

Scho of Basic Sciences SB ANNUAL REPORT 2022

School of Basic Sciences SB

DEAN'S FOREWORD



In recent years, annual reports have opened with reflections on the impact of the pandemic. But in 2022, the world was hit with a series of unprecedented events: war in Europe, extreme weather events, rising autocracies, inflation, energy shortages, and supply chain disruptions, leading to instability and insecurity. Despite all these crises, SB has displayed remarkable resilience and even managed to thrive.

Mathematician Maryna Viazovska made headlines in 2022 when she received a Fields Medal at the International Congress of Mathematics in Helsinki. Her proof of the E8 lattice

as the densest sphere packing in eight dimensions earned her the distinction of being only the second woman to receive this prestigious award. Discover more about her story in the report, where you will also find a story about the official opening ceremony of the Bernoulli Center for Fundamental Studies that was attended by six Fields medalists and a Nobel laureate. Discover other notable achievements in the annual report, which only scratches the surface of all that SB has accomplished, and experience the breadth of our work aligned with EPFL's missions of teaching, research, and innovation.

I extend my gratitude to the various foundations, companies and other organizations that support our school, this year in particular to Lonza that have endowed a chair in Green Synthesis and Bioengineering, held jointly by our school and the School of Life Sciences. My thanks also goes out to all those who contribute to our School for their tireless efforts, as we strive to maintain and extend our standards of exceptional teaching programs and impactful research, in a time of considerable financial challenges. Finally, in the spirit of sustainability, our annual reports will now be exclusively digital, but you can learn more about SB by visiting our website at www.epfl.ch/schools/sb.

PAUL DYSON Dean of the School of Basic Sciences, EPFL

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PRIZES AND AWARDS

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EXTERNAL PRIZES AND AWARDS

Maryna Viazovska is awarded a Fields Medal



Maryna Viazovska has received a Fields Medal, a prestigious honor often described as the Nobel Prize of Mathematics, for her work on the sphere-packing problem in 8 and 24 dimensions. Previously, the problem had been solved for only three dimensions or fewer. Another Fields Medal is awarded to University of Geneva mathematician Hugo Duminil-Copin.

Maryna Viazovska, who holds the Chair of Number Theory at EPFL, has been awarded a Fields Medal, widely considered to be the highest accolade in her discipline and described as the Nobel Prize of Mathematics (a field in which the Nobel Foundation does not sponsor an official award). At 37 years of age, Viazovska has thus become only the second female Fields Medalist - after Marvam Mirzakhani in 2014 and joins a list of over 60 mathematicians to have received the prestigious honor to date. The Fields Medal was created in 1936 and is awarded every four years to one or more mathematicians under the age of 40. The official conferral took place at the International Congress of Mathematicians in Helsinki.

Viazovska, who specializes in number theory, has been awarded a Fields Medal for solving the sphere-packing problem in 8 and 24 dimensions. In doing so, she resolved a question that had stumped mathematicians for more than four centuries: how to pack spheres - such as oranges stacked in a pyramid - as close together as possible. It was in 1611 that Johannes Kepler posited, without proof, that the best solution for packing spheres in a three-dimensional space was in the shape of a pyramid. That hypothesis was finally proven in 1998.

With the third dimension resolved, it was time for mathematicians to move on to other dimensions. "Formulating the problem in the same way complicates matters because each dimension is different, and the optimal solution depends very much on the dimension," says Viazovska. Why did she focus on 8 and 24 dimensions? "Because these are special dimensions, and the solutions are particularly elegant." The way spheres are packed in these particular dimensions is remarkably symmetrical, and uses the E8 and Leech lattices, respectively. More than a decade ago, Henry Cohn (MIT / Microsoft Research) and Noam Elkies (Harvard), found that these lattice patterns were close to perfection - to one billionth of a percent - but were unable develop a proof. Viazovska's brilliant work provided the missing ingredient, demonstrating that these lattices are the densest possible packing patterns in their respective dimensions.

But Viazovska wanted to prove it, suspecting that an auxiliary function existed that could provide the right answer and match the density of the E8 and Leech lattices. In her quest for the right function, she drew on other areas of mathematics - a fact that, according to experts, makes her proof particularly elegant and original. Fueled by creativity and intuition, Viazovska turned to the focus of her dissertation: modular forms, a type of mathematical function with a high level of symmetry. After two years of work, she came up with the right function for 8 dimensions.

UNIVERSAL OPTIMALITY

She announced her results in March 2016. Her proof filled 23 pages: concise for mathematicians. Cohn subsequently got in touch and suggested that she extend her method to 24 dimensions. One week later, Viazovska, Cohn and two other colleagues posted a theorem online demonstrating that the Leech lattice is the optimal sphere-packing configuration for 24 dimensions, confirming the significance of her initial proof for 8 dimensions. This proof was cheered by the mathematical community and has earned Viazovska a number of prestigious distinctions.

Viazovska continues her work on 8 and 24 dimensions, delving deeper into sphere-packing. "These configurations appear in other optimization problems - not only for packing spheres but also in explaining energy expenditure, for example," she says. "That's rather unusual." Viazovska has recently proved the "universal optimality" of the E8 and Leech lattices, demonstrating that these are the best possible configurations across a continuous set of natural problems. It has long been known that sphere-packing plays a key role in information theory and in the theory of error-correcting codes. Viazovska's latest research could one day help solve a wide range of other everyday problems.

AN EARLY PASSION FOR MATHEMATICS

Viazovska was born in Kyiv, Ukraine, on 2 December 1984. Having developed a passion for mathematics at a young age, her path into the discipline was relatively simple. "I've liked mathematics since my schooldays," she says. "It always seemed like the most straightforward subject. And since I liked it, I spent more time on it, and eventually became better at math than other subjects. So then I liked it even more, and so on."

After obtaining a Bachelor's degree from the Taras Shevchenko National University of Kviv. Viazovska moved to Germany to obtain a Master's degree at the Technical University of

Kaiserslautern (2007) before joining the University of Bonn, where she completed her PhD on modular forms in 2013. Since then, she has also started a family. "Studying pure mathematics is bit like reading a book with illustrations," she says. "The images are linked to the text, but they don't match the written word exactly." Viazovska is driven by problem-solving, which she describes as being akin to "doing a jigsaw puzzle," and by understanding abstract concepts "so I can link them to other problems and find practical applications."

It was during her postdoc research at the Berlin Mathematical School and the Humboldt University of Berlin that Viazovska took on and solved the sphere-packing problem in 8 and 24 dimensions. In December 2016, she accepted EPFL's offer to become a tenure-track assistant professor. Just one year later, at 33 years of age, she was promoted to full professor. "I really like the fact that at EPFL there's not just pure mathematics, but also a lot of people working in very applied fields," she says.

sciences.

PRIZES AND AWARDS

SIX YEARS AT EPFL

According to EPFL President Martin Vetterli, Viazovska is an asset to the School for two reasons: "Maryna was already an outstanding researcher when she joined us six years ago. But it's been even more impressive to watch her flourish and play an active part in our Institute of Mathematics. EPFL is becoming a center of excellence in this field, not least through the Bernoulli Center, which is forging a global reputation in mathematics, physics and theoretical computer science. I would like to congratulate not only Maryna, but all the professors and researchers who've been involved in shaping this dynamic ecosystem."

EPFL extends its congratulations to Hugo Duminil-Copin, a professor in the Mathematics Section at the University of Geneva (UNIGE), who has also received a Fields Medal. These two accolades further anchor the Lake Geneva region as a center of excellence in the basic

Zoë Holmes wins Sandoz grant



Zoë Holmes, a new professor at EPFL's School of Basic Sciences, is one of the two winners of the Sandoz Family Foundation's Monique de Meuron Programme for Academic Promotion.

The Sandoz Family Foundation was launched in 1964 by the sculptor and painter Edouard-Marcel Sandoz with the aim to "encourage entrepreneurial commitment through long-term holdings in companies in a variety of sectors."

Each year for the past two decades, the Sandoz Family Foundation chooses two winners of a competition in the framework of the "Programme Fondation Philanthropique Famille Sandoz Monique de Meuron pour la relève universitaire."

The winners are awarded a research grant, which encourages universities to recruit young research talent by providing substantial financial support for up to four years. This support enables each of the laureates to set up their research group and integrate it into their respective research institutions.

This year, Sandoz has chosen Professor Zoë Holmes at EPFL and Professor Roxana Mihet at UNIL.

Zoë Holmes, joined EPFL's Institute of Physics in autumn 2022, after being a researcher with the Los Alamos National Laboratory. Her research focuses on different areas of quantum computing, and she has made important contributions to quantum thermodynamics and fluctuation theory. 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.

Fabrizio Carbone elected **APS Fellow**



EPFL Professor Fabrizio Carbone of the School of Basic Sciences has been elected Fellow of the American Physical Society.

The American Physical Society (APS) is the world's largest organization of physicists. It was founded in 1899 "to advance and diffuse the knowledge of physics." Today, the APS numbers some 50,000 members worldwide, and publishes over a dozen scientific journals, including the prestigious Physical Review and Physical Review Letters. It also runs more than twenty science conferences each year, and is a member society of the American Institute of Physics.

Despite its size, APS Fellows make up a mere 0.5% of the Society's membership, making it a distinct honor. According to its criteria, fellowships is awarded for "exceptional contributions to the physics enterprise; e.g., outstanding physics research, important applications of physics, leadership in or service to physics, or significant contributions to physics education."

This year, the APS has elected into its Fellows Professor Fabrizio Carbone at EPFL's Institute of Physics. Professor Carbone directs the Laboratory for Ultrafast Microscopy and Electron Scattering, where his research focuses on the investigation of matter in out of equilibrium conditions by means of spectroscopy, diffraction and imaging.

The APS citation for Professor Carbone reads: "For pioneering work using ultrafast electron scattering instrumentation to discover andcontrol new states of matter at the nanometer and sub-femtosecond scales."

Maria Colombo receives the **2023 ICIAM Collatz Prize**



Professor Maria Colombo, head of the chair of Mathematical Analysis, Calculus of Variations and PDEs (AMCV) at EPFL has been awarded the 2023 ICIAM Collatz Prize.

The International Council for Industrial and Applied Mathematics (ICIAM) is a society that promotes scientific work in applied mathematics all around the world.

Every four years since 1987 they organize a Congress during which they award special prizes. The ICIAM Collatz prize was started in 1999 upon the initiative of the Association of Applied Mathematics and Mechanics (GAMM) to provide international recognition for scientists under 42 years of age for outstanding work on industrial and applied mathematics.

