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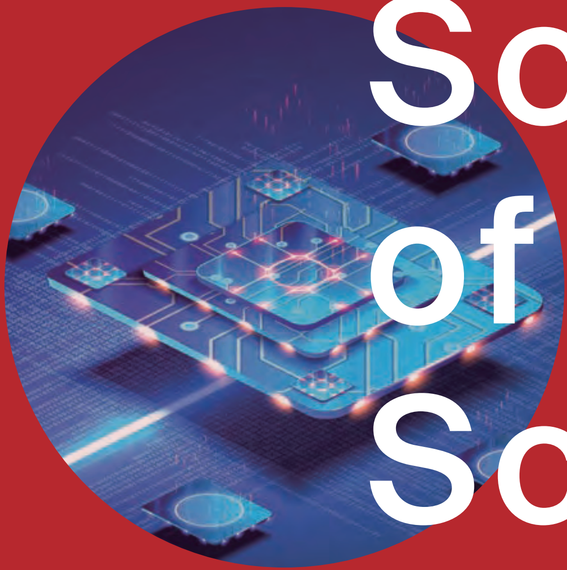

School of Basic Sciences FSB

ANNUAL REPORT 2021

IPHYS ISIC MATH

School of Basic Sciences FSB

DEAN'S FOREWORD

Due to the pandemic, 2021 was another challenging year for all, although thankfully the School of Basic Sciences remained healthy and continued to provide a world-class education due to the flexibility and ingenuity of our teaching cohort. The year also witnessed an abundance of highly innovative research and the School even played a role in helping to take the sting out of the COVID-19 virus, as you will discover later in the annual report. The pandemic was not the only challenge we faced, as Swiss science was excluded from key European research programs, which represent a major source of research income for our professors.

In spite of the challenges posed, 2021 can perhaps best be described as a year of increased interdisciplinarity, facilitated by a number of key instruments aimed at enabling us to better explore basic science at the interfaces of other domains. This interdisciplinarity may be appreciated from the launch of new interfaculty centers and other major initiatives during the year. The Bernoulli Center for Fundamental Studies was relaunched with a wider breadth including mathematics, theoretical computer science and theoretical physics. A Center for Quantum Science and Engineering was created to bring together all those across the EPFL developing future quantum devices, algorithms and applications. Inauguration of the Dubochet Center for Imaging, a joint initiative between the EPFL, the University of Lausanne and beyond, brings a new dimension to the region in cryo-electron microscopy and is already setting world records. The Swiss Plasma Center also became home to a European hub for high-performance computing focused on fusion power and we are reinforcing our connections to the Paul Scherrer Institute, synergizing our respective scientific strengths.

As you browse through this annual report, which contains only a small fraction of our activities and achievements, I hope that you gain a sense of the diversity of our activities, stretching far beyond the typical boundaries of a School of Basic Sciences. This first year for me as Dean has been daunting, enriching and rewarding, and I am confident that in 2021 we have taken some key steps to ensure the School moves forwards and upwards and is ready to contribute to the grand challenges of the future. Finally, I would like to thank all those involved with our School for their dedication and hard work and wish you and all our collaborators, alumni and friends a successful and rewarding year.

PAUL DYSON
Dean of the School of Basic Sciences, EPFL

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RESEARCH HIGHLIGHTS

PRIZES AND AWARDS

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Yimon Aye wins Tetrahedron Young Investigator Award and ICBS award

Founded in 2005, the Tetrahedron Young Investigator Award is given each year by the Executive Board of Editors and the Publisher of Tetrahedron Publications. It is given to two individuals under the age of 40 who have exhibited "exceptional creativity and dedication" in the fields of Organic Synthesis and Bioorganic & Medicinal Chemistry, respectively."

This year, the winner for the latter field is Professor **Yimon Aye**, a chemical biologist within EPFL's School of Basic Sciences, where she leads the Laboratory of Electrophiles And Genome Operation (LEAGO) in the Institute of Chemical Sciences and Engineering (ISIC).

The Award consists of a monetary prize, and Professor Aye has been invited to deliver a plenary lecture at the forthcoming Tetrahedron Symposium in 2022.

Professor Yimon Aye has also won the 2021 Global Lectureship Award from the International Chemical Biology Society.

The International Chemical Biology Society (ICBS) was founded in 2011 as "an independent, not for profit organization dedicated to promoting research and educational opportunities at the interface of chemistry and biology." As an international forum, the ICBS "brings together cross-disciplinary scientists from academia, nonprofit organizations, government, and industry to communicate new research and help translate the power of chemical biology to advance human health and enhance a stable ecosystem for environmental sustainability."

In a communication last week, the ICBS announced it has awarded its 2021 Global Lectureship award to Professor Yimon Aye at EPFL's School of Basic Sciences. The award recognizes "distinguished investigators whose research has significantly advanced the field of chemical biology." The award announcement refers to Professor Aye as "a creative chemical biologist who has generated large impact across the globe, best embodying the spirit of the ICBS Global Lectureship".

Professor Aye leads the Laboratory of Electrophiles And Genome Operation (LEAGO) in the Institute of Chemical Sciences and Engineering (ISIC). In a letter to Professor Aye, the ICBS states that she is being "recognized for [her] pioneering research on the development and application of innovative chemical biology tools to enable the study of reactive electrophilic species (RES) signaling with high spatiotemporal resolution and [her] contributions to the chemical biology field."

Tobias Kippenberg wins R.W. Wood Prize

Professor Tobias J. Kippenberg at EPFL's School of Basic Sciences has been awarded the 2021 Robert W. Wood Prize from The Optical Society.

Established in 1975, the Wood Prize is named after renowned physicist Robert W. Wood, who made pivotal contributions to the field of optics. It recognizes an "outstanding discovery, scientific or technical achievement or invention in the field of optics", measured mainly by whether it impacts the field in a way that "opens a new era of research or significantly expands an established one". The prize is endowed by Xerox Corp.

The Optical Society (OSA) has announced the 2021 recipient of the R.W. Wood Prize is Professor Tobias J. Kippenberg at EPFL's School of Basic Sciences (Institute of Physics). Professor Kippenberg "is honored for pioneering contributions to the realization of chip-scale optical frequency combs."

In 2007, Kippenberg and his team discovered the ability of optical microresonators to generate optical frequency combs via parametric interactions. This discovery showed that as an alternative to the use of mode-locked lasers, a CW laser can be converted into a broadband frequency comb via nonlinear wave mixing, overcoming passive cavity dispersion.

Kippenberg has led the field in novel microfabrication techniques, both in crystalline microresonators and through his introduction and perfection of the photonic damascene process in the silicon nitride platform.

Maria Colombo is the recipient of the Peter Lax award

Professor Maria Colombo, head of the Chair of AMCV, is distinguished with the 2022 Peter Lax Award. She will receive her award at the International Conferences on Hyperbolic Problem (HYP) that will take place in June 2022.

The Peter Lax Award was instituted in honour of Lax's seminal contributions, which laid the foundations of modern theory and computation in the area of hyperbolic conservation laws. It has been introduced in 2020 and is given every two years. This distinction is awarded to a young researcher (10 years within the PhD) in every HYP Conference. The first Peter Lax Awardee is Jacob Bedrossian (University of Maryland).

Professor Maria Colombo will give a distinguished lecture at the HYP2022 conference.

The International Conferences on Hyperbolic Problems is held every two years since 1986 and brings together hundreds of scientists with interests in the theoretical, applied, and computational aspects of hyperbolic partial differential equations and of related mathematical models. Hyperbolic conservation laws were introduced and studies from great mathematicians as L. Euler (1755) and present still incredible challenges. They also deeply connect to related areas such as the study of kinetic equations, nonlocal or/and discrete models, and weakly differentiable flows.

Award-winning year for Michael Grätzel

Professor Michael Grätzel at EPFL's School of Basic Sciences and Professor Paul Alivisatos at UC Berkeley, have won the 2021 Frontiers of Knowledge Award in Basic Sciences for "their fundamental contributions in the development of nanostructured materials for energy-related applications."

Established in 2008, the Awards "recognize and reward contributions of singular impact in science, technology, social sciences and the humanities, privileging those that significantly expand the frontiers of the known world, open up new fields, or emerge from the interaction of various disciplinary areas."

The awarding committee's citation reads: "Graetzel's groundbreaking work includes the invention of a dye-sensitized solar cell named after him. Alivisatos made pioneering contributions in using semiconductor nanocrystals for energy and display applications. Their discoveries have found applications in renewable energy and optoelectronics."

Beyond this, Professor Michael Grätzel at EPFL's School of Basic Sciences is among the winners of the 2022 Rank Prize for optoelectronics.

The Rank Prize was created in 1972 by Lord Arthur J. Rank (1888-1972), a prominent British film producer and philanthropist, to advance research in two fields of research Rank himself pursued during his own career: human and animal nutrition, and optoelectronics.

Since its foundation, the Rank Prize for Optoelectronics is given every two years. The 2022 Prize is awarded to seven internationally leading scientists, from several research laboratories "for pioneering the development of new solar cell technology based on perovskite semiconductors which promises to play a key role in the future of solar power."

Among the seven winners this year is Professor Michael Grätzel at EPFL's School of Basic Sciences. Grätzel, who became world-famous for the invention of dye-sensitized solar cells (popularly known as "Grätzel cells") directs the Laboratory of Photonics and Interfaces within the Institute of Chemical Sciences and Engineering (ISIC).

"The Rank Prize Optoelectronics Committee is delighted to recognise the outstanding achievements of these internationally leading researchers," says Professor Donal Bradley CBE FRS, the Chair of the Optoelectronics Committee. "Their work is a key example of fundamental contributions to physical science being rapidly and successfully translated into new technology, technology moreover that is poised to address truly urgent societal challenges linked to climate change. It is particularly gratifying that we have been able to announce this recognition in the lead up to the COP26 UN Climate Change Conference."

Ardemis Boghossian wins ESP Young Investigator Award

Each year, the European Society for Photobiology (ESP) offers the Young Investigator Award to a young researcher who has conducted original research of exceptionally high quality in a field related to Photobiology. The Award is part of the ESP's continuing effort to promote Photobiology.

The winner of the 2021 European Society of Photobiology (ESP) Young Investigator Award is Professor Ardemis Boghossian at EPFL's School of Basic Sciences. Professor Boghossian's research straddles the interface of nanotechnology and protein engineering, aiming at the commercial development of protein-based constructs for light-harvesting and biosensing applications using inorganic nanomaterials, which demonstrate enhanced photophysical and electronic properties that enable optical devices with unprecedented, quantum optoelectronic properties.

"I'm fascinated with blurring the lines between the living and non-living worlds," says Boghossian. "What's the difference between a biological material and a synthetic material? In the end, they're all built from the same kinds of atoms. So why not make synthetic materials that can evolve, like in biological evolution, or re-program living cells to behave as electronic devices? These are the conceptual walls that my team aims to tear down in creating new optical technologies."

The Award was presented at 19th Congress of the European Society for Photobiology, which was held under virtual congress format over 4 days in Salzburg (Austria), from August 30 to September 3, 2021.

Xile Hu wins Swiss Green & Sustainable Chemistry Award

The Swiss Green & Sustainable Chemistry Award was founded in 2020 by the Swiss Chemical Society, sponsored by Syngenta and hosted by SusChem Switzerland. It is awarded every year to "to encourage and recognize young academic investigators to contribute to the development of sustainable chemical methodologies and technologies." Candidates are scientists from across the entire world who are under 45 and have made "outstanding scientific discoveries within the field of Green and Sustainable Chemistry."

The winner of the 2022 Award is Professor Xile Hu at EPFL's School of Basic Sciences. Professor Hu directs the Laboratory of Inorganic Synthesis and Catalysis who develop catalysts from Earth-abundant elements that can be used chemical transformation related to synthesis, energy, and sustainability. Professor Hu's research focuses on base metal-catalyzed organic synthesis, electrochemical water splitting and CO2 reduction, fuel cell catalysis, and developing synthetic models for the active site of metalloenzymes.

The SCS cites Professor Hu for his "outstanding interdisciplinary research program to develop catalysis for sustainable synthesis of added-value chemicals and for cost-effective production of solar and electric fuels."

The Award was awarded to Professor Hu at the Swiss Chemistry Science Night on 16 September 2022 in Bern.

Adam Marcus part of award-winning team



Professor **Adam W. Marcus**, head of the Chair of Combinatorial Analysis, and colleagues Professors **Daniel A. Spielman** (Yale University) and **Nikhil Srivastava** (University of California, Berkeley) won the **2021 Michael and Sheila Held Prize** for their revolutionary work on the Kadison-Singer problem and Ramanujan graphs. The award is presented with a $100,000 prize.

