## ICFO STORIES

2024

The past year has been a remarkable period of discovery and innovation at ICFO, marked by groundbreaking advancements across our core research areas.

In the realm of energy and environment, ICFO research has contributed to sustainable solutions addressing global challenges, while in biophysics and health, cutting-edge photonic technologies and breakthroughs in bionanophotonics have paved the way for transformative medical applications. In the field of materials science, ICFO researchers have developed novel advanced and low-dimensional materials with enhanced functionalities, offering exciting prospects for electronics and nanotechnology. Quantum physics has remained a focal point, with progress in both fundamental science and quantum technologies.

This Year Booklet highlights key scientific achievements from the institute, reflecting the collaborative efforts and ingenuity that drive ICFO's commitment to scientific excellence for the benefit of society forward.

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# MATERIAL SCIENCE

#### ICFO's 2024 in Material Science

New materials enable researchers to explore key basic science questions and develop deep tech to tackle the most pressing challenges faced by humankind. During 2024, ICFO has contributed in advancing the knowledge around several advanced and low-dimensional materials. It has been a year full of ground-breaking and fundamental research projects, touching a wide variety of different topics.

Quantum dots have been one of the most recurrent subjects in the Functional Optoelectronic Nanomaterials group, exploring their potential for short-wave infrared applications and exploiting their non-toxic and environmentally friendly features.

Another hot topic has been nanocavities, which confine light at the nanoscale. Following different innovative strategies, ICFO researchers from the Quantum Nano-Optoelectronics and the Nanophotonics Theory group have paved the way towards smaller and higher quality cavities.

The Quantum Nano-Optoelectronics group has also played a crucial role in the field of low-dimensional materials, developing on-chip devices to detect molecules, platforms for future miniaturized spectrometers, and expanding fundamental knowledge on one-dimensional superconductors or second-order superlattices.

Other groups, such as the Molecular Nanophotonics, Optoelectronics, and Attoscience and Ultrafast Optics, have used photonics to study materials, molecules and different phenomena occurring within exotic materials, as well as to enhance several existing materials.

### Environmentally friendly InSb/ InP colloidal quantum dots for fast and highly sensitive SWIR photodetectors

Researchers from ICFO have developed a novel method for synthesizing InSb/InP colloidal quantum dots stable under ambient conditions. In their report of ACS Nano, they have employed these quantum dots to fabricate a fast and highly sensitive arsenic free shortwave infrared (SWIR) light sensor. The new strategy expands the possibility for the fabrication of optoelectronic devices based on environmentally friendly CQDs, compliant with the current regulations that limit their use in commercial consumer applications.

Applications such as LIDAR, 3D imaging for mobile devices, automotive and augmented/virtual reality or night vision for surveillance, rely on the development of short-wave infrared (SWIR) photodetectors. These devices are capable of seeing in the region of the spectrum that is invisible to our eye since they operate in the spectral window of 1-2  $\mu$ m.

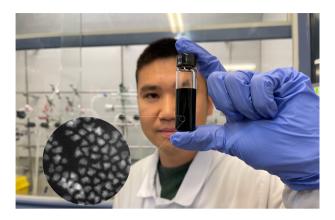
The SWIR light sensor industry has been dominated for years by the epitaxial technology, mainly based on devices made of indium gallium arsenide (InGaAs). However, several factors such as high production costs, low-scale manufacturability and incompatibility with CMOS has confined the epitaxial technology to niche and military markets.

In contrast, the potential of SWIR photodetectors made of colloidal quantum dots (CQDs), nanoscale semiconductor materials, has attracted significant interest in the recent years due to their appealing features, such as low cost and compatibility with CMOS architecture, among others.

While this recent CQD is emerging as a competitor technology for InGaAs based devices, it is important to clarify that current CQDs based SWIR photodetectors use components such as lead (Pb) and mercury (Hg) chalcogenides. Both of these elements are subject to the Restriction of Hazardous Substances (RoHS) European directive, which regulates their usage in commercial consumer applications.

As a consequence of this regulatory framework, there is a pressing urge for the development of SWIR light sensors based on environmentally friendly, heavy-metal-free CQDs.