Professor Maria Colombo, head of the chair AMCV has been awarded the 2023 ICIAM Collatz prize in recognition of her fundamental contributions to the regularity theory and the analysis of singularities in elliptic PDEs, geometric variational problems, transport equations, and incompressible fluid dynamics. She will give a presentation about her work during the upcoming ICIAM Congress in August 2023 in Tokyo.

Sir Adrian Smith, President of the Royal Society said: "It is an honour to welcome so many outstanding researchers from around the world into the Fellowship of the Royal Society. I am also pleased to see so many new Fellows working in areas likely to have a transformative impact on our society over this century, from new materials and energy technologies to synthetic biology and artificial intelligence. I look forward to seeing what great things they will achieve in the years ahead."

Professor Grätzel is world-renowned for inventing the first dve-sensitive solar cell in 1991 with chemist Brian O'Reagan. Just as plants use chlorophyll to turn sunlight into energy, the "Grätzel cells" use industrial dyes, pigments or quantum dots stimulated by sunlight to transmit an electrical charge.

PRIZES AND AWARDS

Michael Grätzel elected to the **Royal Society**

Professor Michael Grätzel has been elected as a Foreign Member of the Royal Society.

The Royal Society is the oldest scientific academy in continuous existence. Its fundamental purpose is "to recognise, promote, and support excellence in science and to encourage the development and use of science for the benefit of humanity."

This year, the Royal Society has elected among its Foreign Members Professor Michael Grätzel at EPFL's School of Basic Sciences. "I was delighted to receive these excellent news," says Grätzel. "It is an immense honor for me to join the ranks of scientific giants of Schrödinger and Heisenberg's caliber."

His 1.650 publications have received over 400.000 citations and have an h-index of 282. In 2019, Stanford University ranked Grätzel first of 100,000 top scientists across all fields. Read more about Michael Graetzel

Annalisa Buffa elected to **French Academy** of Sciences

EPFL mathematician Annalisa Buffa has been elected to Foreign Associate of the prestigious French Academy of Sciences.

The French Academy of Sciences (Académie des sciences) is a learned society, founded in 1666 by Louis XIV at the suggestion of Jean-Baptiste Colbert.

The Academy is "an assembly of scientists, chosen among the most distinguished French and foreign specialists" and aims "to provide policy makers with a framework of expertise, counsel and alert and more broadly to enlighten the debates and choices of our society."

The Academy supports research, is committed to science education, and promotes scientific life at the international level. It also includes up to 150 foreign associates, who contribute to its international reputation.

Following its open 2021 elections, the Academy of Sciences has now elected sixteen new foreign associates. Among them is Professor Annalisa Buffa at EPFL's School of Basic Sciences. Professor Buffa holds the Chair of Numerical Modelling and Simulation at EPFL's Institute of Mathematics, where she directs a research group focusing on the design and analysis of numerical algorithms for partial differential equations.

The reception ceremony for the newly elected members took place on 14 June 2022, at the Institut de France.

Jan Hesthaven elected to Royal **Danish Academy**

Professor Jan S. Hesthaven at EPFL's School of Basic Sciences has been elected as Foreign Member of the Royal Danish Academic of Sciences and Letters.

Founded in 1742 it was created with the purpose "of strengthening the position of science and scholarship in Denmark, in particular promoting basic scientific research and interdisciplinary understanding."

The Academy has now elected Professor Jan S. Hesthaven as a member of the Class of Natural Sciences. Hesthaven is Professor of Mathematics at EPFL's School of Basic Sciences, where he holds the Chair of Computational Mathematics and Simulation Science. Since 2021, he is the Vice President for Academic Affairs at EPFL.

Professor Hesthaven's research focuses on the development, analysis and application of high-order accurate computational methods for time-dependent partial differential equations, while he has also contributed substantially to the development of reduced order models and the application of neural networks and machine-learning techniques to problems in science and engineering.

SIAM honors EPFL mathematicians **Daniel Kressner and Léniac Chizat**

siam iety for Industrial and Applied Mathematics

Professor Daniel Kressner, head of the Chair of Numerical Algorithms and High-Performance Computing (ANCHP) has been named in the 2022 Class of SIAM Fellows and Professor Lénaïc Chizat, a mathematician at EPFL, has won their 2022 Activity Group on Imaging Science Best Paper Prize.

Professor Daniel Kressner has been chosen as one of the 26 members of the 2022 Class of Fellows for "his contributions in numerical linear and multilinear algebra and scientific computing".

The "Society for Industrial and Applied Mathematics" (SIAM) is a big community of more than 14000 applied mathematicians, engineers and computer scientists. SIAM has been founded in 1952 to foster strong interactions between mathematics and other scientific and technological communities through membership activities, publication of journals and books, conferences and prizes.

Every two years, SIAM awards the SIAM Activity Group on Imaging Science Best Paper Prize "to the author(s) of the most outstanding paper on mathematical and computational aspects of imaging published within the four calendar years preceding the year prior to the award year." Candidates include papers on image formation, inverse problems in imaging, image processing, image analysis, image interpretation and understanding, computer graphics, and visualization.

This year, the SIAM selection committee has awarded the Prize to Professor Lénaïc Chizat who holds the Chair of Dynamics of Learning Algorithms at EPFL's School of Basic Sciences (Institute of Mathematics). The selection committee cites Chizat's paper "Sparse optimization on measures with over-parameterized gradient descent", published in May 2021 in the journal Mathematical Programming. The SIAM citation states that Chizat's paper is awarded: "for laying out the mathematical foundations of particles-based methods for off-the-grid sparse regularization."

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PRIZES AND AWARDS

The Prize was awarded during the virtual SIAM Conference on Imaging Science (IS22) in March 2022. As the winner, Chizat presented the paper as a plenary lecture.

Teaching Awards

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

Nicolas Grandjean (IPHYS)

BEST TEACHER AWARD OF THE MATHEMATICS SECTION

Sacha Friedli

BEST TEACHER AWARD OF THE CHEMISTRY AND CHEMICAL ENGINEERING SECTION

Kay Severin

BEST TEACHER AWARD IN THE PHYSICS SECTION AND WINNER OF THE CRÉDIT SUISSE AWARD FOR BEST TEACHING

Jean-Philippe Ansermet

Doctoral **Schools Thesis Awards**

MATHEMATICS DOCTORAL **THESIS AWARD**

Quentin Posva "On the projectivity of some moduli spaces of varieties" THESIS DIRECTOR Prof. Zsolt Patakfalvi

PHYSICS DOCTORAL THESIS AWARD

Dunja Simicic "Advanced metabolite mapping at ultra-high field using 1H-MRS, 1H-MRSI and macromolecules: applications in a rat model of type C hepatic encephalopathy" THESIS DIRECTOR Prof. Rolf Gruetter and Dr. Cristina Cudalbu

CHEMISTRY AND CHEMICAL **ENGINEERING DOCTORAL** THESIS AWARD

Rebekah Wells

"Semiconducting two-dimensional transition metal dichalcogenides via solution-processable route" THESIS DIRECTOR Prof. Kevin Sivula

Elena Braconi "Chiral Diimine Complexes of Earth-Abundant Transition Metals for Asymmetric Catalysis"

THESIS DIRECTOR Prof. Nicolai Cramer

EPFL Thesis **Awards**

VILLE DE LAUSANNE AWARD 2022

Dora Mahecic "High-throughput and adaptive super-resolution fluorescence microscopy of organelles" THESIS DIRECTOR Prof. Suliana Manley

"For innovations in light shaping and real-time adaptation for high-throughput super-resolution microscopy, and their applications to structural biology and cellular biophysics." EPFL Doctorate Award 2021

DIMITRIS N. CHORAFAS FOUNDATION AWARD 2022

Weiyan Ni

"The design and synthesis of nanostructured hydrogen oxidation reaction electrocatalysts for hydroxide exchange membrane fuel cells" THESIS DIRECTOR Prof. Xile Hu

Florent Jean Drave Mathis Duguin Anne Aurélie Marie Fayolle

PHYSICS

Matteo Delladio (5.93)

Nicolas Palazzo Gilbert-Hausmann award for his Diploma work carried out at Harvard University Supervision EPFL: Christophe Galland

Gaëlle Wavre

CHEMISTRY AND CHEMICAL ENGINEERING

BACHELOR **Ole Frederik Dressler** Prix Pelet Section's Highest Bachelor average grade (5.87)

EXCELLENCY AWARD

Ole Frederik Dressler (5.87) Loïc Lucien Cédric Bassement (5.63) Jose Antonio Merkelj Abi-Fadel (5.59) Tom Sorgius (5.43) Ly Yi-Yi (5.42) Frédéric Brantschen (5.41)

MASTER

Prix Firmenich (best master project) Chemistry: Yildiz Kupper Chemical Engineering: Margherita Tonini Prix Syngenta Monthey section's best average grade Chemistry: Samuel Van Gele (5.76) Chemical Engineering: Coline Marie Agathe Boulanger (5.75)

PRIZES AND AWARDS

Bachelor and Master Students Prizes and Awards

MATHEMATICS

Linus Erik Rôsler

EPFL - Best Master average grade and Prix Douchet (for the best grade average in a Math Master cursus) (5.94)

EPFL - Best Bachelor's average grade (5.88)

EPFL - Highest first year average grade (5.97)

EPFL - Youth award - youngest graduated student, born 14.09.2001 (5.6)

EPFL - Second Best Master average grade

Sports award, for her contribution to the creation of the Student's Games

NEWS

 School of Basic Sciences SB

Faculty news 2022

Dr Victor Gorbenko currently Research Fellow at Stanford University, USA, was named as Tenure-Track Assis-

tant Professor of Physics, starting on 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 (Al). 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.

Hirschmann, currently Assistant Professor at the University of Copenhagen, Denmark, as Ten-

Professor Michaela

ure-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 guantum physics and facilitate the development of quantum algorithms.

Professor Guillermina Ramirez-San Juan, currently Assistant Professor at Brandeis University, USA has been appointed as

Tenure-Track Assistant Professor of Physics started on the 1st of August 2022.

Guillermina Ramirez-San Juan considers guestions relating to the fundamental mechanisms affecting how cilia function - an area in which little research has been conducted so far. In her unique skill set, she is able to combine aspects of cell biomechanics and the use of model organisms with expertise in chemical biology and whole tissue imaging. Her research interests thus go beyond traditional biophysics to include the fields of materials science, mechanics and robotics. Guillermina Ramirez-San Juan will forge close links between the EPFL Center for Imaging and the Dubochet Center for Imaging (DCI).