Marcus, Spielman, and Srivastava solved long-standing questions on the Kadison-Singer problem and on Ramanujan graphs, and in the process uncovered a deep new connection between linear algebra, geometry of polynomials, and graph theory that has inspired the next generation of theoretical computer scientists.

Their groundbreaking papers on these questions, both published in 2015, solved problems that mathematicians had been working on for several decades. In particular, their solution to the Kadison-Singer problem, first posited in 1959, has been hailed as one of the most important developments in mathematics of the past decade.

Their proofs provided new tools to address numerous other problems, which have been embraced by other computer scientists seeking to apply the geometry of polynomials to solve discrete optimization problems.

Beyond this Adam Marcus, Daniel Spielman, and Nikhil Srivastava will receive the **2022 Ciprian Foias Prize** in Operator Theory for their highly original work that introduced and developed methods for understanding the characteristic polynomial of matrices.

Professors Adam Marcus, who holds the Chair of Combinatorial Analysis, Daniel Spielman (Yale), and Nikhil Srivastava (UC Berkeley) will receive the 2022 Ciprian Foias Prize in Operator Theory. The award recognizes their highly original work that introduced and developed methods for understanding the characteristic polynomial of matrices, namely the iterative sparsification method (also in collaboration with Batson) and the method of interlacing polynomials.

Together, these ideas provided a powerful toolkit with many applications, notably in the trio's breakthrough paper "Interlacing families II: mixed characteristic polynomials and the Kadison-Singer problem" (Annals of Mathematics, 2015), which solves the famous "paving problem" in operator theory, formulated by Richard Kadison and Isadore Singer in 1959.

Teaching Awards

BEST TEACHER AWARD OF THE SCHOOL OF BASIC SCIENCES (POLYSPHÈRE D'OR)

Paolo Ricci (IPHYS)

BEST TEACHER AWARD OF THE MATHEMATICS SECTION

Michel Cibils

BEST TEACHER AWARD OF THE PHYSICS SECTION

Julien Burnens
Didier Klopfenstein
Daniele Mari
Pierre Wets

EXCELLENCE IN TEACHING AWARD OF THE CHEMISTRY AND CHEMICAL ENGINEERING SECTION

Tom Rizzo

BEST TEACHER AWARD "CRAIE D'OR" BY THE PHYSICS BACHELOR STUDENTS

Paolo Ricci

Doctoral Schools Thesis Awards

MATHEMATICS DOCTORAL THESIS AWARD

Luigi De Rosa
"Non-smooth solutions in incompressible fluid dynamics"
THESIS DIRECTOR
Prof. Maria Colombo and
Prof. Camillo De Lellis (Princeton, USA)

PHYSICS DOCTORAL THESIS AWARD

Gabriel F. Cuomo
"Large Charge, Semiclassics and Superfluids: from Broken Symmetries to Conformal Field Theories "
THESIS DIRECTOR
Prof. Riccardo Rattazzi

CHEMISTRY AND CHEMICAL ENGINEERING DOCTORAL THESIS AWARD

Tomislav Begusic
"Efficient ab initio semiclassical dynamics for linear and nonlinear electronic spectroscopy"
THESIS DIRECTOR
Prof. Jiri Vanicek

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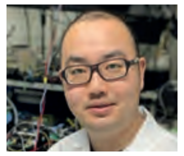
EPFL Thesis Awards

EPFL DOCTORATE AWARD 2021



Liu JunQiu (EDPH)
"Silicon Nitride Nonlinear Integrated Photonics"
THESIS DIRECTOR
Prof. T. J. Kippenberg

ZENO KARL SCHINDLER AWARD 2021

Jovana Milic (EDCH)
"Hybrid Supramolecular Materials for Renewable Energy Conversion in Photovoltaics"
THESIS DIRECTORS
Prof. Michael Grätzel

Bachelor and Master Students Prizes and Awards

MATHEMATICS

Jefferson Baudin
Prix Douchet for the best average in a Math Master cursus (5.88)
Riccardo Tenderini
EPFL highest Master's average, ex aequo (5.94)
Philémon Bordereau
Second best Bachelor's average (5.81)
Kevin Rizk
Third best Bachelor's average (5.79)
Julie Bannwart
Highest Propedeutics's average (5.98)

PHYSICS

Clément Firat
EPFL Prize for the best average in an EPFL Master cursus (5.92)
Alexandre Schiavini
Youth Prize (youngest Master graduate at EPFL at 21 years)
Emilie Hertig
IBM Prize
Diego Visani
Gilbert Hausmann Prize

CHEMISTRY AND CHEMICAL ENGINEERING

Damien Chen
Pelet Prize 2021 for the best average in an EPFL Bachelor cursus
Damien Chen and Louise Foltzer-de Cian
Prix d'excellence
Miyeon Chang
Prix Syngenta for best Master grade Chemistry
Ludovic Zaza
Prix Syngenta for best Master grade in Chemical Engineering)
Miyeon Chang
Prix BASF Monthey for best Master thesis in Chemistry
Nency Patricio Domingues
Prix BASF Monthey for best Master thesis in Chemical Engineering

NEWS

Nominations and Promotions 2021

Dr Lénaïc Chizat formerly Research Associate at Paris-Saclay University, France, was named as Tenure-Track Assistant Professor of Mathematics, starting from the 1st of September 2021.

Lénaïc Chizat's research covers the analysis, development and optimisation of algorithms, particularly those applied to machine learning. This highly competitive area presents one of the major challenges for applied mathematics over the coming years. Lénaïc Chizat and his research programme are at the cutting edge of this field of study. Thanks to his appointment, EPFL will also be able to offer new courses and strengthen connections and interchange between different areas of mathematics.

Professor Florian Richter, formerly Boas Assistant Professor at Northwestern University, Illinois, USA, was named as Tenure Track Assistant Professor of Mathematics in the School of Basic Sciences (SB), starting from the 1st of September.

Florian Richter's work focuses on ergodic theory and discrete dynamical systems. His findings have made a significant contribution to research. In the area of dynamical systems, for example, he has discovered unexpected links with other areas of mathematics, such as additive number theory. By appointing this distinguished researcher, EPFL is strengthening the connections between the various research areas within mathematics.

Dr Victor Gorbenko currently Research Fellow at Stanford University, USA, was named as Tenure-Track Assistant Professor of Physics, starting from the 1st of February 2022.

Victor Gorbenko's main domain of activity is Quantum Field Theory, with important implications to particle physics, cosmology and condensed matter physics. His research has already contributed to important scientific findings, in particular in the area quantum chromodynamics, where he characterized the dynamics of color flux tubes, and in the study of renormalization group flows, where he invented the notion of Complex Conformal Field Theory. This young, very talented physicist shows exceptional potential and has the necessary abilities to succeed at EPFL, where he will also foster interconnection among different areas of fundamental physics.

Dr Philippe Schwaller currently Postdoctoral Researcher at the University of Bern, was named as Tenure-Track Assistant Professor of Chemistry, starting from the 1st of February 2022.

Philippe Schwaller investigates how chemical processes can be simulated using artificial intelligence (AI). His research has a particular focus on the challenge of using artificial chemical intelligence to facilitate the discovery of new catalysts and organic materials. This talented researcher has invented important ways of applying AI methods. He belongs to a new generation of scientists with a very wide-ranging set of skills – in his case a combination of experimental research, computer science, materials science and chemistry.

Dr Georgios Moschidis currently Research Fellow at the University of California, USA, was named as Tenure-Track Assistant Professor of Mathematics, starting from the 1st of September 2022.

Georgios Moschidis' work relates to the general theory of relativity and his research has already achieved important scientific results in areas such as Friedmann equations and anti-de Sitter space. This brilliant mathematician, who excels in the area of analysis and the general theory of relativity, has achieved an international reputation at an early age. His presence will enhance EPFL's efforts in this field and is also likely to attract students from a variety of disciplines.

Dr Zoë Holmes, currently a post-doctoral student at Los Alamos National Laboratory, New Mexico, USA, as Tenure Track Assistant Professor of Physics, starting from the 1st of August 2022.

Zoë Holmes' research focuses on different areas of quantum computing. She has already made important contributions to quantum thermodynamics and fluctuation theory. Furthermore, she is the lead author of numerous academic articles, which not only demonstrate her originality but also show that she can turn her ideas into reality. This well-known researcher will solve pressing scientific problems and strenghten cooperation with other schools at EPFL, including the School of Computer Sciences, in order to develop quantum machine learning algorithms.

Professor Michaela Hirschmann, currently Assistant Professor at the University of Copenhagen, Denmark, as Tenure-Track Assistant Professor of Physics, starting from the 1st of March 2022.

Michaela Hirschmann's research investigates the cosmic development of black holes and galaxies, making it possible to model the formation of galaxies with great precision. She is one of the world's leading theoreticians in this field, and her findings are all the more important now that new terrestrial and space telescopes will be able to observe the first moments of the universe in the coming years. Through her appointment, the school is boosting synergies and partnerships at EPFL in the field of astrophysics and other areas.

Professor Vladimir Manucharyan, currently Associate Professor at the University of Maryland, USA, as Associate Professor of Physics, starting from the 1st of July 2022.

Quantum physics is the main focus of Vladimir Manucharyan's research. He is one of the chief architects of the development of a new type of qubit called the fluxonium qubit, as well as a pioneer in the application of superconductors in the field. The department is thus strengthened by the appointment of one of the leading researchers in the field of quantum science and technology. Among other activities, Vladimir Manucharyan will help solve major challenges in quantum physics and facilitate the development of quantum algorithms.

Nominations and Promotions 2021

Professor Andreas Läuchli, formerly Full Professor and Head of Institute at the University of Innsbruck, Austria, was named as Full Professor of Physics in the School of Basic Sciences (SB) and as Director of the Laboratory for Computational and Theoretical Physics at PSI, starting from the 1st of September 2021.

Andreas Läuchli is a specialist in strongly correlated systems in the physics of condensed matter and atomic gases. He is one of the few people who combine theoretical knowledge with digital expertise. This internationally renowned researcher will boost the range of courses offered by EPFL in one of the core areas of the Institute of Physics while also developing a research programme on condensed matter.

Prof. Zsolt Patakfalvi, currently Tenure-Track Assistant Professor at EPFL, has been promoted to Associate Professor of Mathematics.

Zsolt Patakfalvi's research focuses on algebraic geometry, complex numbers and the properties of geometric bodies, and he is a specialist in the minimal model program (MMP). He has already published numerous academic articles in renowned publications and has won several awards, including an ERC Starting Grant in 2020. This polyvalent researcher is regarded as one of the most promising mathematicians of his generation, in a highly competitive and flourishing field. At EPFL he is the head of the Chair of Algebraic Geometry.

Professor Jeremy Luterbacher, currently Tenure-Track Assistant Professor at EPFL, has been promoted as Associate Professor of Chemical Process Engineering in the School of Basic Sciences (SB)

Jeremy Luterbacher's work on biomass conversion technologies includes looking for an alternative to oil for manufacturing plastics and other common chemicals. He has won a number of prizes (including an ERC Starting Grant in 2017) for his outstanding results in the field of chemical engineering. This highly creative researcher is head of the Laboratory of Sustainable and Catalytic Processing, a field in which he is internationally regarded as a rising star.

Prof. Maria Colombo currently Tenure-Track Assistant Professor at EPFL, has been promoted to Full Professor of Mathematics.

Maria Colombo's research investigates mathematical analysis in combination with probability theory, computational mathematics, statistics and machine learning. In addition to her central role in research, her outstanding leadership and the various grants she has obtained, Maria Colombo also makes a valuable contribution to different areas of EPFL. She is therefore regarded as a pillar of the Mathematics Institute and School. By making this appointment, EPFL is retaining a visionary, world-class researcher whom other universities would be glad to recruit.

Three Professors named Emeritus in 2021

- Professor Majed Chergui, who directed the Laboratory of Ultrafast Spectroscopy at the Institute of Chemical Sciences and Engineering from 2003 to 2021.
- Professor Mikhail Shaposhnikov, who directed the Laboratory of Particle Physics and Cosmology at the Institute of Physics from 2003 to 2021.
- Professor Marco Grioni, who directed the SCI-SB-MG group at the Institute of Physics from 2005 to 2021.

Two Professors left the School of Basic Sciences in 2021

- Professor Marius Lemm, who directed the Chair of Analysis and Mathematical Physics at the Institute of Mathematics from 2020 to 2021.
- Professor Assyr Abdulle, who directed the Chair of Computational Mathematics and Numerical Analysis at the Institute of Mathematics since 2009 passed away on September 1st 2021, after courageously fighting illness for many years.