Indium antimonide (InSb) CQDs have a great potential to deliver high- performance and stability devices. Moreover they are RoHS compliant and have access across the full SWIR range thanks to the low bandgap of bulk InSb. However, its synthesis has proven to be challenging so far due to the most strongly covalent nature of InSb and lack of the highly reactive precursors. Moreover, previous



Lucheng Peng in the lab holding a solution of quantum dots.

studies have reported that InSb CQDs are unstable upon exposure to air due to the strong propensity of Sb to oxidize.

In a new study published in ACS Nano, researchers from ICFO Lucheng Peng, Yongjie Wang, Yurong Ren, Zhuoran Wang, led by Prof. ICREA at ICFO, Gerasimos Konstantatos, in collaboration with Pengfei Cao, from Erns Ruska Centre for Microscopy and Spectroscopy with Electrons, describe a new method to synthesize arsenic free InSb CQDs with access to the SWIR range. Their approach includes the design of an InSb/InP core-shell structure of the synthesized quantum dots that are used to fabricate a fast-response and highly-sensitive SWIR photodetector.

In the new study, the researchers have developed a new synthetic process to produce high-quality wide spectral tunable InSb quantum dots with size uniformity by using commercially available chemical precursors, overcoming some of the hurdles that previous strategies had suffered, including a challenging synthesis process and high surface defect density.

In their study, the researchers adopted the "single-source approach", using a continuous precursor

"the researchers have developed a new synthetic process to produce high-quality wide spectral tunable InSb quantum dots with size uniformity by using commercially available chemical precursors"

injection process, instead of a hot injection option. This strategy was key to obtain InSb CQD with a well-controlled size distribution and distinct absorption over a very broad range of the spectrum (900nm to 1750 nm). By using a range of reaction temperatures spanning from 220 °C to 250 °C, they were able to control the positions of the dots within the resulting solution-processed thin film. "The resultant spectral tuneability from near infrared to short-wave infrared, that is from 900 nm to 1750 nm, is the largest reported to date for InSb CQD", the researchers described.

They observed the processed CQD samples with transmission electron microscopy (TEM) technique and confirmed that the dots had an average size of 2.4 nm, 3.0 nm, 3.5 nm, 5.8 nm and 7.0 nm that enabled the absorption of different wavelengths. The researchers also characterized the surface of the InSb CQDs, since it is known to be crucial to the CQD material's optoelectronic properties. They used X-Ray photoelectron spectroscopy to investigate the oxidation states of Sb that are associated to the surface's unpassivated Sb dangling bonds and they could confirm the formation of Sb-oxide over the unprotected surface.

The next step in their investigation was to develop

a passivation strategy to cover the obtained InSb CQDs creating a shell to protect the QCDs from oxidation. The surface of InSb QCDs was treated with indium trichloride (InCl<sub>3</sub>). This protected the surface dangling bonds of Sb by reducing the defects and improving at the same time the colloidal stability of the CQDs in the following steps of the purification process.

Subsequently, the researchers grew indium phosphide (InP) protection shell with thin thickness over the purified InSb CQD. They used indium oleate and phosphine silylamide as precursors to generate the shell. This caused a significant red shift on the absorption spectrum of the InSb CQDs. The InSb/InP core-shell structure was confirmed later by the photoluminescence spectra analysis.

"InSb/InP core-shell structure means growing another material (in this case, InP) on the surface of the pristine material (in this case, InSb). In comparison to InSb, InP is a wider bandgap material that can sufficiently passivate the surface traps of InSb that are detrimental in optoelectronic devices. Also, the Sb element is quite sensitive to oxygen, so the core-shell structure can largely improve the air stability of the material", explains Lucheng Peng, ICFO researcher and first author of the study.

#### Fabricating faster and more sensitive photodetectors

Once this first step was achieved, the researchers move onto using the optimized InSb/InP core-shell CQDs to fabricate a low temperature, high-speed SWIR photodetector. The light sensor device was formed by several stacked layers: a base of Indium Tin Oxide (ITO), an electron transfer layer (ETL) made by titanium dioxide (TiO<sub>2</sub>), the thin layer containing the InSb/InP CQDs and a final top layer made of gold. They wanted to obtain a photodetector with a fast time response to be used in applications that goes beyond video frame rates, so they used TiO<sub>2</sub>

"This is the best solutionprocessed, CQD SWIR photodetector based on InSb so far considering both performance and stability"

as an ETL because its photochemical stability.

