simulation of composites and multilayered materials, and their production process via both subtracting and additive manufacturing."

CHANGE is a consortium involving the Institute of Mathematics (EPFL), the Institute of Applied Mathematics and Information Technologies of CNR (IMATI-CNR), the Johannes Kepler University of Linz, and the Johann Radon Institute for Computational and Applied Mathematics (RICAM) of Linz.

IPHYS

Particle physicists on a quest for "new physics"



A typical LHCb event fully reconstructed. Particles identified as pions, kaon, etc. are shown in different colours. © LHCb collaboration

The Large Hadron Collider (LHC) at CERN, the European Organization for Nuclear Research, produces hundreds of millions of proton collisions per second. But researchers working on the Large Hadron Collider beauty (LHCb) experiment, which involves physicists from EPFL, can only record 2,000 of those collisions, using one of the detectors installed on the accelerator. So, in the end, this technological marvel leaves the physicists wanting more. They are convinced that the vast volume of uncaptured data holds the answers to several unresolved questions.

In elementary particle physics, the Standard Model – the theory that best describes phenomena in this field – has been well and truly tried and tested, yet the researchers know that the puzzle is not complete. That's why they are looking for phenomena that are not accounted for by the Standard Model. This quest for "new physics" could explain the disappearance of antimatter after the Big Bang and the nature of the dark matter that, although representing around 30% of the universe, can only be detected by astronomical measurements at this point. "To extract more information from the LHC data, we need new technologies for our LHCb detector," says **Aurelio Bay** from EPFL's Laboratory for High Energy Physics. EPFL has teamed up with several research institutes to develop the new equipment that will upgrade the experiment in 2020.

USING SCINTILLATING FIBER TO DETECT PARTICLES

After five years of work, EPFL's physicists, together with some 800 international researchers involved in the LHCb project, have just taken an important preliminary step towards significantly enhancing their experimental equipment. They have decided to build a new detector – a scintillating fiber tracker dubbed SciFi.

Construction of the tracker, which incorporates 10,000 kilometers of scintillating fibers each with a diameter of 0.25mm, has already begun. When particles travel through them, the fibers will give off light signals that will be picked up by light-amplifying diodes. The scintillating fibers will be arranged in three panels measuring five by six meters, installed behind a magnet, where the particles exit the LHC accelerator collision point. The particles will pass through several of these fiber 'mats' and deposit part of their energy along the way, producing some photons of light that will then be turned into an electric signal.

Data on how the particles traverse the fibers will be enough to reconstruct their trajectory. The physicists will then use this information to restore their primitive physical state. "What we will essentially be doing is tracing these particles' journey back to their starting point. This should give us some insight into what happened 14 billion years ago, before antimatter disappeared, leaving us with the matter we have today," says Bay.

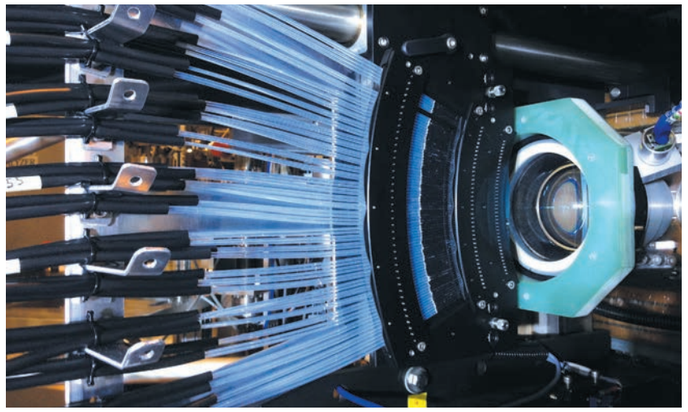
HUGE DATA FLOWS

SciFi is a key component for acquiring data at the highest speed, as it includes filters that are designed to preserve only useful data. In an ideal world, the physicists would collect and analyze all of the data without needing to use too many filters. But that would involve a massive amount of data.

"We may already be at the limit, because we of course have to save the data somewhere. First we use magnetic storage and then we distribute the data on the LHC GRID, which includes machines in Italy, the Netherlands, Germany, Spain, at CERN, and in France and the UK. Many countries are taking part, and numerous studies on this data are being run simultaneously," adds Bay. He points to his computer screen: red is used to denote programs that are not working well or those that have been trying for several days to be included among the priorities. Bay neatly puts this initiative into a physicist's perspective: "If the LHC doesn't have enough energy to uncover new physics, it's all over for my generation of physicists! We will have to come up with a new machine, for the next generation."