  Assyr will be remembered as an energetic, enthusiastic, and passionate colleague, always open to new ideas and engaged in promoting mathematics at EPFL. He played an essential role in creating and shaping a unified Institute of Mathematics at EPFL. Assyr was very much appreciated by students as a teacher and a mentor and will be missed throughout the faculty.

Anna Kiesenhofer wins cycling gold medal in Tokyo Olympics

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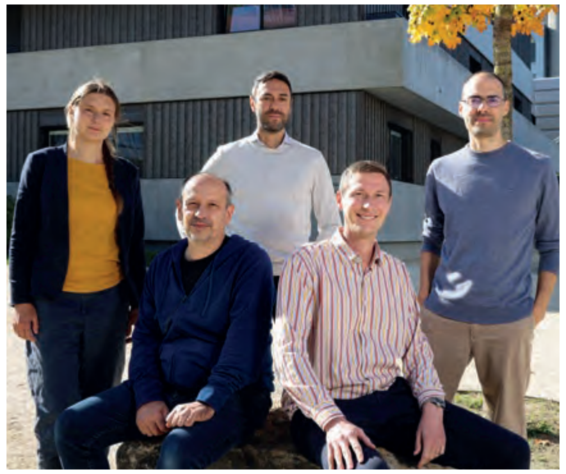
Anna Kiesenhofer, a post-doctoral fellow in Mathematics at EPFL's Faculty of Basic Sciences, won the road race gold medal at the Tokyo Olympic Games.

Anna Kiensenhofer won an incredible victory after a 40-kilometer solo breakaway at the Tokyo Olympics this Sunday. The Austrian athlete, who worked at the time as a scientist at EPFL's Faculty of Basic Sciences, won the gold medal in the road event for her first participation in the Olympic Games.

Anna Kiesenhofer had been a post-doctoral fellow in the Chair of Partial Differential Equations at EPFL's Institute of Mathematics since 2017. Martin Vetterli congratulated Anna for her achievement on the occasion of the EPFL Magistrale celebrated on October 2, 2021.

The new Bernoulli Center for Fundamental Studies broadens its scope



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EPFL's Bernoulli Center has now become the Bernoulli Center for Fundamental Studies, with a broader scope including theoretical computer science and theoretical physics. The Center's focus will also be on education, outreach and on fostering collaborations within the EPFL campus.

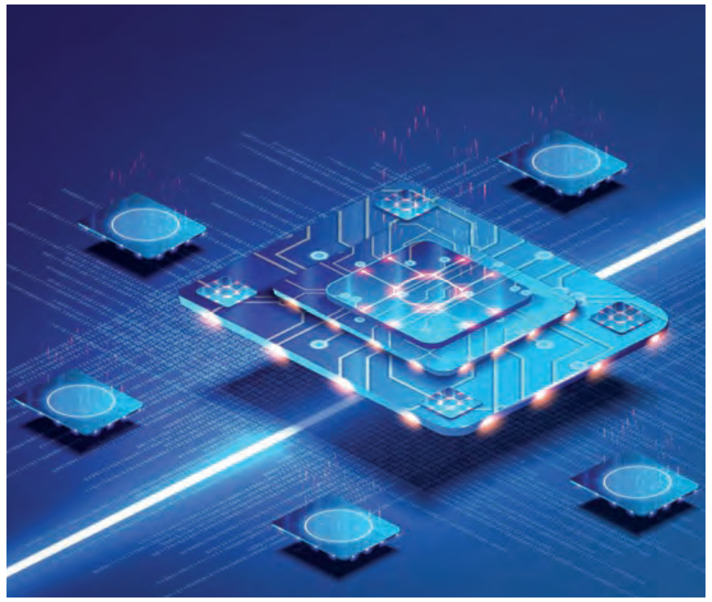
The new Bernoulli Center for Fundamental Studies opened its doors in September. Housed in the GA building on EPFL's Lausanne campus, the Center is headed by Prof. Emmanuel Abbé, holder of EPFL's Chair of Mathematical Data Science, and aims to foster excellence and promote research in the fundamental sciences. "The most important scientific discoveries can be traced back to breakthroughs in the fundamental sciences," says Prof. Abbé. "And these breakthroughs often lie at the crossroads of several different disciplines. That's why it's so important to nurture a synergistic ecosystem in the fundamental sciences right here on EPFL campus."

Until now, the Bernoulli Center supported research mainly in mathematics and related applications. But today, not only does it have a broader remit encompassing computer science and theoretical physics, it also has an expanded management team with professors from several EPFL schools and institutes. In addition to the director, the Center is now led by Maryna Viazovska and Philippe Michel (both from the Institute of Mathematics in EPFL's School of Basic Sciences), Ola Svensson (from the Institute of Computer and Communication Sciences in EPFL's School of Computer and Communication Sciences), and João Penedones (from the Institute of Physics in EPFL's School of Basic Sciences).

Prof. Abbé also stresses the importance of diversity. "We need to do more to encourage under-represented groups, like women, to pursue careers in the fundamental sciences. To that end, we will work closely with EPFL's Associate Vice Presidency for Student Affairs and Outreach," he says.

"We wanted to create a place on campus where fundamental scientists can meet and forge ties across academic levels and disciplines, in an effort to come up with innovative ideas. Some of the most revolutionary scientific ideas came about in these kinds of environments. For example, connections between number theory and nuclear physics emerged at a tea time at Princeton's Institute for Advanced Study, or the elliptic-curve cryptography born out of discussions from Bell Labs visitors," says Prof. Abbé. "The new Center has already made waves on campus. So far, over 50 scientists have joined us from different EPFL schools. There's clearly an interest in creating this kind of forum. The Center will also be an opportunity for EPFL to play a leading role in the fundamental sciences in Europe, reinforce joint initiatives and enhance campus life in general."

EPFL launches new Center for Quantum Science and Engineering



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EPFL's new Center for Quantum Science and Engineering (QSE Center) will establish and promote programs for cross-disciplinary research, education and innovation in the fields of quantum science and engineering.

"Developing quantum technology is an incredible venture that puts us face to face with unprecedented scientific and engineering challenges. Meeting these challenges requires a concerted effort from all technical disciplines – physics, mathematics, chemistry, computer science and engineering – more so than for any previous kind of technological development," says Prof. Vincenzo Savona, the head of EPFL's Laboratory of Theoretical Physics of Nanosystems. "EPFL has a long history of excellence and leadership in these various disciplines and occupies a unique strategic position in quantum science and engineering, both in Switzerland and worldwide."

Prof. Savona, whose expertise spans quantum optics, open quantum systems and quantum information, will be the QSE Center's first director. He will be assisted by a management team composed of professors from EPFL's School of Basic Sciences, School of Engineering and School of Computer and Communication Sciences.

"Thanks to recent progress in science and engineering, we can now use phenomena described by the laws of quantum mechanics to develop revolutionary new technology for computing, communications and measurement," says Prof. Savona. "This will lead to major advancements in several fields and bring significant benefits to society."

By setting up the QSE Center, EPFL aims to coordinate efforts across the board to develop and implement quantum technology in applications that span all disciplines of science and engineering.

What sets the Center apart is its cross-disciplinary approach. Prof. Savona explains: "Quantum technology is highly complex and requires pulling together methods from many scientific fields. The unique feature and key strength of the QSE Center is our ability to bring together experts from different fields – already represented here at EPFL – to apply their knowledge to quantum science and engineering."

Research at the QSE Center will focus on two main areas. The first is quantum computing. "Our goal here will be to develop and implement quantum algorithms [see box] as well as the computer programs needed to use them," says Prof. Savona. "Developing, implementing and integrating these tools will eventually lead to a quantum advantage [see box] in all applications requiring a high level of computing power. These applications could include simulating biological molecules to predict disease and develop new drugs, for example, or running simulations of weather and climate change over extended time horizons. Quantum advantage would also benefit much of the research done here at EPFL, such as in physics, chemistry, materials science, engineering, life science, computer science and data science."

The second research area will involve studying integrated, hybrid and scalable systems using EPFL's advanced nano-fabrication facilities. This will pave the way to technological advancements in quantum hardware, quantum sensing and quantum communications.

The QSE Center will draw on the wide range of skills in quantum science and engineering already available in Switzerland. For instance, it intends to work closely with the University of Geneva through joint R&D projects and jointly hold classes for Master's and PhD students.

Also with regards to education, the Center will introduce a new Master's program in quantum science and engineering at EPFL. This will be a unique, cross-disciplinary program with classes in theoretical physics, computer science and engineering. "We will also offer excellence fellowships for Master's students in order to attract talented young minds from Switzerland and abroad," says Prof. Savona. "This will enable us to lay the foundation for the next generation of quantum scientists and engineers."

In addition, the QSE Center will promote research and innovation by holding events such as workshops, conferences, and programs on specific topics, bringing selected experts to EPFL for long-term stays. These events will foster interaction and collaboration and stimulate creative thinking and progress.

"Current and future breakthroughs in quantum technology mark major turning points in the history of humanity," says Prof. Savona. "We're in a pioneering era that's similar to the emergence of computers in the 1950s and the advent of the internet in the 1990s. This is a one-of-a-kind opportunity to contribute to the progress and advancement of our society."

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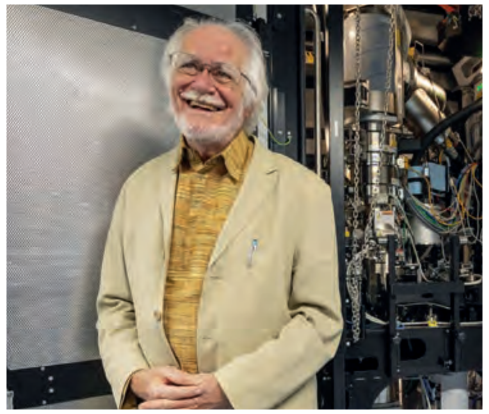
At the Dubochet Center for imaging, atoms are made visible



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Fully operational for two weeks, the Dubochet Center for Imaging was presented to the press on November 22. The DCI houses the world's most advanced cryo-electron microscopes, which promises considerable advances in biomedical research thanks to the precision of the images that these microscopes can obtain.

"Imagine how an old man might feel when a Center like this is named after him..." The emotion could be heard, yesterday, in the voice of Jacques Dubochet. The 2017 Chemistry Nobel Prize laureate was participating in the official launch of the Dubochet Center for Imaging (DCI), a joint platform of EPFL, the University of Lausanne and the University of Geneva.

The Center has more than enough to put the Lake Geneva region on the world map of advanced imaging facilities. "We have here the best model of an electron microscope for life sciences that money can buy. And we have two of it," said Henning Stahlberg, director of the DCI.

These impressive machines, priced in the millions of francs, make use of the discovery that earned Dubochet and his colleagues the prestigious award: cryo-electron microscopy, or cryo-EM for short. "We have developed a technique by which the samples to be studied are instantly vitrified, instead of being frozen," said Dubochet. This speed avoids the formation of ice crystals, which would be harmful to the molecules to be observed. "The properties of water in this state are still mysterious," he added. Once stabilized in this way, the samples can better withstand the flow of electrons that pass through them and are "photographed" in their natural state.

The DCI has two of the most powerful life sciences electron microscopes in the world and will be available to all researchers in the region. In addition, there are smaller cryo-EM instruments to optimize samples, and a prototype cryo-EM instrument will be constructed that will be dedicated to the development of new technologies to further improve image quality.

The most powerful microscopes are temporarily based between the UNIL and EPFL campuses, in the Cubotron building. Two other machines are installed in Geneva. "There are many synergies between the two sites and permanent collaborations," explains Robbie Loewith, Deputy Director of the DCI and head of the Geneva office. "The pooling of all these resources allows us to obtain results with unparalleled speed and precision."

As a clear example, the DCI has determined the complete structure of a ferritin molecule – responsible for the transport of iron in the blood – with a precision of 1.4 Å: a degree of detail that makes it possible to observe each atom individually and its connections with neighboring atoms. The same is true for the SARS-CoV-2 Spike protein, which can now be "walked around" atom by atom.

"This is extremely valuable for biomedical research," says Henning Stahlberg. Because we can understand how biological proteins interact with each other, we can also develop molecules that can block or promote these interactions – for example, in the case of cancer treatments using chemotherapy.

In other words, thanks to this new center, cryo-electron microscopy is now reaching a degree of maturity that will allow considerable scientific advances and for which Western Switzerland will be at the forefront.