The response of the fabricated light sensor was then measured. As the authors wrote, the photodetector "demonstrates remarkable features including a wide linear dynamic range exceeding 128 dB, a maximum external quantum efficiency (EQE) of 25% at 1240 nm (and 12% at 1420 nm), fast photoresponse time of 70 ns, and a specific detectivity of up to 4.4 × 1011 Jones."

As the researchers could verify, the device turned out to be highly resistant to atmospheric conditions without any encapsulation. After two months of exposure to the ambient environment, the photodetector maintained its properties. After 90 hours, the device's stability was also verified when it was functioning in the open air, and it was found to be extremely stable.

"This is the best solution-processed, CQD SWIR photodetector based on InSb so far considering both performance and stability, with figures of merit that can enable high-frame-rate light sensors for machine vision, gated imaging and 3D sensing applications", said ICREA Prof. at ICFO Gerasimos Konstantatos. "The present study not only shows the enormous potential of InSb CQDs as an active material free of heavy metals to be used in SWIR photodetectors, but it also opens the door for future developments in colloidal InSb utilizing wet chemical methods towards the fabrication of high-performing electronic or optoelectronic devices",

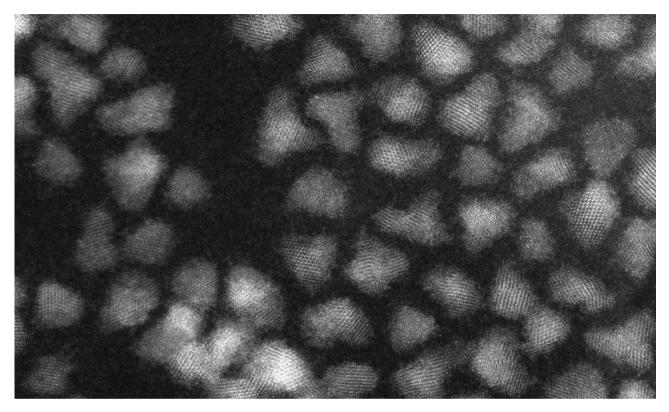


Image of the solution of quantum dots obtained in the study.

#### concluded Konstantatos.

The team is now working on how to further reduce the dark current and increase the quantum efficiency of the CQDs based photosensors. In order to do so, they mainly need to focus on improving the carrier mobility in the thin films that contain the CQDs. Achieving this will allow them to get a faster response speed for the light sensor, aiming to go beyond the 10 ns response speed so that the technology can be used in i-ToF (indirect-time-of-flight), which is useful in LIDAR and 3D imaging.

#### Reference:

Peng, L., Wang, Y., Yurong, R., Wan, Z., Cao, P., Konstantatos, P. (2023) InSb/InP core-shell colloidal quantum dots for sensitive and fast short wave infrared photodetectors. ACS Nano. Doi: https://doi.org/10.1021/acsnano.3c12007

## Spatiotemporal Microscopy as a powerful tool for studying transport phenomena

A review recently published in *Advanced Electronic Materials* by researchers from ICN2, ICFO and Vrije University discusses spatiotemporal microscopy as a promising and versatile technique for observing and controlling transport phenomena. It presents the advantages of this technique over conventional ones, showcasing recent discoveries in particle and heat transport, describes its experimental implementations, and offers insights into potential future applications.

Understanding transport phenomena –processes originating from the spontaneous or force-induced movement of mass, charge, or heat– is fundamental for research on materials and their adaptation to specific applications. The study and control of transport phenomena enables scientists to observe complex processes occurring in matter and potentially learn how to steer and exploit them.

Some conventional techniques used to study charge or heat transport require physical contacts (to apply stimuli and/or read out responses), which can lead to unwanted effects. Additionally, they do not always facilitate distinguishing between different species of particles or carriers. In contrast, optical techniques do not require electronic contacts and allow researchers to focus on specific species of interest, thanks to wavelength selectivity. Amona these techniques, spatiotemporal microscopy (SPTM) is emerging as a particularly promising method to study transport phenomena by visualizing the spatial diffusion or translation of the species under observation as a function of time.