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 strengthen cooperation with other schools at EPFL, including the School of Computer Sciences, in order to develop quantum machine learning algorithms.

School of Basic Sciences SB

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 Angela Steinauer, previous Postdoctoral Researcher at ETH Zurich, has been appointed as Tenure-Track Assistant

Professor of Chemical Biology started on the 1st of October 2022.

Angela Steinauer's research interests bring together chemical synthesis, protein engineering and biological chemistry. She belongs to a new generation of researchers benefiting from a very varied and multidisciplinary education. Angela Steinauer has achieved impressive results in the field of protein development and directed evolution. In addition, she has performed pioneering work on the development of protein cages. Her current research programme grapples with the challenge of designing non-viral vectors for RNA-based therapies.

Faculty news 2022

Professor Xue-Mei Li, former Full Professor at Imperial College London, United Kingdom, has been appointed as Full

Professor of Mathematics on the 1st of November 2022.

Xue-Mei Li's expertise lies at the interface of stochastic analysis and differential geometry. Her research, which has been published in numerous leading journals, has made a significant contribution to the geometric analysis of stochastic processes on differentiable varieties, as well as to Malliavin calculus and infinite-dimensional analysis. The appointment of Xue-Mei Li will considerably strengthen EPFL's excellent reputation in the areas of probability and stochastic processes.

Professor Martin Hairer, pior Full Professor at Imperial College London, United Kinadom. has been appointed

as Full Professor of Mathematics on the 1st of November 2022.

Martin Hairer is a mathematician globally renowned for his breakthrough work at the intersection of analysis and probability. In 2014 he won the Fields Medal for visionary work which introduced a radical new way of constructing solutions for certain nonlinear stochastic partial differential equations which had been intractable before, and which are of great importance in particular to physics. The appointment of Martin Hairer to EPFL will give strong impetus to analysis in particular and mathematics in general, consolidating EPFL as one of the world's leading centres for analysis.

Buonsanti, until now Tenure-Track Assistant Professor, has been promoted as Associate Professor

Professor Raffaella

of Chemical Engineering.

Raffaella Buonsanti conducts research in the field of colloid chemistry. At EPFL she founded the Laboratory of Nanochemistry for Energy and heads a research programme aimed at finding innovative approaches to the controlled synthesis of nanomaterials with novel properties. Her research takes place at the intersection of materials chemistry and catalysis, and pursues a sustainability approach. Raffaella Buonsanti is regarded as an ambitious and forward-thinking researcher. She has already received several awards, including an ERC Starting Grant in 2017

Professor Wendy Queen, currently Tenure-Track Assistant Professor. has been promoted as Associate Professor

of Chemical Engineering.

Wendy Queen's research focuses on the development of metal-organic frameworks (MOFs) for environmental applications. She adopts a collaborative approach aimed at helping to solve some of the important problems faced by society. Wendy Queen has shown herself to be an up-and-coming researcher in this fiercely competitive research area, and her research has made a key contribution to a fast-growing field of study. Her work at EPFL has already resulted in six patents. In addition, she is a popular university lecturer who actively strives to communicate her research findings to a wider audience.

Professor Kumar Agrawal, earlier Tenure-Track Assistant Professor at EPFL, has been promoted as Associate Profes-

sor of Chemistry and Chemical Engineering Sciences in the School of Basic Sciences (SB) at EPFL Valais Wallis.

Kumar Agrawal works on the development of molecular separation systems for industrial product streams. This promising researcher is regarded as a leader in the field of membranes made of two-dimensional materials for filtering gases. A group of chemical engineers under his direction has developed a porous graphene filter which can extract carbon dioxide from the mix of gases emitted by industrial facilities. He and his team aim to expand the applications of nanoporous graphene membranes to include the separation of hydrocarbon mixtures.

Professor Suliana Manley, former Associate Professor at EPFL, has been promoted to Full Professor of Physics.

Suliana Manley's research has a focus on the development of high-resolution optical instruments and their application in studying the organisation and dynamics of proteins. As a pioneer in her field who works closely with the best-known biologists, she took only a few years to become recognised as a leader in her area of research. She received an ERC Starting Grant in 2009 and an ERC Consolidator Grant

researchers.

in 2019. Suliana Manley will make a decisive contribution to super-resolution microscopy at

School of Basic Sciences

SB

EPFL.

Professor Henrik M. Rønnow, until now Associate Professor and Head of the Institute of Physics at EPFL, has been promoted as Full Professor of Physics in

the School of Basic Sciences (SB).

Henrik Rønnow investigates low-dimensional quantum systems. He has not only contributed to fundamental advances in the field of guantum magnetism, resulting in an impressive list of publications in leading journals, but has also developed innovative concepts for neutron scattering instrumentation. He has won a number of awards, including an ERC Starting Grant in 2010 and an ERC Synergy Grant in 2018. Since April 2021 he has been head of the Physics Institute at EPFL. His appointment will help strengthen EPFL and the Paul Scherrer Institute (PSI).

Daniele Mari and Andreas Osterwalder promoted to Adjunct Professor

Dr Daniele Mari, is currently Senior Scientist at the Institute of Physics (IPHYS) and Deputy Director of the Physics Section. Daniele Mari is an expert in mechanical. His research has also had a significant impact on Swiss industry, as numerous collaborations demonstrate.

Dr Andreas Osterwalder, is currently Senior Scientist at the Institute of Chemical Sciences and Engineering (ISIC). he has established himself as one of the world's leading scientists in the field of cold-molecule chemistry. He is a very committed teacher who makes a substantial contribution to the education of young

Faculty news 2022

THREE PROFESSORS NAMED EMERITUS IN 2022

- Prof. Hubert Girault, who directed the Laboratory of Physical and Analytical Electrochemistry at the Institute of Chemical Sciences and Engineering from 1992 to 2022.
- Prof. Jean-Philippe Ansermet, who directed the Laboratory of the Physics of Nanostructured Materials at the Institute of Physics from 1992 to 2022.
- Adj. Prof. Mohammed Nazeeruddin, who directed the group SCI-SB-MN at the Institute of Chemical Sciences and Engineering from 2014 to 2022.

ONE PROFESSOR LEFT THE SCHOOL OF BASIC SCIENCES IN 2022

Prof. Pablo Rivera-Fuentes, who directed the Laboratory of Chemical and Biological Probes at the Institute of Chemical Sciences and Engineering from 2019 to 2022.

Maryna Viazovska included in BBC's "100 Women 2022" list

On December 6, the BBC published its 10th season of "100 Women", a list that includes the most influential women of the year in the categories of "Politics & Education", "Culture & Sport", "Activism & Advocacy", and "Health & Science".

This year's list "also reflects the role of women at the heart of conflict around the world in 2022 - from the protesters bravely demanding change in Iran, to the female faces of conflict and resistance in Ukraine and Russia." For the first time, the BBC also asked for nominations from women who have been previously included in the list.

The BBC 2022 list includes Professor Maryna Viazovska, who holds the Chair of Number Theory at EPFL's School of Basic Sciences (Institute of Mathematics). The citation reads:

"The Ukrainian mathematician who earlier this year became only the second woman in history to win the prestigious Fields Medal - often described as the Nobel Prize of mathematics and given out every four years. Maryna Viazovska won the award for her work on a 400-year-old puzzle, solving the problem of how to pack spheres in the most efficient way into a space with eight dimensions."

Michael Grätzel ranked #1 in Switzerland and the world

Research.com is a leading academic research portal that publishes an annual ranking of researchers in different fields of science. Their ranking is constructed using H-index data gathered by Microsoft Academic and includes only prominent scientists with an H-index of at least 40 for scientific papers.

In their 2022 analysis for Chemistry, Research. com has ranked Professor Michael Grätzel at EPFL's School of Basic Sciences first in Switzerland and the world.

Professor Grätzel is world-renowned for inventing the first dye-sensitive solar cell in 1991 with chemist Brian O'Reagan. Just as plants use chlorophyll to turn sunlight into energy, the "Grätzel cells" use industrial dyes, pigments or quantum dots stimulated by sunlight to transmit an electrical charge. Within fifteen years of the original invention, Grätzel evolved the cells into an applied technology that is now being developed in universities and companies worldwide.

Having discovered molecular photovoltaics, Grätzel's research has focused on designing mesoscopic photosystems based on molecular light harvesters that convert light very efficiently to electricity. He is credited with moving the photovoltaic field beyond the principle of light absorption via diodes to the molecular level.

Recently his research engendered a second revolution in photovoltaics prompting the advent of perovskite solar cells. Within only one decade their power conversion efficiency increased from 3 to over 25% rivaling and even exceeding the performance of conventional photovoltaics.

Grätzel also applied his innovative mesoscopic design concept to enhance the power of lithium-ion batteries and to create photoelectrochemical cells that efficiently generate chemical fuels from sunlight, opening up a new path to provide future sources of renewable energy that can be stored.

Grätzel currently directs EPFL's Laboratory of Photonics and Interfaces within the Institute of Chemical Sciences and Engineering (ISIC). His 1,650 publications have received over 400.000 citations and have an h-index of 282. In 2019, Stanford University ranked Grätzel first of 100,000 top scientists across all fields.

QSE Center organized first **IBM-EPFL** Workshop on Quantum **Algorithms**

The first IBM-EPFL Workshop on Quantum Algorithms organized by the Center for Quantum Science and Engineering (QSE) brought together experts from across Switzerland for two days of sharing and advancing research.

Quantum computers will enable complex problems in fundamental science, engineering, material, and life sciences to be solved more efficiently than today's most powerful supercomputers, offering the promise of great societal benefit. To achieve this ambitious goal, progress in how quantum computers are programmed will be just as important as the progress in quantum hardware.

To advance research and promote discussions in this field, the EPFL Center for Quantum Science and Engineering (QSE) organized the first IBM-EPFL Workshop on Quantum Algorithms. This two-day workshop, held on November 17-18 in the premises of the Bernoulli Center, gathered leading experts on quantum algorithms from EPFL. IBM Research Europe, ETHZ, and CERN to share and discuss their latest advances in this exciting field of research.

Scientists at the workshop discussed cutting-edge research on quantum algorithms that predict the properties of molecules, materials,

and elementary particles, as well as applications in quantum machine learning and artificial intelligence. Speakers included Giuseppe Carleo and Zoë Holmes from the QSE Center, along with Sofia Vallecorsa from CERN, Marina Marinkovic from ETH Zürich, Guglielmo Mazzola from the University of Zürich, and members of the IBM Research team. The meeting led to lively roundtable discussions.