Pierre-Alain Ruffieux: An SB alumnus now CEO of Lonza

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Pierre-Alain Ruffieux received his master's degree in Chemical Engineering and Biotechnology from EPFL in 1993, and continued to with doctorate in 1998. For his PhD, he worked in the lab of Professor Urs von Stockar at ISIC, his thesis advisor. "He was a real mentor for me," he said in an interview with EPFL. "Not only in terms of scientific expertise, but also in how he taught me the value of intellectual honesty and mutual support."

After graduating, Ruffieux immediately moved into industry, marking the start of an outstanding career that now spans more than two decades and four Big Pharma companies. In 1998, he joined Serono in its technical development endeavors. In 2003, he moved to the nascent Novartis, where he spent over a decade, until 2015, when he moved to Roche as Head of Quality and Compliance.

Six years later, in November 2021, Ruffieux accepted the position of CEO of Lonza Group, the Basel-headquartered multinational. Lonza specializes in outsourcing for the biopharmaceutical industry, offering flexible, state-of-the-art, high-capacity production facilities to both industry giants and smaller companies. During the pandemic, Lonza supported Moderna by producing its vaccine against COVID-19. This effort has also involved a number of PhDs and postdoctoral scientists from EPFL.

On October 2, 2021, Ruffieux was presented with an Alumni Award during EPFL's Magistrale, at the SwissTech Convention Center. The award celebrated his exceptional career, rising from his student days to the peaks of one of Switzerland's top-performing companies.

Ruffieux believes that studying at EPFL set him on the right path for his career in industry, through his experiences with different associations. "EPFL taught me about facing challenges," he says. "With time, I have also come to understand how fortunate I was to be able to study here – something that I didn't fully grasp when I was a student. The resources available at EPFL, from the professors to the campus and facilities, are simply extraordinary."

ISIC

Christian Heinis wins ERC Advanced Grant

European Research Council
Established by the European Commission

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Professor Christian Heinis at EPFL's School of Basic Sciences has been awarded a European Research Council (ERC) Advanced Grant for a project that will merge biological and chemical compound libraries to target so-called "undruggable" proteins.

The ERC Advanced Grants are given each year to established, leading principal investigators to fund long-term funding for "ground-breaking, high-risk" research projects in three domains: Life Sciences, Physical Sciences and Engineering, and Social Sciences and Humanities.

The ERC has announced the 209 winners of the 2020 Advanced Grant competition, awarded a total of €507 million. Among them is Professor Christian Heinis at the EPFL School of Basic Sciences (Institute of Chemical Sciences and Engineering). Heinis' winning project, TARGET, aims at "developing and applying a novel method for targeting so-called 'undruggable' proteins by tapping into a new chemical space, generated by 'merging' biological and chemical compound libraries."

"I am very grateful for the opportunity to try this bold plan and hope that my laboratory can contribute with good results to addressing currently unsolved medical challenges," says Professor Heinis.

IPHYS

Four SNSF Ambizione grants awarded in Physics

Swiss National Science Foundation

Aris Tritsis LASTRO | Elena Graverini LPHE-LS | Oliver Müller LASTRO | Johann Riemensberger LPQM

The highly selective Ambizione program is aimed at young researchers who wish to conduct, manage and lead an independent project at a Swiss higher education institution. The awarded projects are funded for a maximum of four years. This year, SNSF has awarded 34 grants in the category "Science Technology Engineering & Mathematics". Four of these have gone to physicists who will perform their project at IPHYS:

Elena Graverini, presently a postdoc at the LPHE-LS, will carry out her project "From beauty to strangeness: a flavour approach to probing new interactions". She proposes a novel approach to challenge the Standard Model (SM) of particle physics, using quark-level decays to probe the SM assumption that lepton interactions are flavour-independent. This test will be performed for the first time at a hadron collider B-factory, the LHCb experiment. She will also develop a new idea to perform real-time neutrino and hidden sector physics at a new experiment, to be built and operated at the Large Hadron Collider: SND@LHC.

Johann Riemensberger, presently a postdoc at LPQM, will perform his project "Ultra-low loss photonic integrated circuits for advanced applications in telecommunication and sensing". He will be using ultra-low loss Si3N4 photonic waveguide technologies that have recently been developed at EPFL. The goals are to demonstrate novel functionality such as continuous wave optical parametric amplification and devices for applications in parallel coherent 3D imaging with high pixel measurement rates and the next generation of optical information technologies with increased optical bandwidth.

Aris Tritsis, currently a post-doctoral researcher at the Research School of Astronomy & Astrophysics of the Australian National University, will join the LASTRO to perform his project "HOMERIC-Halo's magnetic field as evident from striated interstellar clouds". His main challenge will be to construct the first-ever 3D atlas of the strength and orientation of the plane-of-sky component of the Galactic magnetic field using a novel technique, suitable for tomographic measurements. He will also try to unveil the role of the magnetic field in the formation and evolution of molecular clouds and cores through 3D nonideal magnetohydrodynamic simulations.

Oliver Müller, currently a post-doc at LASTRO, will perform his project "Probing the standard model of cosmology with dwarf galaxies". He will extend observations of the abundance and distribution of dwarf galaxies to over 500 other nearby galaxy groups to understand the formation and evolution of galaxies.

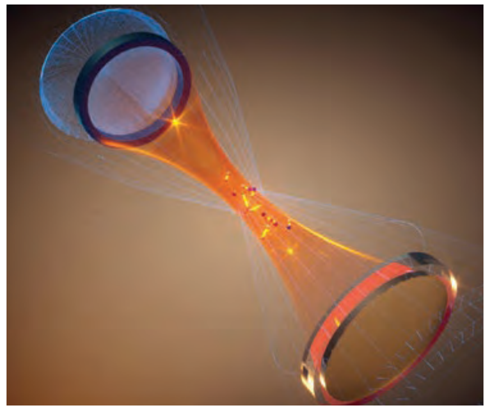
EPFL

RESEARCH HIGHLIGHTS

IPHYS ISIC MATH

IPHYS

Light-matter interactions propel quantum technologies forward



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Physicists at EPFL have found a way to get photons to interact with pairs of atoms for the first time. The breakthrough is important for the field of cavity quantum electrodynamics (QED), a cutting-edge field leading the way to quantum technologies.

There is no doubt that we are moving steadily toward an era of technologies based on quantum physics. But to get there, we first have to master the ability to make light interact with matter – or more technically, photons with atoms.

This has already been achieved to some degree, giving us the cutting-edge field of cavity quantum electrodynamics (QED), which is already used in quantum networks and quantum information processing. Nonetheless, there are still a long way to go. Current light-matter interactions are limited to individual atoms, which limits our ability to study them in the sort of complex systems involved in quantum-based technologies.

In a paper published in Nature, researchers from the group of Jean-Philippe Brantut at EPFL's School of Basic Sciences have found a way to get photons to 'mix' with pairs of atoms at ultra-low temperatures.

The researchers used what is known as a Fermi gas, a state of matter made of atoms that resembles that of electrons in materials. "In the absence of photons, the gas can be prepared in a state where atoms interact very strongly with each other, forming loosely bound pairs," explains Brantut. "As light is sent onto the gas, some of these pairs can be turned into chemically bound molecules by absorbing with photons."

A key concept in this new effect is that that it happens "coherently", which means that photon can be absorbed to turn a pair of atoms into a molecule, then emitted back, then reabsorbed multiple times. "This implies the pair-photon system forms a new type of 'particle' – technically an excitation – which we call 'pair-polariton'," says Brantut. "This is made possible in our system, where photons are confined in an 'optical cavity' – a closed box that forces them to interact strongly with the atoms."

The hybrid pair-polaritons take on some of the properties of photons, meaning that they can be measured with optical methods. They also take on some of the properties of the Fermi gas, like the number of atom pairs it had originally before the incoming photons.

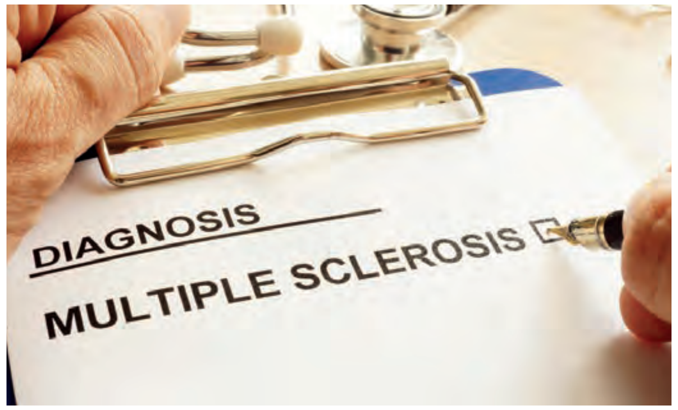
"Some of the very intricate properties of the gas are translated onto optical properties, which can be measured in a direct way, and even without perturbing the system," says Brantut. "A future application would be in quantum chemistry, since we demonstrate that some chemical reactions can be coherently produced using single photons."

REFERENCES

Hideki Konishi, Kevin Roux, Victor Helson, Jean-Philippe Brantut.
"*Universal pair-polaritons in a strongly interacting Fermi gas*".
Nature 25 August 2021.
https://dx.doi.org/10.1038/s41586-021-03731-9

ISIC

A tool to interrogate a new class of drugs



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Reactive electrophilic drugs like Tecfidera, approved for the treatment of relapsing multiple sclerosis, show a lot of potential but are also mystery. Their effects are notoriously difficult to study, which hampers progress testing and approving them. EPFL scientists have now used an innovative chemical method to uncover the biological mechanisms of Tecfidera, providing a powerful tool for exploring other reactive electrophilic drugs.

In 2014, the European Medicines Agency approved the multiple sclerosis drug Tecfidera. The active ingredient of Tecfidera is dimethyl fumarate, a compound that is thought to modulate the immune system, thus acting as an anti-inflammatory that alleviates the symptoms of multiple sclerosis.

But there was a detail of Tecfidera's approval that might have been a little less appreciated: it brought into the market a member of the rel-atively new – and still largely unexplored – class of drugs known as reactive electrophiles.

Reactive electrophilic compounds like dimethyl fumarate are molecules that "seek" to bond with atoms or other molecules that have an availa-ble electron pair. Adding an electrophilic unit to certain drugs significantly increases pharmacological efficacy, which has generated a lot of research activity into this area.

The problem, however, is that we don't know exactly how most reactive electrophilic drugs work. Reactive electrophiles seem to be very "promiscuous", bonding with multiple targets, which can result in unexpected side-effects, drug toxicity, and, in extreme cases, death.

A team of scientists at EPFL led by Professor Yimon Aye, have used a technique called "targetable reactive electrophiles and oxidants", or T-REX for short. The T-REX method releases a specific electrophile to a target protein, and the effects be observed in space and time, and in live cells.

The researchers adapted T-REX to be compatible with zebrafish – a technique they named Z-REX– and used it to systematically investigate the interactions of the electrophilic dimethyl fumarate in Tecfidera, and how those interactions produce the immunomodulating effects of Tecfidera.

The scientists targeted the protein Keap-1, a cancer and metastasis suppressor that could be a target for dimethyl fumarate. Targeting Keap-1 with Z-REX showed that some electrophiles trigger a signaling pathway that results in the apoptosis of neutrophils and macrophages.

That pathway also involves some novel "protein players" that had not been considered before. Removing them abolished the anti-inflammatory effects of Tecfidera, which are what make it a treatment for multiple sclerosis.

The work demonstrates that Z-REX and the REX technologies are effective tools for investigating the interactions of electrophilic compounds in living organisms.

REFERENCES

Jesse R. Poganik, Kuan-Ting Huang, Saba Parvez, Yi Zhao, Sruthi Raja, Marcus J. C. Long, Yimon Aye.
"*Wdr1 and Cofilin are Necessary Mediators of Immune-Cell-Specific Apoptosis Triggered by Tecfidera*".
Nature Communications 30 September 2021.
https://dx.doi.org/10.1038/s41467-021-25466-x

IPHYS

How mitochondria make the cut

With the help of their custom-built super-resolution microscope, EPFL biophysicists have discovered where and why mitochondria divide, putting to rest controversy about the underlying molecular machinery of mitochondrial fission. Mitochondria either split in half or cut off their ends to self-regulate. The results are published in Nature.

Mitochondria either split in half to multiply within the cell, or cut off their ends to get rid of damaged material. That's the take-away message from EPFL biophysicists in their latest research investigating mitochondrial fission. It's a major departure from the classical textbook explanation of the life cycle of this well-known organelle, the powerhouse of the cell. The results are published in Nature.