**Dr. Guillermo Brinatti-Vazquez** and **Giulia Lo Gerfo Morganti** from the Institute of Photonic Sciences

(ICFO, Spain), in collaboration with researchers from the Catalan Institute of Nanoscience and Nanotechnology (ICN2, Spain) and Vrije University of Amsterdam (VU, The Netherlands), are the first authors of a review on spatiotemporal microscopy recently published in *Advanced Electronic Materials*. The essay discusses its experimental implementations and some applications, giving examples of interesting physical phenomena discovered thanks to this technique.

Intended as an overview of the topic, the paper describes the principles of time-resolved optical measurements and the advantage of observing both the time and the spatial evolution of the studied system. The cases of transport governed by particles or quasi-particles and of electronic or phononic heat are considered.

Different experimental implementations of SPTM –namely, time-correlated microscopy, widefield imaging, point scanning, and grating-based techniques—are discussed, highlighting scenarios where one may be preferable over the others. After providing a brief summary of transport theory, the authors proceed to present recent discoveries related to particle transport made possible by

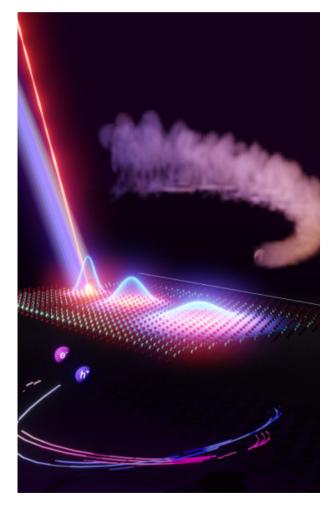
spatiotemporal studies, both in the case of particle and of heat transport. Indeed, this technique offers remarkable advantages in terms of time scale, down to femtoseconds, and length scales, down to nanometres

Finally, an outlook on emerging and future applications or extensions of this technique is provided. The authors suggest that photocurrent based SPMT will play a crucial role in connecting transport dynamics with device functionality and performance. Broad-band and multidimensional SPTM are also promising, as they would allow the separation of transport contributions of different species. Further developments are required to enable the use of this technique to resolve nanometric structures near interfaces or in other situations in which diffraction phenomena can hinder its performance. Another exciting direction of evolution is the replacement of optical beams by electron beams, which would lead to a very high spatial resolution.

The review aims to be a reference introduction to spatiotemporal microscopy for the study of transport phenomena in different contexts and to provide guidelines for scientists interested in including SPTM in their research "toolbox".

#### Reference:

Guillermo D. Brinatti Vazquez, Giulia Lo Gerfo Morganti, Alexander Block, Niek F. van Hulst, Matz Liebel, Klaas-Jan Tielrooij, Spatiotemporal Microscopy: Shining Light on Transport Phenomena. Advanced Electronic Materials, 2023. DOI: https://doi.org/10.1002/aelm.202300584 "The review aims to provide guidelines for scientists interested in including SPTM in their research toolbox"



Artistic illustration of the concept of spatiotemporal microscopy (SPTM), where species spread out in space while time progresses. Credit: Giulia Lo Gerfo Morganti.

## Towards transparent and antimicrobial surfaces for touch displays

A team of ICFO and Corning Incorporated researchers reports in *Communications Materials* journal the development of a durable and transparent antimicrobial surface containing copper nanoparticles. The nanostructured surface was obtained by dewetting ultrathin metal copper films on a glass substrate.

The interest in antimicrobial solutions for personal and multi-user touch screens, such as tablets and mobile devices, has grown in recent years. Traditional methods like sprayable alcohols or wipes are not ideal for these delicate displays. Antimicrobial coatings applied directly to the glass are a promising alternative, but only if they are transparent and long-lasting. Previous proposed coating solutions, such as photocatalytic metal oxides (e.g., TiO<sub>2</sub> and ZnO), have posed some challenges. Additionally, these coatings typically require light and moisture to be antimicrobial and eliminate the microbes present on the surface.



SEM image of the copper dewetted nanoparticles with antimicrobial properties over the glass substrate.