IPHYS - SPC

TCV Tokamak: Successful improvement in temperature and density measurements

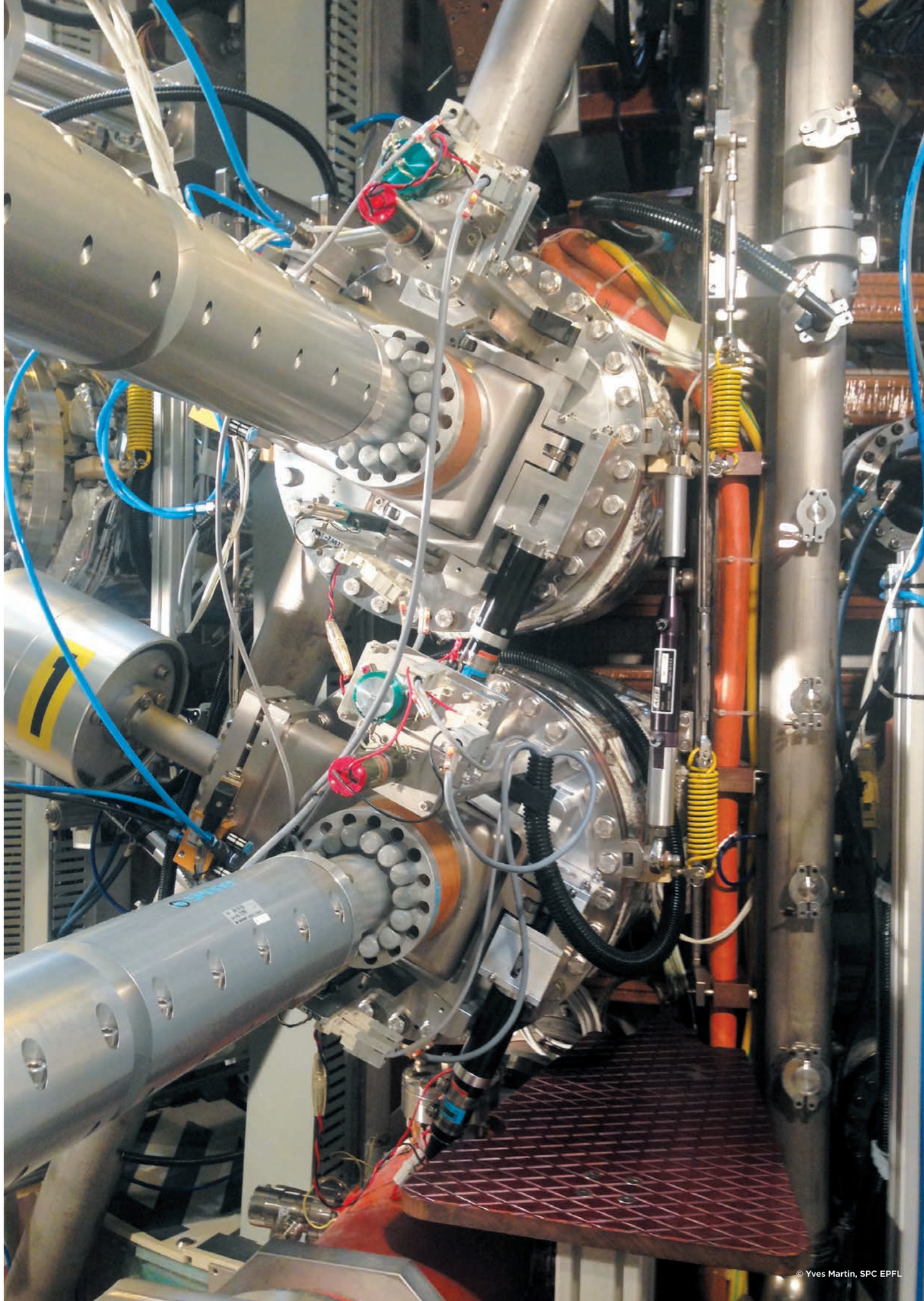


Optical fibers to capture the scattered light

The TCV tokamak of the Swiss Plasma Center (SPC) was recently shut down to upgrade its Thomson Scattering (TS) diagnostic. Right after its commissioning, the first measurements have demonstrated impressive improvement in the diagnostic capabilities. The electron density profile obtained by the new TS system contains many more points than that obtained with the previous setup. This increased resolution enables a better characterization of fine structures that may occur along the profile such as the shoulder around the vertical position of -0.2m called “pedestal”.