"Until this study, it was poorly understood how mitochondria decide where and when to divide," says EPFL biophysicist Suliana Manley and senior author of the study.

"For me, the big question was how do mitochondria know when to proliferate or when to degrade? How does the cell regulate these two opposing functions of mitochondrial fission?" explains EPFL postdoc Tatjana Kleele and first author of the study.

Four years of research and 2000 mitochondria later, Kleele and Manley found that the splitting location of mitochondria is not at all random.

Until now, the dynamics of mitochondrial fission sites had never been measured with high precision and in large numbers. But thanks to their own super resolution microscope (iSIM), the EPFL biophysicists were able to observe many individual mitochondria, in living cancer cell lines and mouse cardiomyocytes, as they split into smaller segments.

"The size of a mitochondrion is just around the diffraction limit for light microscopy, making it impossible to study mitochondrial physiology and shape changes at the sub-organelle level. Using a custom built super-resolution microscope, which allows fast imaging with a two-fold increase in resolution, we were able to analyse a large number of mitochondrial divisions," explains Manley.

From these observations, they could both quantify the position of fission with high precision, and also detect signs of dysfunction in small parts of the organelle with the help of fluorescent biosensors. A low pH within a mitochondrion is a sign that the proton pump necessary for making ATP, energy for the cell, is no longer working optimally. Calcium concentrations provided information about the mitochondria structures.

They observed two types of mitochondrial division: midzone and peripheral. They discovered that midzone division of mitochondria has all of the textbook molecular machinery of fission. In contrast, peripheral division is associated with mitochondrial stress and dysfunction, and the smaller daughter mitochondrion is subsequently degraded.

Next, the biophysicists wanted to know if they could observe the same behavior in heart cells from mice. In collaboration with the laboratory of Thierry Pedrazzini (CHUV), they discovered that mouse heart muscle cells (cardiomyocytes) can independently regulate those two types of fissions, because they use different proteins and machineries.

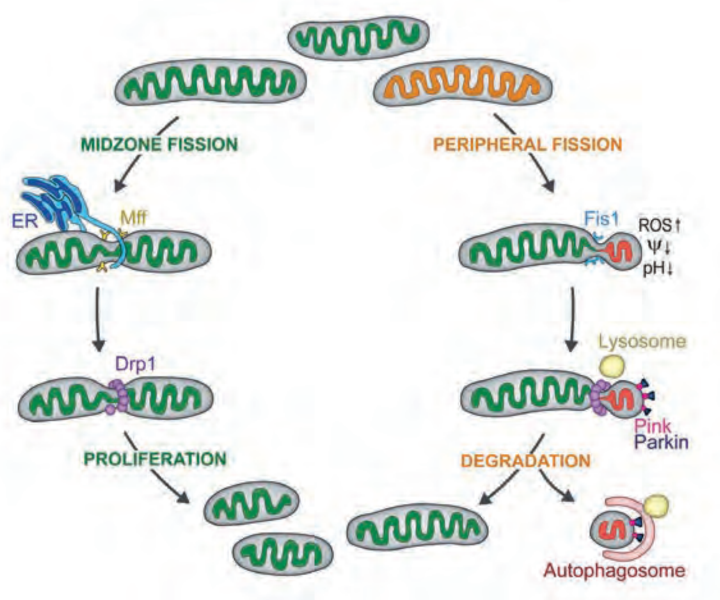
When the scientists stimulated the cardiomyocytes to strongly contract with pharmaceuticals, they found that peripheral division rates increase. In other words, when the cardiomyocytes were over-stimulated or stressed, the mitochondria produced tremendous amounts of energy in order for the heart cells to beat quickly. A by-product of this energy production are free radicals, aka reactive oxygen species, known to lead to dysfunction within the cell, including dysfunction of the mitochondria. The peripheral divisions therefore increase to get rid of damaged mitochondria due to the stress.

When the scientists stimulated the cardiomyocytes to proliferate, they indeed noticed more midzone divisions.

"The behavior of mitochondrial fission that we've observed in the lab is very likely relevant for all mammalian cells," says Kleele.

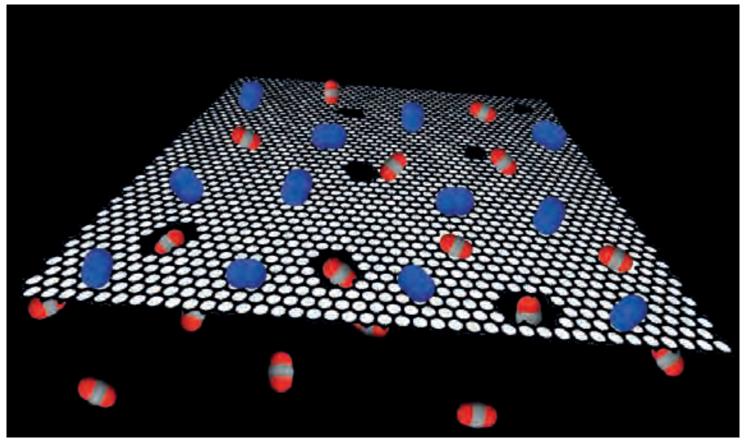
For Manley, this regulation of mitochondrial fission is important for understanding human diseases, such as neurodegeneration and cardiovascular dysfunction, which are both associated with overactive mitochondrial fission. "Therapeutic approaches are rare, since globally targeting mitochondrial fission has many side effects. By identifying proteins which are specifically involved in either biogenesis or degradation, we can now provide more precise targets for pharmacological approaches," concludes Manley.

REFERENCES
Tatjana Kleele , Timo Rey, Julius Winter, Sofia Zaganelli, Dora Mahecic, Hélène Perreten Lambert, Francesco Paolo Ruberto, Mohamed Nemir, Timothy Wai, Thierry Pedrazzini, Suliana Manley.
"*Distinct fission signatures predict mitochondrial degradation or biogenesis*".
Nature 05 May 2021.
https://dx.doi.org/10.1038/s41586-021-03510-6



ISIC

Graphene filter makes carbon capture more efficient and cheaper



An illustration of the graphene carbon dioxide filter.
© KV Agrawal, EPFL

Chemical engineers at EPFL have developed a graphene filter for carbon capture that surpasses the efficiency of commercial capture technologies, and can reduce the cost carbon capture down to $30 per ton of carbon dioxide.

One of the main culprits of global warming is the vast amount of carbon dioxide pumped out into the atmosphere mostly from burning fossil fuels and the production of steel and cement. In response, scientists have been trying out a process that can sequester waste carbon dioxide, transporting it into a storage site, and then depositing it at a place where it cannot enter the atmosphere.

The problem is that capturing carbon from power plants and industrial emissions isn't very cost-effective. The main reason is that waste carbon dioxide isn't emitted pure, but is mixed with nitrogen and other gases, and extracting it from industrial emissions requires extra energy consumption – meaning a pricier bill.

Scientists have been trying to develop an energy-efficient carbon dioxide-filter. Referred to as a "membrane", this technology can extract carbon dioxide out of the gas mix, which can then be either stored or converted into useful chemicals. "However, the performance of current carbon dioxide filters has been limited by the fundamental properties of currently available materials," explains Professor Kumar Varoon Agrawal at EPFL's School of Basic Sciences (EPFL Valais Wallis).

Now, Agrawal has led a team of chemical engineers to develop the world's thinnest filter from graphene, the world-famous "wonder material" that won the Physics Nobel in 2010. But the graphene filter isn't just the thinnest in the world, it can also separate carbon dioxide from a mix of gases such as those coming out of industrial emissions and do so with an efficiency and speed that surpasses most current filters. The work is published in Science Advances.

"Our approach was simple," says Agrawal. "We made carbon dioxide-sized holes in graphene, which allowed carbon dioxide to flow through while blocking other gases such as nitrogen, which are larger than carbon dioxide." The result is a record-high carbon dioxide-capture performance.

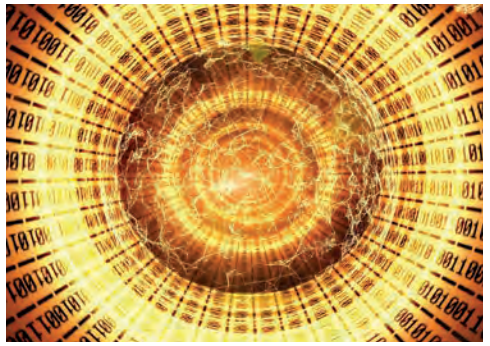
For comparison, current filters are required to exceed 1000 gas permeation units (GPUs), while their carbon-capturing specificity, referred to as their "carbon dioxide/nitrogen separation factor" must be above 20. The membranes that the EPFL scientists developed show more than ten-fold higher carbon dioxide permeance at 11,800 GPUs, while their separation factor stands at 22.5.

"We estimate that this technology will drop the cost of carbon capture close to $30 per ton of carbon dioxide, in contrast to commercial processes where the cost is two-to-four time higher," says Agrawal. His team is now working on scaling up the process by developing a pilot plant demonstrator to capture 10 kg carbon dioxide per day, in a project funded by the Swiss government and Swiss industry.

REFERENCES
S. Huang, S. Li, L. F. Villalobos, M. Dakhchoune, M. Micari, D. J. Babu, M. T. Vahdat, M. Mensi, E. Oveisi, K. V. Agrawal.
"*Millisecond lattice gasification for high-density carbon dioxide and O2-sieving nanopores in single-layer graphene*".
Science Advances 2021, 7, eabf0116, 24 February 2021.
https://dx.doi.org/10.1126/sciadv.abf0116

IPHYS

Running quantum software on a classical computer



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Two physicists, from EPFL and Columbia University, have introduced an approach for simulating the quantum approximate optimization algorithm using a traditional computer. Instead of running the algorithm on advanced quantum processors, the new approach uses a classical machine-learning algorithm that closely mimics the behavior of near-term quantum computers.

EPFL professor Giuseppe Carleo and Matija Medvidović, a graduate student at Columbia University and at the Flatiron Institute in New York, have found a way to execute a complex quantum computing algorithm on tra-ditional computers instead of quantum ones.

The specific "quantum software" they are considering is known as Quantum Approximate Optimization Algorithm (QAOA) and is used to solve classical optimization problems in mathematics; it's essentially a way of picking the best solution to a problem out of a set of possible solutions.

Ultimately, QAOA is meant to help us on the way to the famed "quantum speedup", the predicted boost in processing speed that we can achieve with quantum computers instead of conventional ones. Understandably, QAOA has a number of proponents, including Google.

"But the barrier of "quantum speedup" is all but rigid and it is being continuously reshaped by new research, also thanks to the progress in the development of more efficient classical algorithms," says Carleo.

Carleo and Medvidović address a key open question in the field: can algorithms running on current and near-term quantum computers offer a significant advantage over classical algorithms for tasks of practical interest? "If we are to answer that question, we first need to understand the limits of classical computing in simulating quantum systems," says Carleo. This is especially important since the current generation of quantum processors operate in a regime where they make errors when running quantum "software", and can therefore only run algorithms of limited complexity.

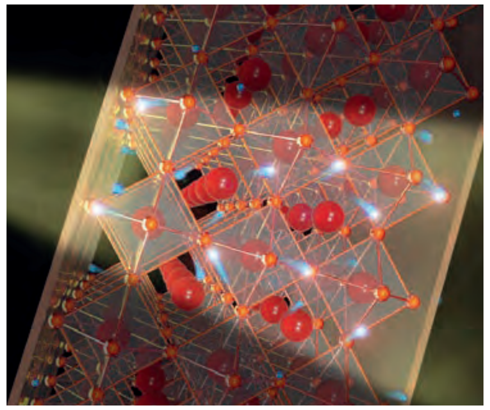
Using conventional computers, the two researchers developed a method that can approximately simulate the behavior of a special class of algorithms known as variational quantum algorithms, which are ways of working out the lowest energy state, or "ground state" of a quantum system. QAOA is one important ex-ample of such family of quantum algorithms, that researchers believe are among the most promising candidates for "quantum advan-tage" in near-term quantum computers.

The approach is based on the idea that modern machine-learning tools, e.g. the ones used in learning complex games like Go, can also be used to learn and emulate the inner workings of a quantum computer. The key tool for these sim-ulations are Neural Network Quantum States, an artificial neural network that Carleo developed in 2016 with Matthias Troyer, and that was now used for the first time to simulate QAOA. The results are considered the province of quantum computing, and set a new benchmark for the future development of quantum hardware.