Copper is a well-known biocidal metal with high efficacy against a wide range of microorganisms, and it has been traditionally used for objects such as door handles and hospital bedrails. However, copper coatings are predominantly opaque, which to date has prevented the realization of a transparent, copper-based antimicrobial solution suitable for displays. Furthermore, the high electrical conductivity of the metal film can negatively interfere with the touch-sensing functionality featured on mobile devices

A team of researchers has designed and implemented a transparent nanostructured copper surface (TANCS) that is non-conductive, and resistant against the growth of certain bacteria. In a recent study, published in the journal Communications Materials, ICFO researchers Christina Graham, Alessia Mezzadrelli led by ICREA Prof. Valerio Pruneri, and colleagues from Corning, including Wageesha Senaratne, Santona Pal, Dean Thelen, Lisa Hepburn and Prantik Mazumder, have described their new approach to develop this surface.

The fabrication process of this surface involved depositing an ultra-thin copper film with a nominal thickness of 3.5nm onto a glass substrate. Then, the

researchers used a rapid thermal annealing process to form dewetted Cu nanoparticles with optimal size and distribution. The specific design and method provided an antimicrobial effect, transparency, color neutrality, and electrical insulation. Finally, additional layers of SiO<sub>2</sub> and fluorosilanes were deposited on top of the nanoparticles, providing environmental protection and improved durability properties with use-test cases.

The authors of the study examined the fabricated coating morphology, optical response, antimicrobial efficacy, and mechanical durability. The TANCS showed the ability to eliminate over 99.9% of "Staphylococcus Aureus" present in the tested surfaces within two hours, under stringent dry test conditions. Moreover, the substrate demonstrated optical transparency allowing for 70-80% light transmission in the visible range (380-750nm), color neutrality. Finally, the surfaces showed to have a prolonged effectiveness with use-test cases, maintaining their antimicrobial activity even after a rigorous wipe testing procedure.

"This is a great example of creating a multi attribute product while co-optimizing the attributes high efficacy antimicrobial properties that work under dry test conditions for touch enabled, display use test cases. Our goal was to show the connections with biological performance and physical attributes, and provide further guidance for future research," said Wageesha Senaratne, researcher at Corning and leading co-author of the study.

"This new approach of considering the dewetting process opens to a variety of new possibilities to exploit some specific properties of metals while being able to thoughtfully change the others. Here for example, we were able to preserve the powerful antimicrobial effect of the copper while obtaining transparency and insulation despite the use of a metal," said Alessia Mezzadrelli, author of the study and PhD student of the Nano-Glass project.

### "This is a great example of creating a multi co-optimized attribute product"

The introduction of these transparent antimicrobial surfaces holds significant promise in a world increasingly reliant on touchable displays, including smartphones or tablets.

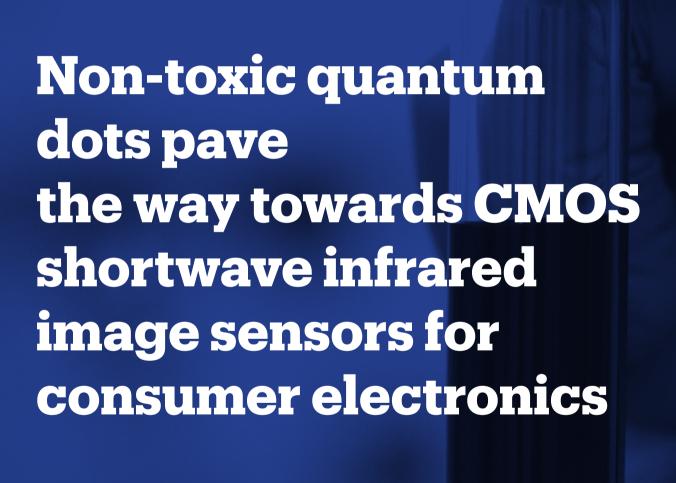
"While further development is necessary for full-fledged commercial deployment, this is a step in the right direction to enable antimicrobial touch screens for public or personal displays," said Prantik Mazumder, researcher at Corning and co-author of the study.

"The proof-of-concept surface we have developed with Corning is an example of our continuous joint efforts in the development of enhanced multifunctional display screen glass using nanostructuring," said Valerio Pruneri, ICREA professor at ICFO and coordinator of the Nano-Glass project.

#### Reference:

Graham, C., Mezzadrelli, A., et. al. (2024). Towards transparent and durable copper-containing antimicrobial surfaces. Communications Materials.