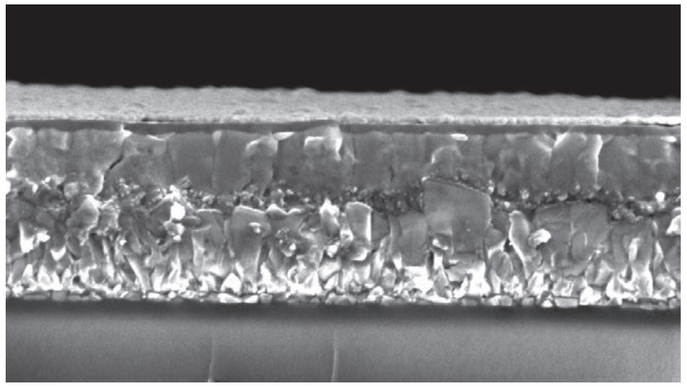
The upgrade was driven by the recent interest in plasma edge phenomenon requiring enhanced spatial resolution in the so-called plasma pedestals. It has been partly funded by EUROfusion, the European consortium for fusion research. Its primary objectives were to almost double the number of installed polychromators passing from 47 to 89 and to completely redesign the fiber optic system collecting the scattered light to cope with the increase of polychromators.

Very early in tokamak fusion research, laser diffusion onto the plasma electrons, called Incoherent Thomson Scattering, has provided crucial spatial and temporal electron temperature and density measurements. The principle is to send a powerful laser beam through the plasma and to collect the laser light scattered by plasma electrons. The scattered light is then analyzed spectrally by polychromators, which allows precise measurements of local electron temperature and density. Such system has been working on the TCV tokamak since its beginning. However, multiplying the number of collection volumes and corresponding polychromators led to a much better spatial resolution.



ISIC

Record stability for perovskite solar cells, efficiency over 20%



Cross-sectional scanning electron microscopy micrograph of a complete CuSCN solar cell displaying various layers

Perovskite solar cells (PSCs) can offer high light-conversion efficiency with low manufacturing costs. But to be commercially viable, perovskite films must also be durable and not degrade under solar light over time. EPFL scientists have now greatly improved the operational stability of PSCs, retaining more than 95% of their initial efficiencies of over 20 % under full sunlight illumination at 60°C for more than 1000 hours. The breakthrough, which marks the highest stability for perovskite solar cells, is published in *Science*.

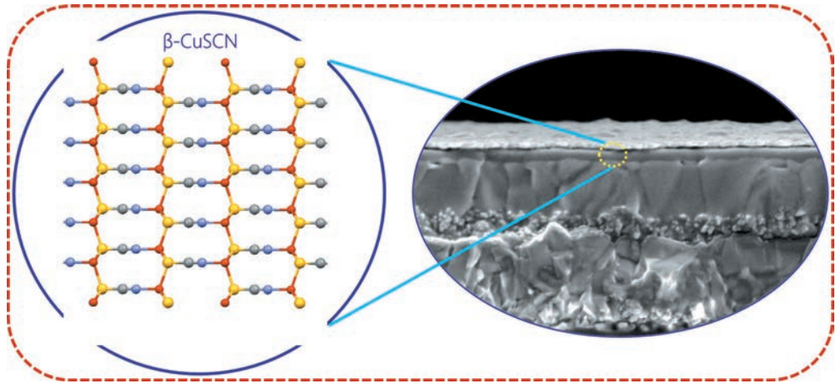
CHALLENGES OF STABILITY

Conventional silicon solar cells have reached a point of maturation, with efficiencies plateauing around 25% and problems of high-cost manufacturing, heavyweight, and rigidity has remained largely unresolved. On the contrary, a relatively new photovoltaic technology based on perovskite solar cells has already achieved more than 22% efficiency. Given the vast chemical versatility, and the low-cost processability of perovskite materials, the PSCs hold the promise to lead the future of photovoltaic technology by offering cheap, lightweight and highly efficient solar cells. But until now, only highly expensive, prototype organic hole-transporting materials (HTMs, selectively transporting positive charges in a solar cell) have been able to achieve power-conversion efficiencies over 20%. And by virtue of their ingredients, these hole-transporting materials adversely affect the long-term operational stability of the PSC.