REFERENCES
Medvidović, M., Carleo, G.
"*Classical variational simulation of the Quantum Approximate Optimization Algorithm*".
npj Quantum Inf 7, 101 (2021).
https://dx.doi.org/10.1038/s41534-021-00440-z

ISIC

3D chemistry boosts perovskite efficiency to 23.9%



Highly luminescent and stable alpha-FAPbI3 perovskite via HCOO- anion engineering. © Jin Young Kim (UNIST)

An international collaboration led by EPFL chemical engineers has overcome a problem in the manufacturing of perovskites that reduces their efficiency as solar panels. The approach produced perovskite solar panels with an efficiency of 23.9% and operational stability longer than 1000 hours.

Perovskites are hybrid compounds made from metal halides and organic constituents, and show great potential in a range of applications, e.g. LED lights, lasers, and photodetectors. However, their major contribution is in solar cells, where they are poised to overtake the market and replace their silicon counterparts.

Among the leading candidates for highly efficient and stable solar cells are lead iodide perovskites, which show excellent light-harvesting capabilities. However, their efficiency depends greatly on their manufacturing, and a key factor is removing defects from their light-harvesting surface.

The way this is typically done is with a method called "passivation", which coats the surface of perovskite films with chemicals (alkylammonium halides) to make them more resistant and stable. The process adds a two-dimensional perovskite layer on top of the primary perovskite light absorber, which improves the stability of the device.

The problem is that passivation actually backfires by forming so-called "in-plane" perovskite layers that don't "move" electrical charge as well, especially under heat. This is an obvious disadvantage for scaling up and commercializing potential solar panels.

In a new study, scientists led by Mohammad Nazeeruddin at EPFL's School of Basic Sciences, have found a way to solve the problem by treating them with different isomers of an iodide used to make perovskites. In chemistry, isomers are compounds that have the same molecular formulas but their atoms are arranged differently in three-dimensional space.

The scientists studied the minimum energy required to form two-dimensional perovskites from different isomers of the iodide PDEAI2 (phenylenediethylammonium). The isomers were designed for what the researchers call "tailored defect passivation", meaning that their passivation effect on perovskites was very well characterized in advance.

The approach turned out to be very effective in staving off the negative effects of passivation on perovskite efficiency. Specifically, the most effective PDEAI2 isomer was also the most "sterically hindered", a term that refers to a slowing of chemical reactivity simply because of the compound's molecular bulk. In fact, steric hindrance is often used to prevent or minimize unwanted reactions.

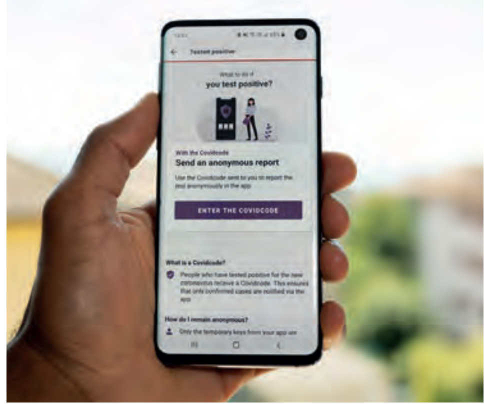
The perovskite solar cells produced with this method showed an efficiency of 23.9% with operational stability beyond 1000 hours. The work also achieved a record efficiency of 21.4% for perovskite modules with an active area of 26 cm^2.

REFERENCES

Cheng Liu, Yi Yang, Kasparas Rakstys, Arup Mahata, Marius Franckevicius, Edoardo Mosconi, Raminta Skackauskaite, Bin Ding, Keith G. Brooks, Onovbaramwen Jennifer Usiobo, Jean-Nicolas Audinot, Hiroyuki Kanda, Simonas Driukas, Gabriele Kavaliauskaite, Vidmantas Gulbinas, Marc Dessimoz, Vytautas Getautis, Filippo De Angelis, Yong Ding, Songyuan Dai, Paul J. Dyson, Mohammad Khaja Nazeeruddin. "*Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules*". Nature Communications 12, 6394 (04 November 2021). https://dx.doi.org/10.1038/s41467-021-26754-2

IPHYS

Improving contact-tracing apps in the COVID-19 era



© Jamani Caillet (EPFL)

An international collaboration with EPFL has developed a method to improve the performance of COVID-19 contact-tracing apps by taking into account a user's recent contacts, risk levels and shared information about tests and symptoms.

Contact-tracing apps like SwissCovid have enormous potential to mitigate the spread of the COVID-19 pandemic. Users allow the apps to track their contact with each other and estimate the chances that they might have come into contact with someone infected with the SARS-CoV-2 coronavirus. If they have, the app issues a notification.

Understandably, contact-tracing technology has raised a lot of ethical and privacy questions, all of which are weighed against the need to safeguard public health. Nonetheless, there has been comparably less effort in optimizing the performance and accuracy of contact-tracing apps, despite their great potential in addressing the pandemic.

Now, a collaboration of scientists has developed a statistical method that can improve the performance of contact-tracing apps by taking into account a user's recent contacts, risk levels and shared information about tests and symptoms. Published in PNAS, the work was carried out by scientists at EPFL, Italy, and France.

The scientists used Bayesian statistics, which calculate the probability of events. Here, they used this approach to estimate the risk that an individual is infected, based on their intrinsic degree of risk, the list of their recent contacts and the estimated risk level of those contacts.

"We wanted to quantify what epidemiological gain we could have if users who were recently in contact could also exchange messages of information," says Professor Lenka Zdeborová at EPFL's School of Basic Sciences and School of Computer and Communication Sciences, one of the study's main authors. "By just adding simple message-passing, we could estimate the risk of contracting COVID-19 with much higher accuracy than simple contact tracing."

The scientists' mathematical approach quickly transformed into fully distributed algorithms that work just off communication between individuals who have recently been in contact. The communication can be completely encrypted and anonymous so that it can potentially comply with future privacy regulations.

Testing out their "probabilistic risk" method, the scientists found that it is an efficient way to mitigate epidemics like COVID-19. Of course, the approach works best within a window of the epidemic, typically after the manual tracing of all contacts of infected people becomes practically impossible but before the fraction of infected people reaches the scale where a lock-down becomes unavoidable.

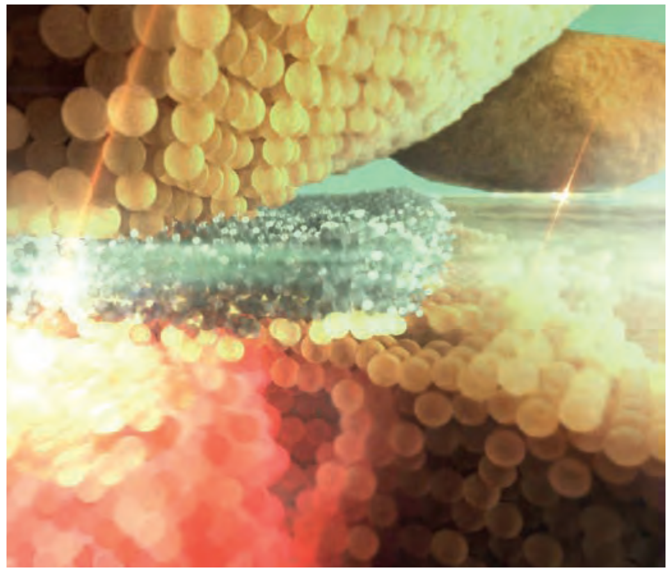
But as this kind of probabilistic risk estimation can enhance the performance of contact-tracing technology enough to make a real difference in the spread of an epidemic – or pandemic – the authors recommend, based on their data, that developers should consider implementing it in their apps.

REFERENCES

Antoine Baker, Indaco Biazzo, Alfredo Braunstein, Giovanni Catania, Luca Dall'Asta, Alessandro Ingrosso, Florent Krzakala, Fabio Mazza, Marc Mézard, Anna Paola Muntoni, Maria Refinetti, Stefano Sarao Mannelli, Lenka Zdeborová. "*Epidemic mitigation by statistical inference from contact tracing data*". PNAS 10 August 2021. https://dx.doi.org/10.1073/pnas.2106548118

IPHYS

Green light on gold atoms



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Scientists at EPFL discover that laser-driven rearrangement of just a few gold atoms inside nanoscale antennas can be observed by the naked eye.

Because individual atoms or molecules are 100 to 1000 times smaller than the wavelength of visible light, it is notoriously difficult to collect information about their dynamics, especially when they are embedded within larger structures.

In an effort to circumvent this limitation, researchers are engineering metallic nano-antennas that concentrate light into a tiny volume to dramatically enhance any signal coming from the same nanoscale region. Nano-antennas are the backbone of nanoplasmonics, a field that is profoundly impacting biosensing, photochemistry, solar energy harvesting, and photonics.

Now, researchers at EPFL led by Professor Christophe Galland at the School of Basic Sciences have discovered that when shining green laser light on a gold nano-antenna, its intensity is locally enhanced to a point that it "knocks" gold atoms out of their equilibrium positions, all the time maintaining the integrity of the overall structure. The gold nano-antenna also amplifies the very faint light scattered by the newly formed atomic defects, making it visible to the naked eye.

This nanoscale dance of atoms can thus be observed as orange and red flashes of fluorescence, which are signatures of atoms undergoing rearrangements. "Such atomic scale phenomena would be difficult to observe in situ, even using highly sophisticated electron or X-ray microscopes, because the clusters of gold atoms emitting the flashes of light are buried inside a complex environment among billions of other atoms," says Galland.

The unexpected findings raise new questions about the exact microscopic mechanisms by which a weak continuous green light can put some gold atoms into motion. "Answering them will be key to bringing optical nano-antennas from the lab into the world of applications – and we are working on it," says Wen Chen, the study's first author.

REFERENCES

Wen Chen, Philippe Roelli, Aqeel Ahmed, Sachin Verlekar, Huatian Hu, Karla Banjac, Magalí Lingenfelder, Tobias J. Kippenberg, Giulia Tagliabue, Christophe Galland.
"*Intrinsic luminescence blinking from plasmonic nanojunctions*".
Nature Communications 21 May 2021.
https://dx.doi.org/10.1038/s41467-021-22679-y

ISIC

Extending the power of attosecond spectroscopy

Scientists at EPFL have shown that the powerful transient absorption spectroscopy technique can unravel ultrafast motion of electrons and nuclei in a molecule in real time and with atomic spatial resolution.

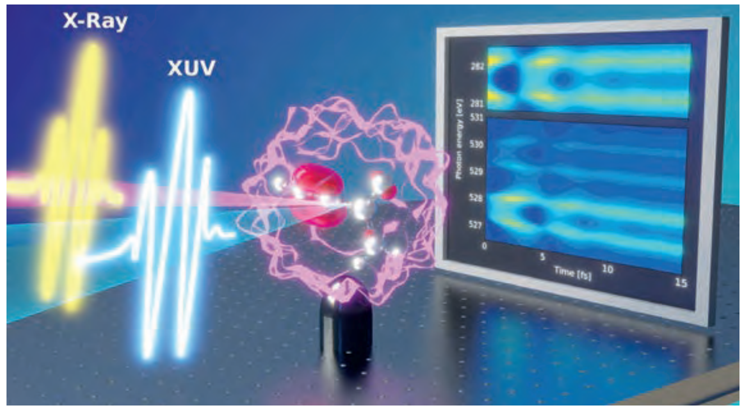
The last few decades have seen impressive progress in laser-based technologies, which have led to significant advancements in atomic and molecular physics. The development of ultrashort laser pulses now allows scientists to study extremely fast phenomena, like charge transport in molecules and elementary steps of chemical reactions. But beyond that, our ability to observe such processes on the attosecond scale (one quintillionth of a second) means that it is also possible to steer and probe the dynamics of individual electrons on their natural timeframes.

One of the emerging ultrafast technologies is attosecond transient absorption spectroscopy (ATAS), which can track the movement of electrons at a specific site of a molecule. This is a particularly appealing feature of ATAS, because it permits tracing the evolution of the molecular system with spatial resolution at the atomic scale.

Modern lasers can push chemistry into unexplored domains of light-matter interactions, where the role of theory in interpreting the results of ATAS measurements will be more important than ever before. But so far, the theory behind ATAS has been developed only for atoms or for molecules either in the absence of nuclear motion or in the absence of electronic coherence.

Now, a team of physicists from EPFL's Laboratory of Theoretical Physical Chemistry (LCPT) have extended ATAS theory to molecules, including a full account of the correlated electron-nuclear dynamics.

The work, in collaboration with Alexander Kuleff at Heidelberg University, is published in Physical Review Letters.