QSE Center.

next year.

School of Basic Sciences SB

2022 EPFL

"The development of useful quantum algorithms for near-term quantum computers is a rapidly emerging field that is still in its infancy. This workshop was a great opportunity to set new research goals and establish synergies between the leading Swiss researchers," says Vincenzo Savona, Academic Director of the

The first IBM-EPFL Workshop on Quantum Algorithms led to new ideas, fostered fruitful collaborations, and promoted the excellence of Swiss research in this exciting field, and is just the start of a great tradition of collaborative workshops between the QSE Center, the Bernoulli Center, and quantum industry both in Switzerland abroad. This workshop is planned to become an annual event, with the second edition being hosted at the IBM offices in Zürich

Ascending peaks of knowledge - Bernoulli Center Inaugural Event

Left to right: M. Vetterli, A. Fontcuberta i Morral, D. Haldane (Nobel Prize '16), E. Abbé, M. Viazovska (Fields Medal '22), H. Duminil-Copin (Fields Medal '22), J. Penedones, M. Hairer (Fields Medal '14), A. Wigderson (Abel Prize '21) © Alain Herzog, EPFL

The Bernoulli Center for Fundamental Studies at EPFL on the shores of Lake Geneva is a new hub for the advancement of fundamental research in mathematics, theoretical physics, and theoretical computer science. The inauguration event in November 2022 was attended by students, faculty, researchers, and invited guests including Nobel laureates, Fields medalists, Abel Prize winners and other prominent scientists.

The keynote speakers at the event included EPFL's own Fields Medalist, Maryna Viazovska, who spoke about solving the sphere-packing problem in high dimensions, Abel Prize laureate Avi Wigderson, who discussed the role of "imitation games" in various fields, Nobel Prize laureate Duncan Haldane, who presented his contributions to topologically protected quantum entanglement, and Fields Medalist Hugo Duminil-Copin, who gave a humorous tour of the creation of mathematical models of real-world systems. The center was originally inspired by the Institut des Hautes Études Scientifiques (IHES) in Paris and was originally opened as the Centre Interdisciplinaire Bernoulli serving as a visitors center for mathematicians. However, under the direction of Nicolas Monod from 2014 to 2021, the center grew into a meeting place for theoretical mathematicians to exchange ideas and collaborate. The center would host hundreds of visiting scientists and researchers every year before the pandemic and was highly sought after for its opportunities for projects and workshops.

Due to a lack of dedicated facilities and disruptions from the COVID pandemic, the Bernoulli Center was briefly suspended in 2021, but was re-inaugurated in November 2022 in its new facilities with much more space and resources to support its mission. EPFL President Martin Vetterli, cut the ribbon at the new center, symbolizing the fresh start in new facilities, building on a solid foundation with many lessons learned. The event was a celebration of science, understanding, and excellence, with a focus on pushing the boundaries of knowledge and encouraging collaboration and discovery.

RESEARCH HIGHLIGHTS

SPC

EPFL and DeepMind use AI to control plasmas for nuclear fusion

Plasma inside the TCV tokamak © Curdin Wüthrich /SPC/EPFL

Scientists at EPFL's Swiss Plasma Center and DeepMind have jointly developed a new method for controlling plasma configurations for use in nuclear fusion research.

EPFL's Swiss Plasma Center (SPC) has decades of experience in plasma physics and plasma control methods. DeepMind is a scientific discovery company acquired by Google in 2014 that's committed to "solving intelligence to advance science and humanity." Together, they have developed a new magnetic control method for plasmas based on deep reinforcement learning, and applied it to a real-world plasma for the first time in the SPC's tokamak research facility, TCV. Their study has just been published in Nature.

Tokamaks are donut-shaped devices for conducting research on nuclear fusion, and the SPC is one of the few research centers in the world that has one in operation. These devices use a powerful magnetic field to confine plasma at extremely high temperatures - hundreds of millions of degrees Celsius, even hotter than the sun's core - so that nuclear fusion can occur between hydrogen atoms. The energy released from fusion is being studied for use in generating electricity. What makes the SPC's tokamak unique is that it allows for a variety of plasma configurations, hence its | tion and gathering experience. Based on the

name: variable-configuration tokamak (TCV). That means scientists can use it to investigate new approaches for confining and controlling plasmas. A plasma configuration relates to its shape and position in the device.

CONTROLLING A SUBSTANCE AS HOT AS THE SUN

Tokamaks form and maintain plasmas through a series of magnetic coils whose settings, especially voltage, must be controlled carefully. Otherwise, the plasma could collide with the vessel walls and deteriorate. To prevent this from happening, researchers at the SPC first test their control systems configurations on a simulator before using them in the TCV tokamak. "Our simulator is based on more than 20 years of research and is updated continuously," says Federico Felici, an SPC scientist and co-author of the study. "But even so, lengthy calculations are still needed to determine the right value for each variable in the control svstem. That's where our joint research project with DeepMind comes in."

DeepMind's experts developed an Al algorithm that can create and maintain specific plasma configurations and trained it on the SPC's simulator. This involved first having the algorithm try many different control strategies in simula-

collected experience, the algorithm generated a control strategy to produce the requested plasma configuration. This involved first having the algorithm run through a number of different settings and analyze the plasma configurations that resulted from each one. Then the algorithm was called on to work the other way - to produce a specific plasma configuration by identifying the right settings. After being trained, the Al-based system was able to create and maintain a wide range of plasma shapes and advanced configurations, including one where two separate plasmas are maintained simultaneously in the vessel. Finally, the research team tested their new system directly on the tokamak to see how it would perform under real-world conditions.

The SPC's collaboration with DeepMind dates back to 2018 when Felici first met DeepMind scientists at a hackathon at the company's London headquarters. There he explained his research group's tokamak magnetic-control problem. "DeepMind was immediately interested in the prospect of testing their AI technology in a field such as nuclear fusion, and especially on a real-world system like a tokamak," says Felici. Martin Riedmiller, control team lead at DeepMind and co-author of the study, adds that "our team's mission is to research a new generation of AI systems - closed-loop controllers - that can learn in complex dynamic environments completely from scratch. Controlling a fusion plasma in the real world offers fantastic, albeit extremely challenging and complex, opportunities."

ing plasmas."

REFERENCES

RESEARCH **HIGHLIGHTS**

A WIN-WIN COLLABORATION

After speaking with Felici, DeepMind offered to work with the SPC to develop an Al-based control system for its tokamak. "We agreed to the idea right away, because we saw the huge potential for innovation," says Ambrogio Fasoli, the director of the SPC and a co-author of the study. "All the DeepMind scientists we worked with were highly enthusiastic and knew a lot about implementing Al in control systems." For his part, Felici was impressed with the amazing things DeepMind can do in a short time when it focuses its efforts on a given project.

DeepMind also got a lot out of the joint research project, illustrating the benefits to both parties of taking a multidisciplinary approach. Brendan Tracey, a senior research engineer at DeepMind and co-author of the study, says: "The collaboration with the SPC pushes us to improve our reinforcement learning algorithms, and as a result can accelerate research on fus-

This project should pave the way for EPFL to seek out other joint R&D opportunities with outside organizations. "We're always open to innovative win-win collaborations where we can share ideas and explore new perspectives, thereby speeding the pace of technological development," says Fasoli.

Degrave, J., Felici, F., Buchli, J. et al. Magnetic control of tokamak plasmas through deep reinforcement learning. Nature 602, 414-419 (2022), https://doi.org/10.1038/s41586-021-04301-9

ISIC

Localis-rex: a new tool for studying electrophile signaling

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A team of researchers led by Professor Yimon Aye at EPFL's School of Basic Sciences has developed a new screening method to explore an important biological process known as electrophile signaling.

In general, an electrophile is a highly reactive compound that "seeks" to bond with atoms or other molecules that have an available electron pair. In the buzzing hive of activity that is the cell, electrophile signaling is a process that regulates the signaling properties of proteins.

Electrophile signaling is also directly related to drug-target discovery and in our understanding of drug mode of action. In fact, there is an entire field of pharmacology that aims to improve the efficacy of certain drugs by adding electrophilic "parts" to them.

Intriguingly, as the proteins move across the cell's subcellular compartments, they may encounter different reactive small-molecule metabolites, which are low-molecular weight compounds, typically involved in a biological process as a substrate or product. Some of these compounds are themselves electrophilic. Thus, it is interesting to ponder how a specific protein's "electrophile-sensing" properties may change across different parts of the cell.

In 2021, Aye's group developed an innovative chemical method to study the biological mechanisms of the electrophilic drug Tecfidera, which is used to treat multiple sclerosis. Now, the team has developed a new tool, named "Localis-rex", that allowed them to delve deeper into electrophile biology and address some unanswered questions in the field. The study is published in PNAS.

LOCALIS-REX: SOLVING ELECTROPHILE SIGNALING MYSTERIES

"Electrophile signaling is typically viewed in one of two ways," says Aye. "First, the random collision of small reactive molecules and reactive proteins that leads to a muddled response that may affect some cell signaling pathways. Second, the localized production of an electrophile labeling a protein due to proximity, leading to downstream signaling."

The problem is that proteins themselves can change their own sensing properties as they move through different areas of the cell; something that the field has given little thought to, according to Aye. "Even less thought has been invested into how the electrophile-modified state, itself significantly more stable and diffusive than the electrophile signals themselves. may signal across organelles," she adds.

The aim of Localis-rex was to explore all those questions by identifying metabolite "sensors" located in subcellular compartments - in this case the nucleus or the outer membrane of the mitochondrion. The method works by releasing a transient burst of an electrophilic compound in a specific subcellular compartment. There, the compound reveals (or not) potential reactive metabolites that sense and regulate a sig-

NOVEL FINDINGS

naling protein.

"Using Localis-rex, we identified 32 locale-specific sensor proteins sensing a native lipid-carbonyl-based metabolite, namely, hydroxynonenal," says Aye. "Twenty percent of these proteins were not previously identified as being sensitive to electrophiles or covalent-drugs at all, while others were not even known to be sensitive specifically to hydroxynonenal, a quintessential lipid-derived electrophilic-metabolite." Hydroxynonenal is of particular interest to Aye's group, because they recently showed it to be a novel covalent fragment for kinase-isoform-specific drug development, an important field of pharmacology.