Therefore, investigating cheap and stable hole-transporters that produce equally high efficiencies is in great demand to enable large-scale deployment of perovskite solar cells. Among various inorganic HTMs, cuprous thiocyanate (CuSCN) stands out as a stable, efficient and cheap candidate ($0.5/gr versus $500 /gr for the commonly used spiro-OMeTAD). But previous attempts to use CuSCN as a hole transporter in perovskite solar cells have yielded only moderately stabilized efficiencies and poor device stability, due to problems associated with depositing a high-quality CuSCN layer atop of the perovskite film, as wells as the chemical instability of the CuSCN layer when integrated into a perovskite solar cell.

A STABLE SOLUTION

Now, researchers at **Michael Grätzel**'s lab at EPFL, in a project led by postdocs Neha Arora and M. Ibrahim Dar, have introduced two new concepts that overcome the major shortcomings of CuSCN-based perovskite solar cells. First, they developed a simple dynamic solution-based method for depositing highly conformal, 60-nm thick CuSCN layers that allows the fabrication of perovskite solar cells with stabilized power-conversion efficiencies exceeding 20%. This is comparable to the efficiencies of the best performing, state-of-the-art spiro-OMeTAD-based perovskite solar cells.



Structure of β-CuSCN and cross-sectional SEM micrograph of a complete solar cell

Second, the scientists introduced a thin spacer layer of reduced graphene oxide between the CuSCN and a gold layer. This innovation allowed the perovskite solar cells to achieve excellent operational stability, retaining over 95% of their initial efficiency while operating at a maximum power point for 1000 hours under full-sun illumination at 60 °C. This surpasses even the stability of organic HTM-based perovskite solar cells that are heavily researched and have recently dominated the field.

The researchers also discovered that the instability of the perovskite devices originates from the degradation of CuSCN/gold contact during the solar cell's operation.

"This is a major breakthrough in perovskite solar-cell research and will pave the way for large-scale commercial deployment of this very promising new photovoltaic technology," says Michael Grätzel. "It will benefit the numerous scientists in the field that have been intensively searching for a material that could replace the currently used, prohibitively expensive organic hole-transporters," adds M. Ibrahim Dar.

CONTRIBUTORS

Universität Tübingen, Germany

FUNDING

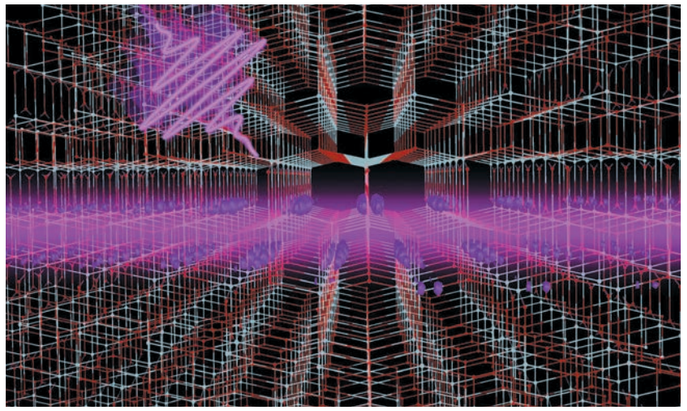
- **Greatcell Solar SA**
- **EU Horizon 2020 (FET project GOTSolar and Graphene Flagship Core1)**

REFERENCE

Neha Arora, M. Ibrahim Dar, Alexander Hinderhofer, Norman Pellet, Frank Schreiber, Shaik Mohammed Zakeeruddin, Michael Grätzel. **Perovskite solar cells with CuSCN hole extraction layers yield stabilized efficiencies >20%.** *Science* 28 September 2017. DOI: 10.1126/science.aam5655

ISIC

Shedding light on the absorption of light by titanium dioxide



Lattice structure of anatase TiO_2 with a graphical representation of the 2D exciton that is generated by the absorption of light (purple wavy arrow). This 2D exciton is the lowest energy excitation of the material.