Fingerprints of ultrafast electron-nuclear dynamics obtained with attosecond transient absorption spectroscopy.
© N. Golubev, EPFL

"We present a simple quasi-analytical expression for the absorption cross-section of molecules, which accounts for the nuclear motion and non-adiabatic dynamics and is composed from physically intuitive terms," says Nikolay Golubev, a postdoc at LCPT and the study's lead author.

By extending ATAS theory, the scientists also show that this spectroscopy technique has sufficient resolution to "see" the follow-up decoherence of electron motion caused by the molecule's nuclear rearrangement.

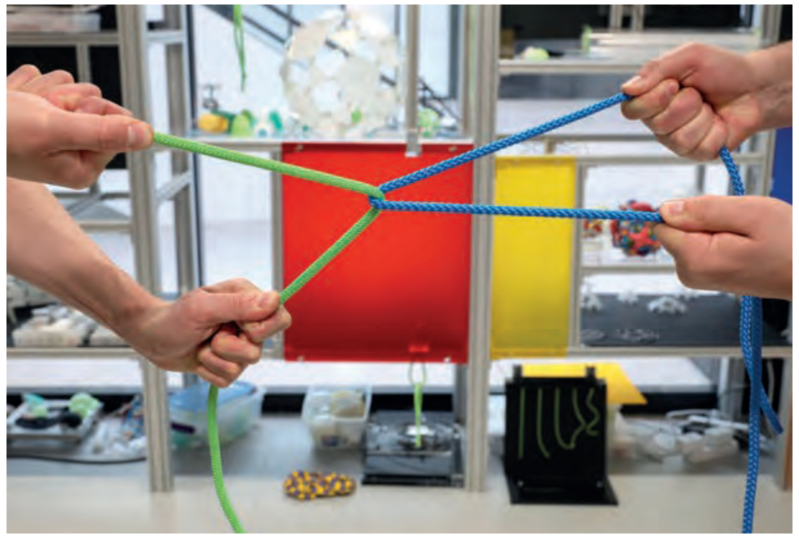
Putting theory into practice, the team tested the polyatomic molecule propiolic acid as an example. "The simulation of X-ray ATAS of the propiolic acid was made possible by combining high-level ab initio electronic structure methods with efficient semiclassical nuclear dynamics," says Jiří Vaníček, head of the LCPT. By advancing our knowledge of the correlated motion of electrons and nuclei in molecules, the findings of the LCPT researchers could also help our understanding of various other "attochemistry" phenomena.

REFERENCES

Nikolay V. Golubev, Jiří Vaníček, Alexander I. Kuleff.
"*Core-valence attosecond transient absorption spectroscopy of polyatomic molecules*".
Physical Review Letters 127, 123001 (2021).
https://dx.doi.org/10.1103/PhysRevLett.127.123001

MATH

Theory and experiments to understand a contact between two filaments



The orthogonal clasp

Mechanical engineers and mathematicians at EPFL have joined forces to gain a better understanding of the geometry and mechanics of two filaments in contact – as in the cases of knots and woven fabrics.

Pedro Reis, head of EPFL's Flexible Structures Laboratory, and John Maddocks, head of EPFL's Laboratory for Computation and Visualization in Mathematics and Mechanics, have something in common: a fascination with ropes and knots. Reis, an engineer, is an avid rock climber while Maddocks, a mathematician, has a passion for sailing. But their mutual interest in knots is not restricted to their hobbies, as knots are used in a variety of applications – take surgical sutures, for example. And although knots have been part of our daily lives since the dawn of time, their mechanics are still poorly understood.

Reis, Maddocks and the researchers at their labs have been studying a specific configuration of contact between two filaments – the orthogonal clasp – which can be regarded as the most basic building block for every knot. "This intertwining is the simplest of all knots; or to be more specific, it's the link that knots are based on. It's also the most widely used knot. It's found in the thread patterns in our clothing, for example," says Reis. He, Maddocks and their research team conducted a detailed study of the contact region between the two filaments, and their findings have just been published in Proceedings of the National Academy of Sciences of the United States of America (PNAS).

For over 30 years, Maddocks has been investigating (among other things) the mathematical theories that explain the mechanics of knots, and in particular the complex geometry of the curves that make up the contact region between filaments. In 2003, his colleague at the time Eugene Starostin published a paper specifically on the orthogonal clasp. The contact zone resembles a diamond shape, and the four corners mark the main pressure peaks. However, his theory could never be empirically corroborated due to technical limitations. "When Pedro and I decided to work together, we wondered whether Starostin's earlier results would still be relevant in practice," says Maddocks. "We then carried out tests, measurements and experiments to answer this question." Reis adds: "the contact region has always been calculated according to an ideal hypothesis, but never experimentally verified."

The researchers at Reis' lab conducted experiments using a tomograph, which employs X-rays and computer models to generate 3D images of objects. "Tomography lets us look inside the contact region between the two filaments. We then corroborated our experimental results with computer simulations. We didn't expect to find such a heterogeneous pressure distribution between the two filaments," says Paul Grandgeorge, a postdoc at Reis' lab. Their experiments showed that the pressure region between two filaments coincided with Starostin's earlier geometrical calculations. "This is a small step forward in understanding filaments in contact," says Maddocks.

Spurred on by these results, the research team wanted to take things a step further. They therefore studied the contact region between two filaments under the effect of friction. Their initial hypothesis was that friction could be explained by the capstan equation. "The concept behind the capstan equation is simple: when a rope is wrapped around a cylindrical tube, such as a mooring bollard, the tensions in the two hanging strands are separated. The more loops there are around the tube, the greater the difference in tension between the two strands. We assumed that we could use this equation to calculate the tension ratio between the two strands in our experiments," says Grandgeorge.

However, after running several experiments, the researchers concluded that the capstan equation was not applicable in the case of filaments in a frictional state. "The capstan equation assumes that the tube does not deform and is larger in diameter than the rope wrapped around it. In our experiments, however, the elastic rod that functions as the tube can be deformed and has the same diameter as the second rod that functions as the rope," says Reis. But the research team doesn't see these findings as a setback – in fact, quite the opposite. "This gives us even more incentive to find a theoretical model that can explain this physical phenomenon," says Grandgeorge. "It may appear to be a simple problem, but geometrically it's actually quite complicated," adds Maddocks. The researchers expect that there will be many studies conducted on knots in the coming years, bringing a better theoretical understanding to real-world situations.

REFERENCES

Paul Grandgeorge, Changyeob Baek, Harmeet Singh, Paul Johanns, Tomohiko G. Sano, Alastair Flynn, John H. Maddocks, Pedro M. Reis. "Mechanics of two filaments in tight orthogonal contact". Proceedings of the National Academy of Sciences Apr 2021, 118 (15) e2021684118. https://dx.doi.org/10.1073/pnas.2021684118

ISIC

Laser improves the time resolution of CryoEM

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EPFL scientists have devised a new method that can speed up the real-time observation capabilities of cryo-electron microscopy.

In 2017, Jacques Dubochet, Joachim Frank, and Richard Henderson won the Nobel Prize in Chemistry for their contributions to cryo-electron microscopy (cryoEM), an imaging technique that can capture pictures of biomolecules such as proteins with atomic precision.

In cryoEM, samples are embedded in vitreous ice, a glass-like form of ice that is obtained when water is frozen so rapidly that crystallization cannot occur. With the sample vitrified, high-resolution pictures of their molecular structure can be taken with an electron microscope, an instrument that forms images using a beam of electrons instead of light.

CryoEM has opened up new dimensions in life sciences, chemistry, and medicine. For example, it was recently used to map the structure of the SARS-CoV-2 spike protein, which is the target of many of the COVID-19 vaccines.

Proteins constantly change their 3D structure in the cell. These conformational rearrangements are integral for proteins to perform their specialized functions, and take place within millionths to thousandths of a second. Such fast movements are too fast to be observed in real time by current cryoEM protocols, rendering our understanding of proteins incomplete.

But a team of scientists led by Ulrich Lorenz at EPFL's School of Basic Sciences has developed a cryoEM method that can capture images of protein movements at the microsecond (a millionth of a second) timescale. The work is published in Chemical Physics Letters.

The method involves rapidly melting the vitrified sample with a laser pulse. When the ice melts into a liquid, there is a tunable time window in which the protein can be induced to move in the way they do in their natural liquid state in the cell.

"Generally speaking, warming up a cryo sample causes it to de-vitrify," says Ulrich Lorenz. "But we can overcome this obstacle by how quickly we melt the sample."

After the laser pulse, the sample is re-vitrified in just a few microseconds, trapping the particles in their transient configurations. In this "paused" state, they can now be observed with conventional cryoEM methods.

"Matching the time resolution of cryoEM to the natural timescale of proteins will allow us to directly study processes that were previously inaccessible," says Lorenz.

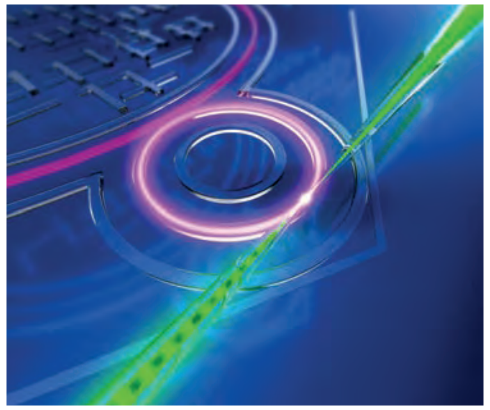
The team of scientists tested their new method by disassembling proteins after structurally damaging them, and trapping them in partially unraveled configurations.

REFERENCES

Jonathan M. Voss, Oliver F. Harder, Pavel K. Olshin, Marcel Drabbels, and Ulrich J. Lorenz.
"*Rapid Melting and Revitrification as an Approach to Microsecond Time-Resolved Cryo-Electron Microscopy*".
Chemical Physics Letters 11 June 2021.
https://dx.doi.org/10.1016/j.cplett.2021.138812

IPHYS

Integrated photonics meet electron microscopy



The experimental setup, showing a transmission electron microscope and silicon nitride microresonator used to demonstrate the electron-photon interaction. © Murat Sivis

Scientists in Switzerland and Germany have achieved efficient electron-beam modulation using integrated photonics – circuits that guide light on a chip. The experiments could lead to entirely new quantum measurement schemes in electron microscopy.

The transmission electron microscope (TEM) can image molecular structures at the atomic scale by using electrons instead of light, and has revolutionized materials science and structural biology. The past decade has seen a lot of interest in combining electron microscopy with optical excitations, trying, for example, to control and manipulate the electron beam by light. But a major challenge has been the rather weak interaction of propagating electrons with photons.

In a new study, researchers have successfully demonstrated extremely efficient electron beam modulation using integrated photonic microresonators. The study was led by Professor Tobias J. Kippenberg at EPFL and by Professor Claus Ropers at the Max Planck Institute for Biophysical Chemistry and the University of Göttingen.

In the experiments conducted by Ropers' group, an electron beam was steered through the optical near field of a photonic circuit, to allow the electrons to interact with the enhanced light. The researchers then probed the interaction by measuring the energy of electrons that had absorbed or emitted tens to hundreds of photon energies.

The photonic chips were engineered by Kippenberg's group, built in such a way that the speed of light in the microring resonators exactly matched the speed of the electrons, drastically increasing the electron-photon interaction.

The technique enables a strong modulation of the electron beam, with only a few milli-Watts from a continuous wave laser – a power level generated by a common laser pointer. This entails a dramatic simplification and efficiency increase in the optical control of electron beams, which can be seamlessly implemented in a regular transmission electron microscope.

"Integrated photonics circuits based on low-loss silicon nitride have made tremendous progress and are intensively driving the progress of many emerging technologies and fundamental science such as LiDAR, telecommunication, and quantum computing, and now prove to be a new ingredient for electron beam manipulation," says Kippenberg.

"Interfacing electron microscopy with photonics has the potential to uniquely bridge atomic scale imaging with coherent spectroscopy," adds Ropers. "For the future, we expect this to yield an unprecedented understanding and control of microscopic optical excitations."

The silicon nitride samples were developed in the Center of MicroNanoTechnology (CMi) at EPFL.