About forty percent of the sensor proteins that Localis-rex identified sensor electrophilic-metabolites in areas of the cell where these proteins normally neither localize nor are active. The researchers focused on CDK9, a protein that is involved in transcription, the process of converting a gene from DNA to mRNA. Their work showed CDK9, which primarily resides in the nucleus is indeed a cytosol-specific sensor of electrophiles.

apeutics targeting it.

REFERENCES

School of Basic Sciences SB

RESEARCH **HIGHLIGHTS**

It is important to note here that transcription, which is as critical to life as it is studied, has never before been thought to be regulated by electrophiles and there are few advanced ther-

"Localis-rex is likely to be most informative for rigorous identification of the best electrophile-sensors," says Aye. "Our work has important ramifications for covalent drug design and also profiling of drug-sensitive cells with high spatiotemporal resolution, as well as establishing interesting and relevant means through which endogenous signaling electrophiles and reactive metabolites can impact biological signaling processes."

Yi Zhao, Pierre A. Miranda Herrera, Dalu Chang, Romain Hamelin, Marcus J. C. Long, Yimon Aye. Function-guided proximity mapping unveils electrophilic-metabolite sensing by proteins not present in their canonical locales. PNAS 01 February 2022; 119 (5) e2120687119 DOI: 10.1073/pnas.2120687119

IPHYS

Single photon emitter takes a step closer to quantum tech

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To get closer to quantum technology we need to develop non-classical light sources that can emit a single photon at a time and do so on demand. Scientists at EPFL have now designed one of these "single photon emitters" that can work at room temperature and are based on quantum dots grown on cost-effective silicon substrates.

Conventional light sources like incandescent light bulbs or LEDs emit bunches of photons at a time. Laser sources can emit streams of single photons, but not on-demand.

The main advantage of SPEs is that they can do both: emit a single photon and do so on-demand - or, in more technical terms, their single-photon purity, which they can maintain at an ultrafast timeframe. Thus, for a light source to qualify as an SPE, it must feature a single-photon purity above 50%; of course, the closer to 100%, the closer we will be to an ideal SPE.

Researchers at EPFL, led by Professor Nicolas Grandjean, have now developed "bright and pure" SPEs based on wide-bandgap semiconductor quantum dots grown on cost-effective silicon substrates.

The quantum dots are made of gallium nitride and aluminum nitride (GaN/AIN) and feature single-photon purity of 95% at cryogenic temperatures, while also maintaining excellent good resilience at higher temperatures, with a purity of 83% at room temperature.

The SPE also shows photon emission rates up to 1 MHz while maintaining a single-photon purity over 50%. "Such brightness up to room temperature is possible because of the unique electronic properties of the GaN/AIN guantum dots, which preserves the single-photon purity due to the limited spectral overlap with competing neighboring electronic excitation," says Stachurski, the PhD student who investigated these quantum systems.

"A very appealing feature of GaN/AIN quantum dots is that they belong to the III-nitride semiconductor family, namely that behind the solid-state lighting revolution (blue and white LEDs) whose importance was recognized by the Nobel prize in Physics in 2014," state the researchers. "It is nowadays the second semiconductor family in terms of consumer market right after silicon that dominates the microelectronic industry. As such, Ill-nitrides benefit from a solid and mature technological platform, which makes them of high potential interest for the development of quantum applications."

An important future step will be to see if this platform can emit one photon and only one per laser pulse, which is an essential prerequisite to determine its efficiency.

"Since our electronic excitations exhibit room temperature lifetimes as short as 2 to 3 billionth of a second, single photon rates of several tens of MHz could be within reach," state the authors. "Combined with resonant laser excitation, which is known to significantly improve single-photon purity, our quantum-dot platform could be of interest for implementing room-temperature quantum key distribution based on a true SPE, as opposed to current commercial systems that run with attenuated laser sources."

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IPHYS Stabilizing polarons opens up new physics

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Physicists at EPFL have developed a formulation to solve the longstanding problem of electron self-interaction when studying polarons - quasiparticles produced by electron-phonon interactions in materials. The work can lead to unprecedented calculations of polarons in large systems, systematic studies of large sets of materials, and molecular dynamics evolving over long time periods.

One of the many peculiarities of quantum mechanics is that particles can also be described as waves. A common example is the photon, the particle associated with light.

In ordered structures, known as crystals, electrons can be seen and described as waves that spread across the entire system - a rather harmonious picture. As electrons move through the crystal, ions - atoms carrying a negative or positive charge - are periodically arranged in space.

Now, if we were to add an extra electron to the crystal, its negative charge could make the ions around it move away from their equilibrium positions. The electron charge would localize in space and couple to the surrounding structural - "lattice" - distortions of the crystal, giving rise to a new particle known as a polaron.

"Technically, a polaron is a quasi-particle, made up of an electron "dressed" by its self-induced phonons, which represent the quantized vibrations of the crystal," says Stefano Falletta at EPFL's School of Basic Sciences. He continues:

Working with Professor Alfredo Pasquarello at EPFL, they have published two papers in Physical Review Letters and Physical Review B describing a new approach for solving a major shortcoming of a well-established theory that physicists use to study the interactions of electrons in materials. The method is called density functional theory or DFT, and is used in physics, chemistry, and materials science to study the electronic structure of many-body systems like atoms and molecules.

periods."

REFERENCES

RESEARCH **HIGHLIGHTS**

"The stability of polarons arises from a competition between two energy contributions: the gain due to charge localization, and the cost due to lattice distortions. When the polaron destabilizes, the extra electron delocalizes over the entire system, while the ions restore their equilibrium positions."

DFT is a powerful tool for performing ab-initio calculations of materials, by simplified treatment of the electron interactions. However, DFT is susceptible to spurious interactions of the electron with its own self - what physicists refer to as the "self-interaction problem". This self-interaction is one of the greatest limitations of DFT, often leading to incorrect description of polarons, which are often destabilized.

"In our work, we introduce a theoretical formulation for the electron self-interaction that solves the problem of polaron localization in density functional theory," says Falletta. "This gives access to accurate polaron stabilities within a computationally-efficient scheme. Our study paves the way to unprecedented calculations of polarons in large systems, in systematic studies involving large sets of materials, or in molecular dynamics evolving over long time

Stefano Falletta, Alfredo Pasquarello, Manv-Body Self-Interaction and Polarons. Phys. Rev. Lett. 129, 126401, 14 September 2022. DOI: 10.1103/PhysRevLett.129.126401

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ISIC

Nanotubes illuminate the way to living photovoltaics

Light-harvesting bacteria infused with nanoparticles can produce electricity in a "living photovoltaic". © Giulia Fattorini

Scientists at EPFL have gotten bacteria to spontaneously take up fluorescent carbon nanotubes for the first time. The breakthrough unlocks new biotechnology applications for prokaryotes, such as near-infrared bacteria tracking and "living photovoltaics" - devices that generate energy using light-harvesting bacteria.

"We put nanotubes inside of bacteria," says Professor Ardemis Boghossian at EPFL's School of Basic Sciences. "That doesn't sound very exciting on the surface, but it's actually a big deal. Researchers have been putting nanotubes in mammalian cells that use mechanisms like endocytosis, that are specific to those kinds of cells. Bacteria, on the other hand, don't have these mechanisms and face additional challenges in getting particles through their tough exterior. Despite these barriers, we've managed to do it, and this has very exciting implications in terms of applications."

Boghossian's research focuses on interfacing artificial nanomaterials with biological constructs, including living cells. The resulting "nanobionic" technologies combine the advantages of both the living and non-living worlds. For years, her group has worked on the nanomaterial applications of single-walled carbon nanotubes (SWCNTs), tubes of carbon atoms with fascinating mechanical and optical properties.

These properties make SWCNTs ideal for many novel applications in the field of nanobiotechnology. For example, SWCNTs have been placed inside mammalian cells to monitor their metabolisms using near-infrared imaging. The insertion of SWCNTs in mammalian cells has also led to new technologies for delivering therapeutic drugs to their intracellular targets, while in plant cells they have been used for genome editing. SWCNTs have also been implanted in living mice to demonstrate their ability to image biological tissue deep inside the body.

FLUORESCENT NANOTUBES IN BACTERIA: A FIRST

In an article published in Nature Nanotechnology, Boghossian's group with their international colleagues were able to "convince" bacteria to spontaneously take up SWCNTs by "decorating" them with positively charged proteins that are attracted by the negative charge of the bacteria's outer membrane. The two types of bacteria explored in the study, Synechocystis and Nostoc, belong to the Cyanobacteria phylum, an enormous group of bacteria that get their energy through photosynthesis - like plants. They are also "Gram-negative", which means that their cell wall is thin, and they have an additional outer membrane that "Gram-positive" bacteria lack

The researchers observed that the cyanobacteria internalized SWCNTs through a passive, length-dependent and selective process. This process allowed the SWCNTs to spontaneously penetrate the cell walls of both the unicellular Synechocystis and the long, snake-like, multicellular Nostoc.

Following this success, the team wanted to see if the nanotubes can be used to image cyanobacteria - as is the case with mammalian cells. "We built a first-of-its-kind custom setup that allowed us to image the special near-infrared fluorescence we get from our nanotubes inside the bacteria," says Boghossian.

Alessandra Antonucci, a former PhD student at Boghossian's lab adds: "When the nanotubes are inside the bacteria, you could very clearly see them, even though the bacteria emit their own light. This is because the wavelengths of the nanotubes are far in the red, the near-infrared. You get a very clear and stable signal from the nanotubes that you can't get from any other nanoparticle sensor. We're excited because we can now use the nanotubes to see what is going on inside of cells that have been difficult to image using more traditional particles or proteins. The nanotubes give off a light that no natural living material gives off, not at these wavelengths, and that makes the nanotubes really stand out in these cells."

INHERITED NANOBIONICS

The scientists were able to track the growth and division of the cells by monitoring the bacteria in real-time. Their findings revealed that the SWCNTs were being shared by the daughter cells of the dividing microbe. "When the bacteria divide, the daughter cells inherent the nanotubes along with the properties of the nanotubes," says Boghossian. "We call this 'inherited nanobionics.' It's like having an artificial limb that gives you capabilities beyond what you can achieve naturally. And now imagine that your children can inherit its properties from you when they are born. Not only did we impart the bacteria with this artificial behavior, but this behavior is also inherited by their descendants. It's our first demonstration of inherited nanobionics."

LIVING PHOTOVOLTAICS

"Another interesting aspect is when we put the nanotubes inside the bacteria, the bacteria show a significant enhancement in the electricity it produces when it is illuminated by light," says Melania Reggente, a postdoc with Boghossian's group. "And our lab is now working towards the idea of using these nanobionic bacteria in a living photovoltaic."