© Joerg Harms

ISIC scientists uncovered the hidden properties of titanium dioxide, one of the most promising materials for light-conversion technology.

Titanium dioxide (TiO_2) is one of the most promising materials for photovoltaics and photocatalysis nowadays. This material appears in different crystalline forms, but the most attractive one for applications is called "anatase". Despite decades of studies on the conversion of the absorbed light into electrical charges in anatase TiO_2, the very nature of its fundamental electronic and optical properties was still unknown. EPFL scientists, with national and international partners, have now shed light onto the problem by a combination of cutting-edge steady-state and ultrafast spectroscopic techniques, as well as theoretical calculations. The work is published in *Nature Communications*.

Anatase TiO_2 is involved in a wide range of applications, ranging from photovoltaics and photocatalysis to self-cleaning glasses, and water and air purification. All of these are based on the absorption of light and its subsequent conversion into electrical charges. Given its widespread use in various applications, TiO_2 has been one of the most studied materials in the twentieth century, both experimentally and theoretically.

When light shines on a semiconducting material such as TiO_2, it generates either free negative (electrons) and positive (holes) charges or a bound neutral electron-hole pair, called an exciton. Excitons are of great interest because they can transport both energy and charges on a nanoscale level, and form the basis of an entire field of next-generation electronics, called "excitonics". The problem with TiO_2 so far is that we have not been able to clearly identify the nature and properties of the physical object that absorbs light and characterize its properties.

The group of **Majed Chergui** at EPFL, along with Swiss and international colleagues, have shed light on this long-standing question by using a combination of cutting-edge experimental methods: steady-state angle-resolved photoemission spectroscopy (ARPES), which maps the energetics of the electrons along the different axis in the solid; spectroscopic ellipsometry, which determines the optical properties of the solid with high accuracy; and ultrafast 2D deep-ultraviolet spectroscopy, used for the first time in the study of materials, along with state-of-the-art first-principles theoretical tools.

They discovered that the threshold of the optical absorption spectrum is due to a strongly bound exciton, which exhibits two remarkable novel properties: First, it is confined on a two-dimensional (2D) plane of the three-dimensional lattice of the material. This is the first such case ever reported in condensed matter. And secondly, this 2D exciton is immune against temperature and defects as it is present in any type of TiO_2 — single crystals, thin films, and even nanoparticles used in devices.

This "immunity" of the exciton to long-range structural disorder and defects implies that it can store the incoming energy in the form of light and guide it at the nanoscale in a selective way. This promises a huge improvement compared to current technology, in which the absorbed light energy is dissipated as heat to the crystal lattice, making the conventional excitation schemes extremely inefficient.

Furthermore, the properties of the newly discovered exciton are very sensitive to a variety of external and internal stimuli in the material (temperature, pressure, excess electron density), paving the way to a powerful, accurate and cheap detection scheme for sensors with an optical read-out.

"Given that it is cheap and easy to fabricate anatase TiO_2 materials, these findings are crucial for many applications and beyond," says Majed Chergui. "To know how electrical charges are generated after light is absorbed is a key ingredient for efficient photocatalysts."

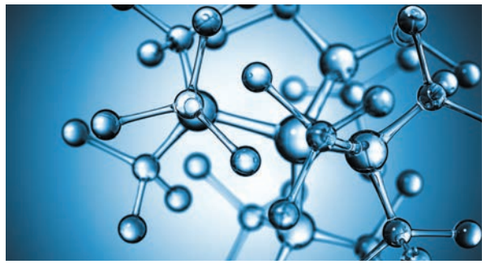
This work was carried out in a collaboration of the EPFL's Laboratoire de Spectroscopie Ultrarapide (LSU) and the Institute of Physics (IPHYS) within the Lausanne Centre for Ultrafast Science (LACUS), with the Max Planck Institute for the Structure and Dynamics of Matter, the University of Fribourg, the Università Campus Bio-Medico di Roma, the Università Roma "Tor Vergata", and the Universidad del Pais Vasco. It was funded by the Swiss National Science foundation (SNSF; NCCR:MUST), the European Research Council Advanced Grants "DYNAMOX" and "Qspec-Newmat", the Grupos Consolidados del Gobierno Vasco and COST Actions, EUSpec.