REFERENCES

Jan-Wilke Henke, Arslan Sajid Raja, Armin Feist, Guanhao Huang, Germaine Arend, Yujia Yang, F. Jasmin Kappert, Rui Ning Wang, Marcel Moeller, Jiahe Pan, Junqiu Liu, Ofer Kfir, Claus Ropers, Tobias J. Kippenberg.
"*Integrated photonics enables continuous-beam electron phase modulation*".
Nature, 23 December 2021.
https://dx.doi.org/10.1038/s41586-021-04197-5

IPHYS

New high-performance computing hub aims to harness the sun's energy

© Photo Sarah Kenderdine Authors: Joram Posma, Sarah Kenderdine, Jeremy Nicholson

EUROfusion – or the European Consortium for the Development of Fusion Energy, which consists of organizations from 28 European countries – has just selected EPFL as the site for its Advanced Computing Hub. This research hub will be led by the Swiss Plasma Center and bring together a diverse group of scientists from EPFL's Institute of Mathematics, SCITAS (which houses a high-performance scientific computing platform), Swiss Data Science Center (a national center of excellence in big data), and Laboratory for Experimental Museology (eM+). These experts will provide scientific and technical support as well as supercomputing capacity to European researchers working in the field of fusion power.

The Swiss Plasma Center is one of the world's leading fusion research laboratories. According to its head Ambrogio Fasoli, "Being selected to host the Advanced Computing Hub reflects our recognized expertise in fusion theory and simulation, and points to the interdisciplinary nature of our work. It proves that our research is of interest to other scientific communities, like those in mathematics and big data. These scientists will soon be able to pool their knowledge and start working together on a high-level international initiative."

The research team has its work cut out for it – they will be updating computer simulation codes used by experimental fusion reactors known as tokamaks. The most well-known of these types of reactors, ITER, is currently being built in the south of France. The aim of tokamaks is to demonstrate the feasibility of large-scale nuclear fusion. Fusion power – generated from the same reactions that occur inside the Sun – could be an alternative for providing clean energy for the entire planet, without producing long-term radioactive waste.

Creating a fusion reaction here on Earth, however, is an incredibly complicated task, from both an experimental and theoretical point of view. "The field of fusion power entails not just building massive reactors such as ITER, but also performing cutting-edge research to better understand, interpret and predict physical phenomena. These predictions are based on large-scale simulations that require the world's most powerful computers. Researchers need operational support to perform such calculations," says Paolo Ricci, a professor at the Swiss Plasma Center and the hub's chief scientist.

The purpose of the hub is to provide comprehensive, Europe-wide support for fusion simulations. Incredibly powerful computers are needed to simulate the complex phenomena involved in the fusion process, and these computers must be used wisely and upgraded regularly. "We'll try to work in a scalable, adaptable manner. EUROfusion researchers need to be able to benefit from future advancements in computing technology. Our job at the Advanced Computing Hub will be to update existing simulation codes so that researchers can take full advantage of new capabilities offered by upcoming generations of supercomputers," says Gilles Fourestey, head of the hub's operations.

The hub will also draw on one of EPFL's new areas of expertise: 3D data visualization, using technology developed at the Laboratory for Experimental Museology (eM+), headed by Prof. Sarah Kenderdine. To help the scientists better understand the highly complex data generated by the supercomputers, Kenderdine's lab will supply immersive augmented reality technology and state-of-the art facilities for performing highly advanced 3D visualizations.

The goal will be to graphically display the results of simulations and, ultimately, to allow researchers to interact with them in real time. "What we're going to be doing is taking data feeds live from the Swiss Plasma Center and importing them into these big systems. This allows multiple researchers to come together in a visualization space. The emergence of real time graphics is a big, booming area, where so much is possible. But how you construct these worlds is not yet clear. So that's what we're going to figure out together," says Kenderdine.

The Advanced Computing Hub initiative will kick off on 1 July 2021 and run through 2025. However, most of the scientists involved believe that it could become a long-term fixture on EPFL's campus. "In any case, I'll work hard to make sure that this cross-disciplinary effort continues well beyond the European framework program," says Fasoli.

ISIC

Machine learning cracks the oxidation states of crystal structures

Chemists voting on the oxidation states of metal-organic frameworks. © David Abbasi Pérez

Chemical engineers at EPFL have developed a machine-learning model that can predict a compound's oxidation state, a property that is so essential that many chemists argue it must be included in the periodic table.

Publishing in Nature Chemistry, chemical engineers at EPFL's School of Basic Sciences investigate the element's oxidation state, also known as oxidation number. Simply put, the oxidation state describes how many electrons an atom must gain or lose in order to form a chemical bond with another atom.

"In chemistry, the oxidation state is always reported in the chemical name of a compound," says Professor Berend Smit who led the research. "Oxidation states play such an important role in the fundamentals of chemistry that some have argued that they should be represented as the third dimension of the periodic table." A good example is chromium: in oxidation state III it is essential to the human body; in oxidation state IV, it is extremely toxic.

But although figuring out the oxidation state of a single element is pretty straightforward, when it comes to compounds made up of multiple elements, things become complicated. "For complex materials, it is in practice impossible to predict the oxidation state from first principles," says Smit. "In fact, most quantum programs require the oxidation state of the metal as input."

The current state-of-the-art in predicting oxidation states is still based on a something called "bond valence theory" developed in the early 20th century, which estimates the oxidation state of a compound based on the distances between the atoms of its constituent elements. But this doesn't always work, especially in materials with crystal structures. "It is well known that it is not only the distance that matters but also the geometry of a metal complex," says Smit. "But attempts to take this into account have not been very successful."

Until now, that is. In the study, the researchers were able to train a machine-learning algorithm to categorize a famous group of materials, the metal-organic frameworks, by oxidation state.

The team used the Cambridge structural database, a repository of crystal structures in which the oxidation state in given in the name of the materials. "The database is very messy, with many errors and a mixture of experiments, expert guesses, and different variations of the bond valence theory are used to assign oxidation states," says Smit. "We assume that chemistry is self-correcting," he adds. "So while there are many errors on individual accounts, the community as a whole will get it right."

"We basically made a machine-learning model that has captured the collective knowledge of the chemistry community," says Kevin Jablonka, a PhD student in Smit's group at EPFL. "Our machine learning is nothing more than the television game "Who Wants To Be A Millionaire?" If a chemist does not know the oxidation state, one of the lifelines is to ask the audience of chemistry what they think the oxidation state should be. By uploading a crystal structure and our machine-learned model is the audience of chemists that will tell them what the most likely oxidation state is."

REFERENCES

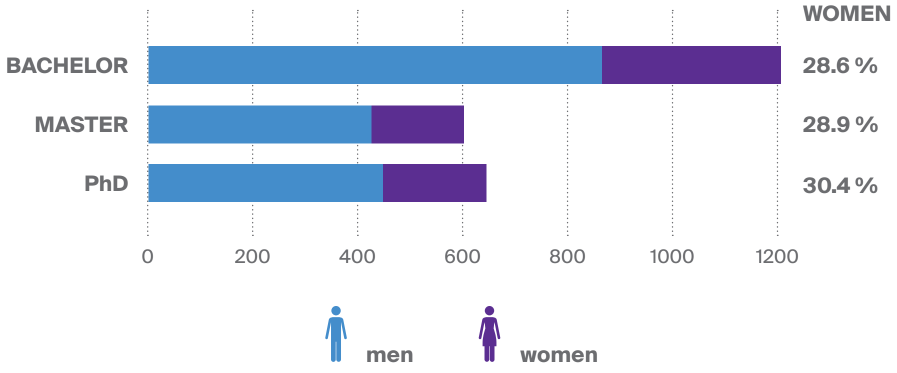
Kevin Maik Jablonka, Daniele Ongari, Seyed Mohamad Moosavi, and Berend Smit.
"*Using collective knowledge to assign oxidation states of metal-cations in metal-organic frameworks*".
Nature Chemistry 05 July 2021.
https://dx.doi.org/10.1038/s41557-021-00717-y

2021 IN FIGURES

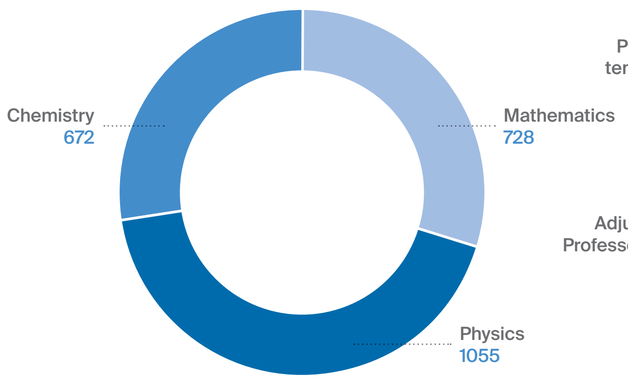
IPHYS ISIC MATH

PEOPLE

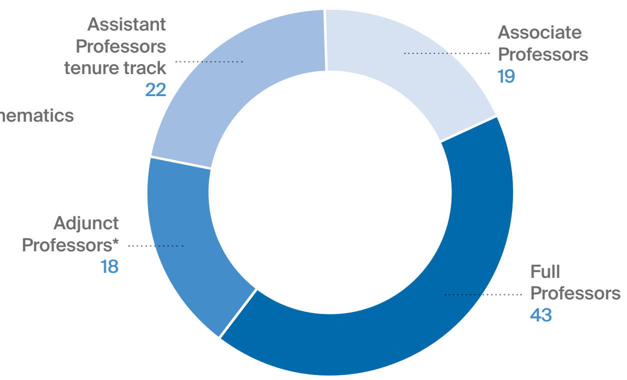
FSB Students



FSB Students (incl. PhD)

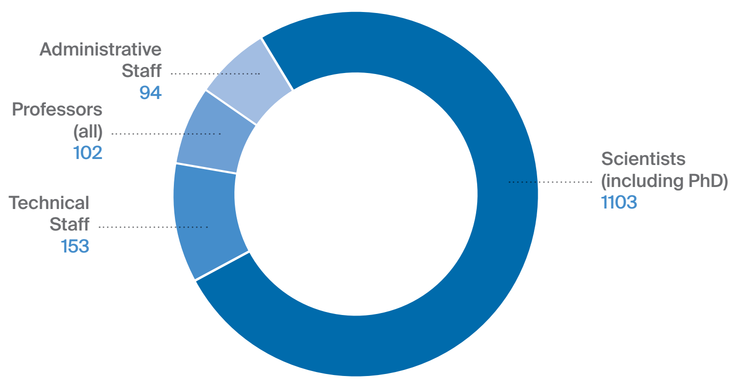


FSB Professors



* Including one Assistant Professor non tenure track

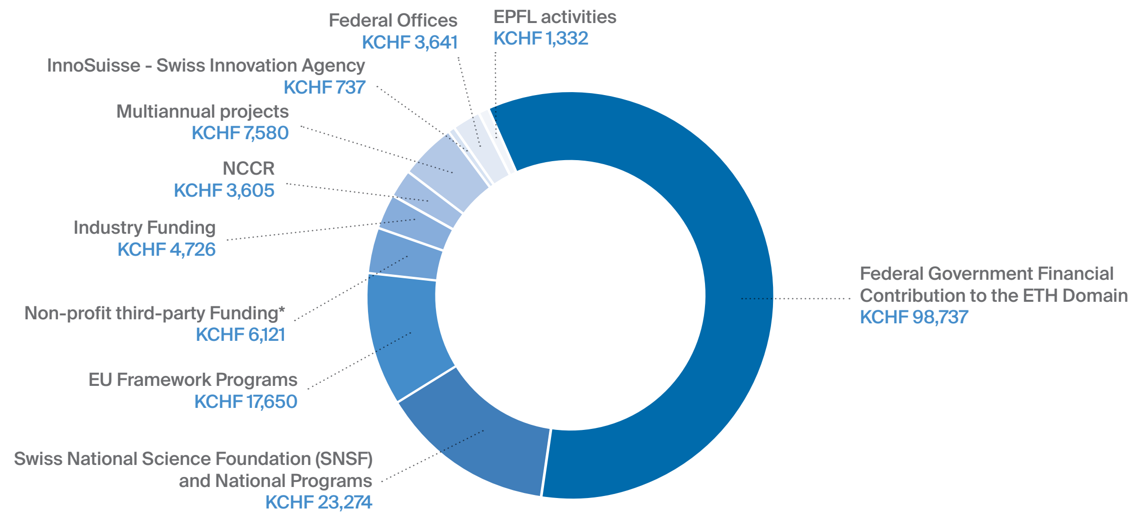
FSB Staff



FSB Staff

STAFF	TOTAL	WOMEN %
PhD students	644	30
Scientific staff / postdocs	459	22
Technical / IT staff	153	16
Administrative staff	94	70
Emeriti Professors	75	4
Full professors	43	14
Apprentices	38	40
Senior Scientists / MER	27	7
Tenure-Track Assistant Professors	22	23
Associate Professors	19	20
Adjunct Professors / Titulaires	17	24
SNSF Funded Professors	1	0

FUNDING



* includes Foundations and Associations

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RESEARCH

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