"Living" photovoltaics are biological energy-producing devices that use photosynthetic microorganisms. Although still in the early stages of development, these devices represent a real solution to our ongoing energy crisis and efforts against climate change.

on a large scale."

With an eye towards large-scale implementation, Boghossian and her team are looking to synthetic biology for answers: "Our lab is now working towards bioengineering cyanobacteria that can produce electricity without the need for nanoparticle additives. Advancements in synthetic biology allow us to reprogram these cells to behave in totally artificial ways. We can engineer them so that producing electricity is literally in their DNA."

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RESEARCH **HIGHLIGHTS**

"There's a dirty secret in photovoltaic community," says Boghossian. "It is green energy, but the carbon footprint is really high; a lot of CO₂ is released just to make most standard photovoltaics. But what's nice about photosynthesis is not only does it harness solar energy, but it also has a negative carbon footprint. Instead of releasing CO₂, it absorbs it. So it solves two problems at once: solar energy conversion and CO₂ sequestration. And these solar cells are alive. You do not need a factory to build each individual bacterial cell; these bacteria are self-replicating. They automatically take up CO₂ to produce more of themselves. This is a material scientist's dream."

Boghossian envisions a living photovoltaic device based on cyanobacteria that have automated control over electricity production that does not rely on the addition of foreign particles. "In terms of implementation, the bottleneck now is the cost and environmental effects of putting nanotubes inside of cyanobacteria

Alessandra Antonucci, Melania Reggente, Charlotte Roullier, Alice J. Gillen, Nils Schuergers, Vitalijs Zubkovs, Benjamin P. Lambert, Mohammed Mouhib, Elisabetta Carata, Luciana Dini, Ardemis A Boghossian Nature Nanotechnology 12 September 2022, DOI: 10.1038/s41565-022-01198-x

IPHYS

Cosmic web orchestrates the progression of galaxies

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The shape of galaxies and how they evolve depend on a web of cosmological filaments that run across the Universe. According to a recent study headed by EPFL's Laboratory of Astrophysics, this cosmic web plays a much bigger role than previously thought.

To get deeper insight, an international team of scientists led by Prof. Pascale Jablonka and Gianluca Castignani from EPFL's Laboratory of Astrophysics (LASTRO) examined the vast environment surrounding Virgo, a representative cluster in the local Universe. It contains some 1,500 galaxies and is located around 65 million light-years away from our own galaxy, the Milky Way.

"Many properties of galaxies, like their morphology, gas content and star formation rate, are directly influenced by their environment," says Jablonka. "We know that galaxies form fewer stars in very dense environments and adopt a more elliptical shape. But the exact role that filaments play in this transformation is still not clear. That's what we wanted to investigate with our research."

The scientists analyzed the properties of galaxies located around the Virgo cluster, across a region spanning 12 times the radius of the main cluster. Theirs is the largest study conducted to date on this topic and covers a sample size of some 7,000 galaxies, including 250 that are

big enough for scientists to be able to precisely estimate their gas content - and especially the amount of cold, dense atomic hydrogen that stars are made out of. Measurements were taken using the decametric radio telescope in Nancay, France, and the IRAM-30m telescope in Pico Veleta, Spain.

A TRANSITIONAL ENVIRONMENT

By combining the new data they collected with measurements from the literature, the scientists found that the properties of galaxies clearly change as the galaxies progress from more isolated positions towards filaments and eventually into clusters.

Filaments therefore seem to serve as a transitional environment where galaxies are pre-processed before falling into a cluster. In this environment, star formation slows or even stops altogether, elliptical shapes appear more frequently, and there is less atomic and molecular hydrogen, indicating that the galaxies are reaching the end of their active life. The scientists observed that a galaxy's evolution through its life cycle corresponds to the local galaxy density: galaxies producing few or no stars made up less than 20% of the sample of isolated galaxies, but they accounted for 20-60% of galaxies in the filaments and some 80% of galaxies in the Virgo cluster. These findings open up new avenues of research on theories to explain galaxy formation and how galaxies evolve in tandem with major cosmic bodies.

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ISIC "Grätzel" solar cells achieve a new record

Grätzel cells installed at the SwissTech Convention Center © Alain Herzog

Scientists at EPFL have increased the power conversion efficiency of dye-sensitized solar cells ("Grätzel cells") beyond 15% in direct sunlight and 30% in ambient light conditions.

Mesoscopic dye-sensitized solar cells (DSCs) were invented in 1990s by Brian O'Regan and Michael Grätzel, EPFL Professor, taking on the latter's name - the world-famous Grätzel cells. DSCs convert light into electricity through photosensitizers - dve compounds that absorb light and inject electrons into an array of oxide nanocrystals and are subsequently collected as electric current.

DSCs are transparent, can be fabricated in multiple colors for low cost, and are already being used in skylights, greenhouses, as well as glass facades, such as those adorning the SwissTech Convention Center. In addition, lightweight flexible versions of DSCs are now commercially sold on a large scale for electrical powering of portable electronic devices such as earphones and e-readers, as well in the Internet of Things by using ambient light.

Recent advancements in photosensitizers and other components of DSCs have improved the performance of DSCs under both solar sunlight and ambient light conditions. But the key to enhance DSC efficiency, lies in understanding and controlling the assembly of dye molecules on the surface of titanium dioxide nanoparticle films that favor the generation of electrical charge.

REFERENCES

RESEARCH **HIGHLIGHTS**

Now, scientists from the groups of Grätzel and Anders Hagfeldt at EPFL have developed a way of improving the packing of two newly designed photosensitizer dye molecules to enhance the DSC's photovoltaic performance. Together, the new photosensitizers can harvest light quantitatively across the entire visible domain. The new technique involves pre-adsorbing a monolayer of a derivative of hydroxamic acid on the surface of nanocrystalline mesoporous titanium dioxide. This slows down the adsorption of the two sensitizers, enabling the formation of a well ordered and densely packed layer of sensitizer at the titanium dioxide surface.

With this approach, the team was able to develop DSCs with a power conversion efficiency of 15.2% for the first time under standard global simulated sunlight, with long-term operational stability tested over 500 hours. By increasing the active area to 2.8 cm², the power conversion efficiency spanned 28.4% - 30.2% over a wide range of ambient light intensities along with outstanding stability.

The authors write: "Our findings pave the way for facile access to high performance DSCs and offer promising prospects for applications as power supply and battery replacement for low-power electronic devices that use ambient light as their energy source."

Yameng Ren, Dan Zhang, Jiajia Suo, Yiming Cao, Felix T. Eickemeyer, Nick Vlachopoulos, Shaik M. Zakeeruddin, Anders Hagfeldt, Michael Grätzel. Hydroxamic Acid Preadsorption Raises Efficiency of Cosensitized Solar Cells. Nature 26 October 2022. DOI: 10.1038/s41586-022-05460-z

5P5I

ISIC **Chemistry boosts drug libraries**

© Mischa Schüttel (EPEL)

Scientists at EPFL have found a way to synthesize large numbers of macrocyclic compounds, which are needed for developing drugs against difficult disease targets.

Pharmaceutical companies actually have libraries of 1-2 million "small-molecule" compounds collected over years. But in many cases, screening classical small-molecule compounds can't identify drug candidates simply because they don't contain a compound that binds sufficiently strong to the target.

A solution has been found in the "macrocycles", an emerging class of molecules that have proven to be ideal for binding difficult targets like proteins with flat surfaces or even proteins bound to other proteins. The problem is that current macrocycle libraries only contain less than 10,000 compounds, which limits the chance of finding drug candidates that can bind a given disease target.

But a group of chemists at EPFL have now found a way to generate large numbers of macrocycles, which can significantly increase the sizes of available libraries. The breakthrough is the work of the group of Professor Christian Heinis at EPFL's School of Basic Sciences.

"Our approach is based on combining a large number 'm' of different macrocyclic scaffolds with a myriad of 'n' chemical fragments to generate 'm×n' different macrocyclic compounds," says Heinis. "For example, we generated a library of 19,968 macrocycles by reacting 192 macrocycle scaffolds with 104 carboxylic acid fragments."

With the help of EPFL's Biomolecular Screening Facility, the scientists performed the reactions in tiny volumes of 40 nanoliters and by transferring the reagents using acoustic waves, which is enormously fast. Through the miniaturization and the high speed, the library of 19,968 macrocyclic compounds was put together in just half a day.

Working with scientists from the universities of Padova and Venice, the team got an X-ray structure of the thrombin inhibitor while it bound the protein. "The structural analysis validated the approach of screening compounds containing macrocyclic cores and laterally linked chemical fragments," says Sevan Habeshian, the PhD student leading the project.

"We are currently applying the approach for developing macrocyclic compounds to a range of disease targets for which pharmaceutical companies are struggling to generate drugs based on classical small molecules," says Heinis. "Given the small size and the limited polar surface of macrocyclic compounds, they have a high chance of being passing through cell membranes, which means that they can be used to developing drugs for intracellular targets or even drugs that are taken orally."

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ISIC **New PET-like plastic made directly** from waste biomass

A 3D-printed "leaf" made with the new bioplastic © Alain Herzog (EPFL)

EPFL scientists have developed a new, PET-like plastic that is easily made from the non-edible parts of plants. The plastic is tough, heat-resistant, and a good barrier to gases like oxygen, making it a promising candidate for food packaging. It can be chemically recycled and degrade back to harmless sugars in the environment.

It is becoming increasingly obvious that moving away from fossil fuels and avoiding the accumulation of plastics in the environment are key to addressing the challenge of climate change. In that vein, there are considerable efforts to develop degradable or recyclable polymers made from non-edible plant material referred to as "lignocellulosic biomass".

Of course, producing competitive biomassbased plastics is not straightforward. There is a reason that conventional plastics are so widespread, as they combine features that any alternative plastic replacements must match or surpass. And so far, the task has been challenging.

Until now, that is. Scientists led by Professor Jeremy Luterbacher at EPFL's School of Basic Sciences have successfully developed a biomass-derived plastic. similar to PET. that meets the criteria for replacing several current plastics while also being more environmentally friendly.

"By using a different aldehyde – glyoxylic acid instead of formaldehyde - we could simply clip 'sticky' groups onto both sides of the sugar molecules, which then allows them to act as plastic building blocks," says Lorenz Manker, the study's first author. "By using this simple technique, we are able to convert up to 25% of the weight of agricultural waste, or 95% of purified sugar, into plastic."

natives."