REFERENCE

E. Baldini, L. Chiodo, A. Dominguez, M. Palummo, S. Moser, M. Yazdi-Rizi, G. Auböck, B.P.P. Mallett, H. Berger, A. Magrez, C. Bernhard, M. Grioni, A. Rubio, M. Chergui. Strongly bound excitons in anatase TiO_2 single crystals and nanoparticles. *Nature Communications* **13 April 2017. DOI: 10.1038/s41467-017-00016**

IPHYS

New computer model shows how proteins are controlled “at a distance”



© iStock photos

Enzymes are large proteins that are involved in virtually every biological process, facilitating a multitude of biochemical reactions in our cells. Because of this, one of the biggest efforts in drug design today aims to control enzymes without interfering with their so-called active sites — the part of the enzyme where the biochemical reaction takes place. This “at a distance” approach is called “allosteric regulation”, and predicting allosteric pathways for enzymes and other proteins has gathered considerable interest. Scientists from EPFL, with colleagues in the US and Brazil, have now developed a new mathematical tool that allows more efficient allosteric predictions. The work is published in *PNAS*.

ALLOSTERIC DRUGS

Allosteric regulation is a fundamental molecular mechanism that modulates numerous cell processes, fine-tuning them and making them more efficient. Most proteins contain parts in their structure away from their active site that can be targeted to influence their behavior “from a distance”. When an allosteric modulator molecule — whether natural or synthetic — binds such a site, it changes the 3D structure of the protein, thereby affecting its function.

The main reason allosteric sites are of such interest to drug design is that they can be used to inhibit or improve the activity of a protein, eg. the binding strength of an enzyme or a receptor. For example, diazepam (Valium) acts on an allosteric site of the $GABA_A$ receptor in the brain, and increases its binding ability. Its antidote, flumazenil (Lanexat), acts on the same site, but instead inhibits the receptor. Generally speaking, an allosteric drug would also be used at a comparatively lower dose than a drug acting directly on the protein’s active site, thus providing more effective treatments with fewer side effects.

DEVELOPING AN ALLOSTERIC MODEL

Despite the importance of allosteric processes, we still do not fully understand how a molecule binding on a distant and seemingly unimportant part of a large protein can change its function so dramatically. The key lies in the overall architecture of the protein, which determines what kinds of 3D changes an allosteric effect will have.

The lab of **Matthieu Wyart** at EPFL sought to address several questions regarding our current understanding of allosteric architectures. Scientists classify these into two types: hinges, which cause scissor-like 3D changes, and shear, which involve two planes moving side-by-side. Despite being clear mechanically, the two models do not capture all cases of allosteric effects, where certain proteins cannot be classified as having either hinge or shear architectures.

The researchers explored alternative allosteric architectures. Specifically, they looked at the structure of proteins as randomly packed spheres that can evolve to accomplish a given function. When one sphere moves a certain way, this model can help scientists track its structural impact on the whole protein. Using this approach, the scientists addressed several questions that conventional models do not answer satisfactorily. Which types of 3D “architecture” are susceptible to allosteric effects? How many functional proteins with a similar architecture are they? How can these be modeled and evolved in a computer to offer predictions for drug design?

Using theory and computer power, the team developed a new model that can predict the number of solutions, their 3D architectures and how the two relate to each other. Each solution can even be printed in a 3D printer to create a physical model.

The model proposes a new hypothesis for allosteric architectures, introducing the concept that certain regions in the protein can act as levers. These levers amplify the response induced by binding a ligand and allow for action at a distance. This architecture is an alternative to the hinge and shear designs recognized in the past. The computational approach can also be used to study the relationship between co-evolution, mechanics, and function, while being open to many extensions in the future.

This work involves a collaboration of EPFL’s Physics of Complex Systems Laboratory with the University of California Santa Barbara and the Universidade Federal do Rio Grande do Sul in Brazil. It was funded by the National Science Foundation (NSF), the Swiss National Science Foundation (SNSF), and the Simons Foundation.