"The plastic has very exciting properties, notably for applications like food packaging," says Luterbacher. "And what makes the plastic unique is the presence of the intact sugar structure. This makes it incredibly easy to make because you don't have to modify what nature gives you, and simple to degrade because it can go back to a molecule that is already abundant in nature."

REFERENCES

"We essentially just 'cook' wood or other non-edible plant material, such as agricultural wastes, in inexpensive chemicals to produce the plastic precursor in one step," says Luterbacher. "By keeping the sugar structure intact within the molecular structure of the plastic, the chemistry is much simpler than current alter-

The technique is based on a discovery that Luterbacher and his colleagues published in 2016, where adding an aldehyde could stabilize certain fractions of plant material and avoid their destruction during extraction.

The well-rounded properties of these plastics could allow them to be used in applications ranging from packaging and textiles to medicine and electronics. The researchers have already made packaging films, fibers that could be spun into clothing or other textiles, and filaments for 3D-printing.

Lorenz P. Manker, Graham R. Dick, Adrien Demongeot, Maxime A, Hedou, Christèle Ravroud, Thibault Rambert, Marie J. Jones, Irina Sulaeva, Yves Leterrier, Antie Potthast, Francois Marechal, Veronique Michaud, Harm-Anton Klok and Jeremy S. Luterbacher. Sustainable polyesters via direct functionalization of lignocellulosic sugars. Nature Chemistry 23 June 2022. DOI: 10.1038/s41557-022-00974-5

IPHYS

How cells correct errors under time pressure

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How does a cell balance risk and speed when dividing? EPFL scientists have developed and experimentally tested the first mathematical theory that describes the cell's best strategy for dividing safely and efficiently.

Cells go through a life cycle that includes growing to the right size, being equipped to perform its functions, and finally dividing into two new cells. The cell cycle is critical because it ensures the perpetuation of the cell population and by extension of the greater structure they are a part of - for example a tissue in the body.

The cell cycle itself is tightly regulated by checkpoints, which prevent errors like mutations or DNA damage from being passed onto the next generation of cells. Each checkpoint acts as a kind of quality-control monitor (a biological "checklist") that ensures the order, integrity, and fidelity of the cell cycle. But checkpoints themselves often fail or are overridden after a prolonged stop of the cell cycle. If this happens in the human body, the result could be unregulated cell growth and division, which is what happens in cancer.

"Checkpoints monitor cells or whole organisms and can stop either the cell cycle or the organism's development when they detect problems," says Sahand Jamal Rahi at EPFL's School of Basic Sciences. "But if cells or organisms are stuck with an error for a very long time, in many cases, they just continue dividing or growing; they don't stop forever. There is a real risk of dying if checkpoints do not stop at all, but also waiting forever is effectively equivalent to dying."

THE MATH OF CHECKPOINT OVERRIDE

The question is then, how does the cell balance risk and speed when dividing? Although critical, checkpoint override is not very well understood, neither theoretically nor experimentally. But in a new paper, Rahi and his colleagues put forward the first mathematical theory to describe the process of checkpoint override. "Many organisms have to predict what's going to happen," he says. "You have a problem and you have to assess how bad that problem could be because the consequences are not certain. You could survive this or you might not survive this. So, the cell makes a bet either way. And in this study, we analyze the odds of that bet."

For a real-life model organism, the researchers looked at the budding yeast Saccharomyces cerevisiae, which has been used in wine making, baking and brewing for centuries. "There are systems that monitor organisms, and among these systems, possibly the best studied is the DNA damage checkpoint in yeast," says Rahi. "So, we thought, let's look at that and see whether we can make sense of checkpoint overrides. We started with a mathematical analysis behind which was a very simple question: what if these organisms are balancing risk and speed because they have to predict the

THE RISK-SPEED TRADEOFF

future?"

This tradeoff between risk and speed is similar to the quality control system of a factory assembly line: how fast can you produce things before the quality is affected? How do you balance quality and efficiency? "People have thought about this risk-speed tradeoff for checkpoints before, but they've only thought about it qualitatively," says Rahi. "It's not something that has been actually analyzed or taken seriously. So, I guess we can claim ownership of the idea!"

The scientists looked into the relationship between risk and speed. "The theory is basically balancing different probabilities, so we're computing the change in fitness if you wait versus if you continue with self-replication," says Rahi. "The organism has to come up with a strategy that involves continuously making the decision to wait or go depending on the gravity of the organism's situation at that time. Of course, waiting means that you will make fewer and fewer progeny. So the alternative is to take a risk, so the cell divides and there's a probability that it survives, and there's a probability that it dies." The theory calculates when risk and speed balance one another, determining the optimal "time". "The result turned out to be a very simple equation," Rahi adds.

describes."

RESEARCH **HIGHLIGHTS**

Despite being developed for yeast, the theory applies broadly to cells because it only takes into account risk and speed, factors that affect all organisms. "There isn't a one-to-one correspondence between what happens in yeast and mammalian cells because mammalian cells have other constraints on them than just maximizing their own growth," says Rahi.

THE CANCER DIMENSION

"But when cells become cancerous, they decouple their fitness from the fitness of their host. And then Darwinian evolution suggests that they should remodel their checkpoints to maximize growth. It's something we are interested in; one of our next steps is seeing whether cells rewire their checkpoints in an optimal way once they become cancerous."

Rahi does not expect that cancerous cells would abolish their checkpoint systems altogether. "They don't get rid of their checkpoints because then they take on too much risk in each division," he says. "Having no checkpoints whatsoever compared to when they were precancerous is also not optimal because then as soon as there's a problem they will die. So, we're interested to see whether they too aim for this state of optimal balance that our theory

Ahmad Sadeghi, Roxane Dervey, Vojislav Gligorovski, Marco Labagnara, Sahand Jamal Rahi. The optimal strategy balancing risk and speed predicts DNA damage checkpoint override times. Nature Physics 12 May 2022.

DOI: 10.1038/s41567-022-01601-3

ISIC

Imaging chemical kinetics at liquid-liquid interfaces

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Scientists led by EPFL have developed a new method to measure chemical kinetics by imaging progress of a reaction at a liquid-liquid interface embedded in a laminar-flow liquid microjet. This method is ideal for studies of dynamics on the sub-millisecond timescale, which is very difficult to do with current applications.

"It is a new application of so-called water flatjets," says Andreas Osterwalder at EPFL's School of Basic Sciences. "We prepare a controlled interface between two aqueous solutions and use it to measure chemical kinetics."

Free-flowing liquid microjets allow chemists to create a controllable smooth (and in some cases flat) surface of a liquid that can be used for surface scattering or spectroscopy studies. The free flow of the liquid in air or in a vacuum creates unobstructed optical access to gas-liquid and liquid-vacuum interfaces.

Some of the main applications of microjets include X-ray photoelectron spectroscopy, evaporation dynamics, attosecond-pulse generation, and gas-liquid chemistry. A popular implementation is a single cylindrical jet, made by forcing a liquid to exit through a nozzle 10–50 micrometers in diameter and under a pressure of a few bars, resulting in a laminar jet with a flow velocity of tens of meters per second.

These microjets have recently garnered a lot of interest for in-vacuum applications, where the jets travel freely, and remain liquid, for some millimeters before decaying into droplets and freezing. "Many experiments require a planar surface that prevents unwanted averaging over effects from the angle-dependent surface," says Osterwalder. As a result of this need, scientists have been developing different arrangements of laminar-flow planar surfaces, producing so-called liquid flat-jets.

A common form of such an arrangement is to cross two cylindrical jets of a liquid. The resulting flat-jet is a chain of leaf-shaped structures of the flowing liquid. The "leaves" are sheets only a few microns thick, and each one is bound by a relatively thick fluid rim and stabilized by surface tension and fluid inertia.

The scientists tested the flat-jet arrangement by using it to study the kinetics of the luminol oxidation chemiluminescence reaction, a glow-in-the-dark reaction that emits a blue light when the organic compound luminol is oxidized. The reaction is popular with criminal investigators looking for trace amounts of blood, but is also widely used in biological research assays.

"We believe this is a promising approach towards measuring chemical kinetics on the sub-millisecond timescale, a range that is very difficult to reach with currently existing technologies, and to study fundamental dynamics at liquid-liquid interfaces," says Osterwalder.

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ISIC

Chemical data management: an open way forward

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Writing in Nature Chemistry, three EPFL scientists propose an open platform for managing the vast amounts of machine-searchable data produced in chemical research.

"For a long time, we needed to compress information due to the limited page count in printed journal articles," says Professor Berend Smit, who directs the Laboratory of Molecular Simulation at EPFL Valais Wallis.

The scientists envision the platform as "seamlessly" integrating three crucial steps: data collection, data processing, and data publication - all with minimal cost to researchers. The guiding principle is that data should be FAIR: easily findable, accessible, interoperable, and re-usable. "At the moment of data collection, the data will be automatically converted into a standard FAIR format, making it possible to automatically publish all 'failed' and partially successful experiments together with the most successful experiment," says Smit.

But the authors go a step further, proposing that data should also be machine-actionable. "We are seeing more and more data-science studies in chemistry," says Jablonka. "Indeed, recent results in machine learning try to tackle some of the problems chemists believe are unsolvable.

School of Basic Sciences SB

them interoperable."

REFERENCES

Finally, the authors propose concrete steps that the field must take to create a FAIR data-management plan.

"We think there is no need to invent new file formats or technologies," says Patiny. "In principle, all the technology is there, and we need to embrace existing technologies and make

"Our perspective offers a vision of what we think are the key components to bridge the gap between data and machine learning for core problems in chemistry," says Smit. "We also provide an open science solution in which EPFL can take the lead."

Kevin Maik Jablonka, Luc Patiny, Berend Smit. Making the collective knowledge of chemistry open and machine-actionable. Nature Chemistry 04 April 2022. DOI: 10.1038/s41557-022-00910-7

SPC A new law unchains fusion energy

The tokamak thermonuclear fusion reactor at Swiss Plasma Center. © Alain Herzog (EPFL)

Physicists at EPFL, within a large European collaboration, have revised one of the fundamental laws that has been foundational to plasma and fusion research for over three decades, even governing the design of megaprojects like ITER. The update shows that we can actually safely use more hydrogen fuel in fusion reactors, and therefore obtain more energy than previously thought.

Fusion is one of the most promising sources of future energy. It involves two atomic nuclei combining into one, thereby releasing enormous amounts of energy. In fact, we experience fusion every day: the Sun's warmth comes from hydrogen nuclei fusing into heavier helium atoms.