REFERENCE

Le Yan, Riccardo Ravasio, Carolina Brito, Matthieu Wyart. Architecture and Co-Evolution of Allosteric Materials. *PNAS* 20 February 2017. DOI: 10.1073/pnas.1615536114

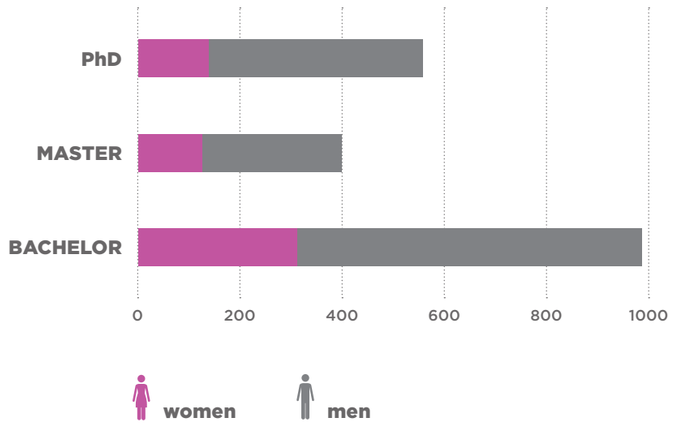
FSB IN FIGURES

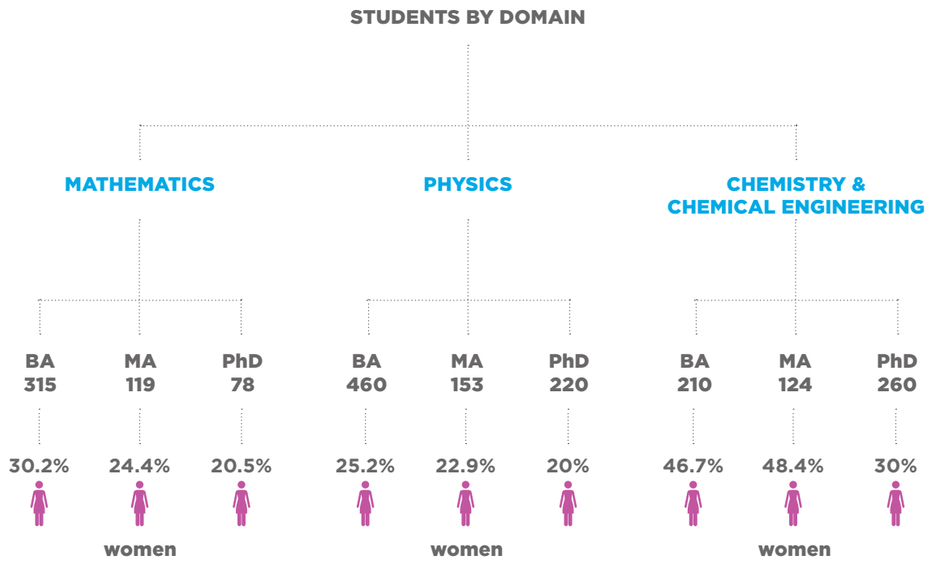
PEOPLE
FUNDING
RESEARCH
KEY FIGURES

IPHYS ISIC MATH

PEOPLE

FSB students



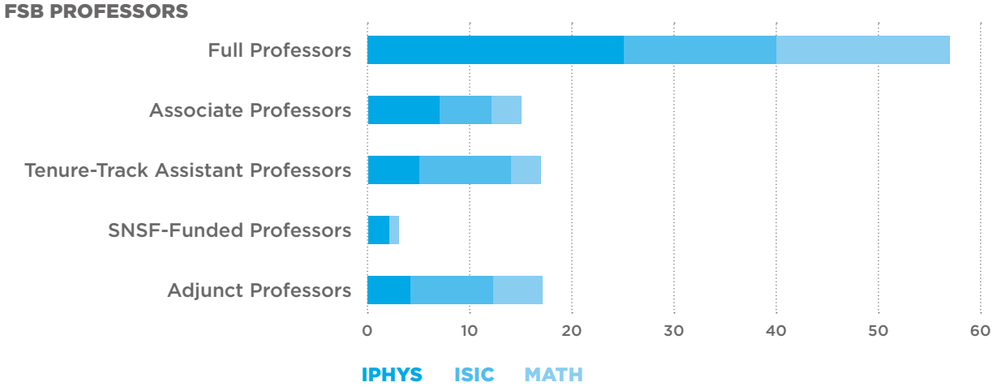


FSB staff

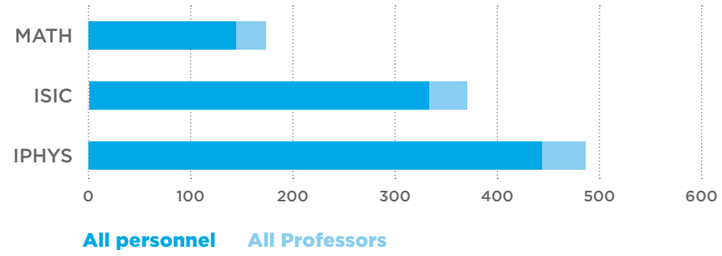
	IPHYS	ISIC	MATH	ALL
Full Professors	25	15	17	57
Associate Professors	7	5	3	15
Tenure-Track Assistant Professors	5	9	3	17
SNSF-funded Professors	2	0	1	3
Adjunct Professors	4	8	5	17
Emeritus Professors	32	13	14	59
Senior Scientists	21	9	2	32
Scientific Collaborators*	185	163	67	415
Administrative Collaborators	60	47	33	140
Technical Collaborators	102	64	0	166

* does not include PhD candidates

FSB PROFESSORS

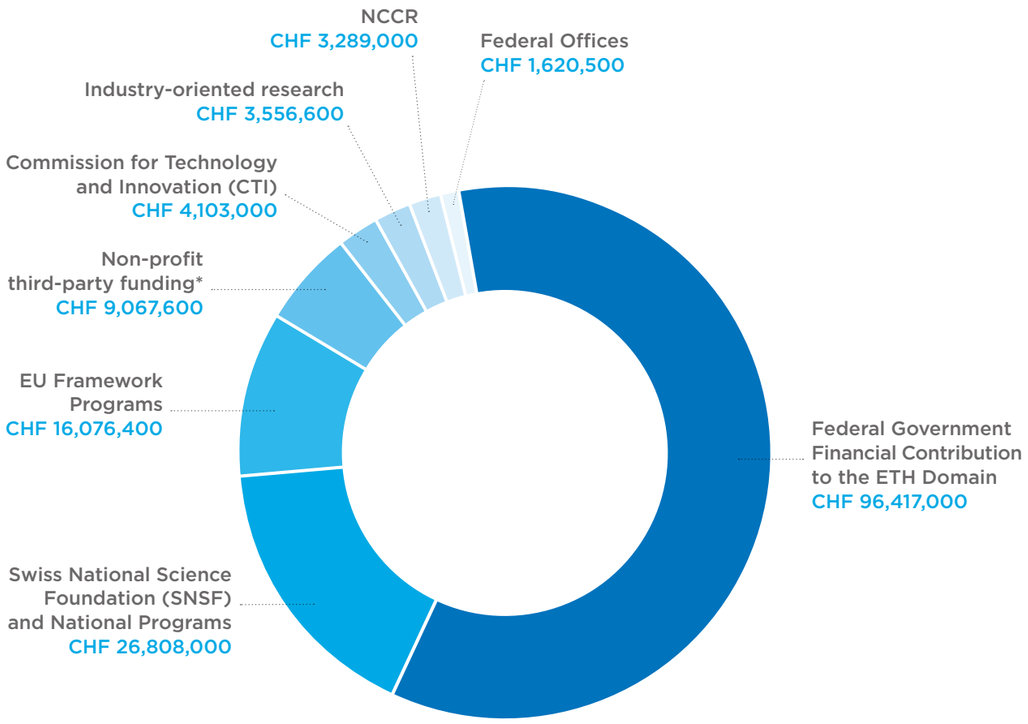


FSB STAFF



FUNDING

FSB funding in 2017



* includes Foundations and Associations

RESEARCH

FSB publications in 2017

905	Journal articles
54	Conference papers
41	Reviews
7	Books and book chapters
1007	Total peer-reviewed publications
107	Theses
11	Patents

KEY FIGURES

120	Research groups
3	Research Institutes
1939	Students
109	Professors
756	Collaborators

School of Basic Sciences FSB

EPFL
Bâtiment PH
Station 3
CH-1015 Lausanne
sb@epfl.ch

sb.epfl.ch

@epflSB