There is currently an international fusion research megaproject called ITER, which aims to replicate the fusion processes of the Sun to create energy on the Earth. Its aim is the creation of high temperature plasma that provides the right environment for fusion to occur, producing energy.

Plasmas – an ionized state of matter similar to a gas - are made up of positively charge nuclei and negatively charged electrons, and are almost a million times less dense than the air we breathe. Plasmas are created by subjecting "the fusion fuel" - hydrogen atoms - to extremely high temperatures (10 times that of the core of

the Sun), forcing electrons to separate from their atomic nuclei. The process takes place inside a donut-shaped ("toroidal") structure called a "tokamak".

"In order to create plasma for fusion, you have to consider three things: high temperature, high density of hydrogen fuel, and good confinement," says Paolo Ricci at the Swiss Plasma Center, one of the world's leading research institutes in fusion located at EPFL.

Working within a large European collaboration, Ricci's team has now released a study updating a foundational principle of plasma generation - and showing that the upcoming ITER tokamak can actually operate with twice the amount of hydrogen and therefore generate more fusion energy than previously thought.

"One of the limitations in making plasma inside a tokamak is the amount of hydrogen fuel you can inject into it," says Ricci. "Since the early days of fusion, we've known that if you try to increase the fuel density, at some point there would be what we call a 'disruption' - basically you totally lose the confinement, and plasma goes wherever. So in the eighties, people were trying to come up with some kind of law that could predict the maximum density of hydrogen that you can put inside a tokamak."

An answer came in 1988, when fusion scientist Martin Greenwald published a famous law that correlates fuel density to the tokamak's minor radius (the radius of the doughnut 's inner circle) and the current that flows in the plasma inside the tokamak. Ever since then, the "Greenwald limit" has been a foundational principle of fusion research; in fact, ITER's tokamak-building strategy is based on it.

"Greenwald derived the law empirically, that is completely from experimental data - not a tested theory, or what we'd call 'first principles'," explains Ricci. "Still, the limit worked pretty well for research. And, in some cases, like DEMO (ITER's successor), this equation constitutes a big limit to their operation because it says that you cannot increase fuel density above a certain level "

Working with fellow tokamak teams, the Swiss Plasma Center, designed an experiment where it was possible to use highly sophisticated technology to precisely control the amount of fuel injected into a tokamak. The massive experiments were carried out at the world's largest tokamaks, the Joint European Torus (JET) in the UK, as well as the ASDEX Upgrade in Germany (Max Plank Institute) and EPFL's own TCV tokamak. This large experimental effort was made possible by the EUROfusion Consortium, the European organization that coordinates fusion research in Europe and to which EPFL now participates through the Max Planck Institute for Plasma Physics in Germany.

At the same time, Maurizio Giacomin, a PhD student in Ricci's group, began to analyze the physics processes that limit the density in tokamaks, in order to derive a first-principles law that can correlate fuel density and tokamak size. Part of that though, involved using advanced simulation of the plasma carried out with a computer model.

"The simulations exploit some of the largest computers in the world, such as those made available by CSCS, the Swiss National Supercomputing Center and by EUROfusion," says

Ricci. "And what we found, through our simulations, was that as you add more fuel into the plasma, parts of it move from the outer cold layer of the tokamak, the boundary, back into its core, because the plasma becomes more turbulent. Then, unlike an electrical copper wire, which becomes more resistant when heated, plasmas become more resistant when they cool down. So, the more fuel you put into it at the same temperature, the more parts of it cool down - and the more difficult is for current to flow in the plasma, possibly leading to a disruption."

In the end, Ricci and his colleagues were able to crack the code, and put "pen to paper" to derive a new equation for fuel limit in a tokamak, which aligns very well with experiments. Published in Physical Review Letters, it does justice to Greenwald's limit, by being close to it, but updates it significant ways.

The new equation posits that the Greenwald limit can be raised almost two-fold in terms of fuel in ITER: that means that tokamaks like ITER can actually use almost twice the amount of fuel to produce plasmas without worries of disruptions. "This is important because it shows that the density that you can achieve in a tokamak increases with the power you need to run it," says Ricci. "Actually, DEMO will operate at a much higher power than present tokamaks and ITER, which means that you can add more fuel density without limiting the output, in contrast to the Greenwald law. And that is very good news."

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This was challenging to simulate. "Turbulence in a fluid is actually the most important open issue in classical physics," says Ricci. "But turbulence in a plasma is even more complicated because you also have electromagnetic fields."

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IPHYS

Photonics chip allows light amplification

The photonic integrated circuits used in this study @Tobias Kippenberg (EPFL)

Scientists at EPFL have developed photonic integrated circuits that demonstrated a new principle of light amplification on a silicon chip. It can be employed for optical signals like those used in Lidar, trans-oceanic fiber amplifiers or in data center telecommunications.

The ability to achieve quantum-limited amplification of optical signals contained in optical fibers is arguably among the most important technological advances that are underlying our modern information society. In optical telecommunications, the choice of 1550 nm wavelength band is motivated not only by he loss minimum of silicon dioxide optical fibers (a development recognized with the 2009 Nobel Prize in Physics), but equally to the existence of ways to amplify these signals, crucial to achieve trans-oceanic fiber optical communication.

Optical amplification plays a key role in virtually all laser-based technologies such as optical communication, used for instance in data-centers to communicate between servers and between continents through trans-oceanic fiber links, to ranging applications like coherent Frequency Modulated Continuous Wave (FMCW) LiDAR - an emerging technology that can detect and track objects farther, faster, and with greater precision than ever before. Today, optical amplifiers based on rare-earth ions like erbium, as well as III-V semiconductors, are widely used in real-world applications.

These two approaches are based on amplification by optical transitions. But there is another paradigm of optical signal amplification: traveling-wave parametric amplifiers, which achieve signal amplification by varying a small system "parameter", such as the capacitance or the nonlinearity of a transmission line.

OPTICAL PARAMETRIC AMPLIFIERS

It has been known since the 80's that the intrinsic nonlinearity of optical fibers can also be harnessed to create travelling-wave optical parametric amplifiers, whose gain is independent of atomic or semiconductor transitions. which means that it can be broad-band and virtually cover any wavelength.

Parametric amplifiers also do not suffer from a minimum input signal, which means that they can be used to amplify both the faintest signals and large input power in a single setting. And finally, the gain spectrum can be tailored by waveguide geometry optimization and dispersion engineering, which offers enormous design flexibility for target wavelengths and applications.

Most intriguingly, parametric gain can be derived in unusual wavelength bands that are out of reach of conventional semiconductors or rare-earth-doped fibers. Parametric amplification is inherently quantum-limited, and can even achieve noiseless amplification.

SILICON LIMITATIONS

Despite their attractive features, optical parametric amplifiers in fibers are compounded by their very high pump power requirements resulting from the weak Kerr nonlinearity of silica. Over the past two decades, the advances in integrated photonic platforms have enabled significantly enhanced effective Kerr nonlinearity that cannot be achieved in silica fibers, but have not achieved continuous-wave-operated amplifiers.

"Operating in the continuous-wave regime is not a mere 'academic achievement'," says Professor Tobias Kippenberg, head of EPFL's Laboratory of Photonics and Quantum Measurements at EPFL. "In fact, it is crucial to the practical operation of any amplifier, as it implies that any input signals can be amplified - for example, optically encoded information, signals from LiDAR, sensors, etc. Time- and spectrum-continuous, travelling-wave amplification is pivotal for successful implementation of amplifier technologies in modern optical communication systems and emerging applications for optical sensing and ranging."

BREAKTHROUGH PHOTONIC CHIP

A new study led by Dr Johann Riemensberger in Kippenberg's group has now addressed the challenge by developing a traveling-wave amplifier based on a photonic integrated circuit operating in the continuous regime. "Our results are a culmination of more than a decade of research effort in integrated nonlinear photonics and the pursuit of ever lower waveguide losses," says Riemensberger.

"The application areas of such amplifiers are unlimited," says Kippenberg. "From optical communications where one could extend signals beyond the typical telecommunication bands, to mid-infrared or visible laser and signal amplification, to LiDAR or other applications where lasers are used to probe, sense and interrogate classical or quantum signals."

REFERENCES

RESEARCH **HIGHLIGHTS**

The researchers used an ultralow-loss silicon nitride photonic integrated circuit more than two meters long to build the first traveling-wave amplifier on a photonic chip 3x5 mm² in size. The chip operates in the continuous regime and provides 7 dB net gain on-chip and 2 dB net gain fiber-to-fiber in the telecommunication bands. On-chip net-gain parametric amplification in silicon nitride was also recently achieved by the groups of Victor Torres-Company and Peter Andrekson at Chalmers University.

In the future, the team can use precise lithographic control to optimize the waveguide dispersion for parametric gain bandwidth of more than 200 nm. And since the fundamental absorption loss of silicon nitride is very low (around 0.15 dB/meter), further fabrication optimizations can push the chip's maximum parametric gain beyond 70 dB with only 750 mW of pump power, exceeding the performance of the best fiber-based amplifiers.

Johann Riemensberger, Junqiu Liu, Nikolai Kuznetsov, Jijun He, Rui Ning Wang, Tobias J. Kippenberg. Photonic chip-based continuous-travelling-wave parametric amplifier. Nature 30 November 2022. DOI: 10.1038/s41586-022-05329-1

2022 IN FIGURES

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PEOPLE

SB Students

SB Students (incl. PhD)

* Including one Assistant Professor non tenure-track

SB Staff

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SB Staff

STAFF	TOTAL	WOMEN %
PhD students	645	29
Scientific staff / postdocs	394	19
Technical / IT staff	153	14
Administrative staff	97	70
Emeriti Professors	80	5
Full professors	45	18
Apprentices	38	39
Senior Scientists / MER	22	5
Tenure-Track Assistant Professors	25	28
Associate Professors	12	23
Adjunct Professors / Titulaires	18	22
SNSF Funded Professors	2	0

FUNDING Federal Offices

EPFL activities (incl. pluriannual projects) KCHF 2,083

InnoSuisse - Swiss Innovation Agency KCHF 1,320

NCCR KCHF 3,483

KCHF 3.115

Industry Funding KCHF 4,654

Non-profit third-party Funding* KCHF 5,932

> EU Framework Programs KCHF 21,058

Swiss National Science Foundation (SNSF) and National Programs KCHF 25,955

KEY FIGURES

Federal Government Financial Contribution to the ETH Domain KCHF 99,740

* includes Foundations and Associations

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