DOI: https://doi.org/10.1038/s43246-024-00472-w



### Non-toxic quantum dots pave the way towards CMOS shortwave infrared image sensors for consumer electronics

ICFO and Qurv researchers have fabricated a new high-performance shortwave infrared (SWIR) image sensor based on non-toxic colloidal quantum dots. In their study published in *Nature Photonics*, they report on a new method for synthesizing functional high-quality non-toxic colloidal quantum dots integrable with complementary metal-oxide-semiconductor (CMOS) technology.

Invisible to our eyes, shortwave infrared (SWIR) light can enable unprecedented reliability, function and performance in high-volume, computer vision first applications in service robotics, automotive and consumer electronics markets. Image sensors with SWIR sensitivity can operate reliably under adverse conditions such as bright sunlight, fog, haze and smoke. Furthermore, the SWIR range provides eye-safe illumination sources and opens up the possibility of detecting material properties through molecular imaging.

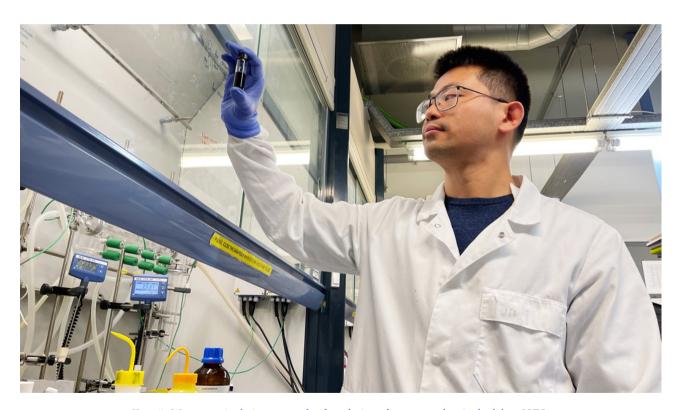
Colloidal quantum dots (CQD) based image sensor technology offers a promising technology platform to enable high-volume compatible image sensors in the SWIR. CQDs, nanometric semiconductor crystals, are a solution-processed material platform that can be integrated with CMOS and enables accessing the SWIR range. However, a fundamental roadblock exists in translating SWIR-sensitive quantum dots into key enabling technology for mass-market applications, as they often contain heavy metals

like lead or mercury (IV-VI Pb, Hg-chalcogenide semiconductors). These materials are subject to regulations by the Restriction of Hazardous Substances (RoHS), a European directive that regulates their use in commercial consumer electronic applications.

In a new study published in Nature Photonics, ICFO researchers Yongjie Wang, Lucheng Peng, and Aditya Malla led by ICREA Prof. at ICFO Gerasimos Konstantatos, in collaboration with researchers Julien Schreier, Yu Bi, Andres Black, and Stijn Goossens, from Qurv, have reported on the development of high-performance infrared photodetectors and a shortwave infrared (SWIR) image sensor operating at room temperature based on non-toxic colloidal quantum dots. The study describes a new method for synthesizing size tuneable, phosphine-free silver telluride (Ag<sub>2</sub>Te) quantum dots while preserving the advantageous properties of traditional heavymetal counterparts paving the way to the introduction of SWIR colloidal quantum dot technology in high-volume markets.

While investigating how to synthetize silver bismuth telluride (AgBiTe<sub>2</sub>) nanocrystals to extent the spectral coverage of the AsBiS<sub>2</sub> technology to enhance the performance of photovoltaic devices, the researchers obtained silver telluride (Ag<sub>2</sub>Te) as a by-product. This material showed a strong and tuneable quantum confined absorption akin to quantum dots. They realized its potential for SWIR photodetectors and image sensors and pivoted their efforts to achieve and control a new process

In their new synthetic method, the team used different phosphine-free complexes such as a tellurium and silver precursors that led them to obtain quantum dots with a well-controlled size distribution and excitonic peaks over a very broad range of the spectrum. After fabricating and characterizing them, the new synthesized quantum dots exhibited remarkable performances, with distinct excitonic peaks over 1500 nm—an unprecedented achievement compared to previous



Yongije Wang manipulating a sample of a solution of quantum dots in the lab at ICFO.

to synthesize phosphine-free versions of silver telluride quantum dots, as phosphine was found to have a detrimental impact on the optoelectronic properties of the quantum dots relevant to photodetection. phosphine-based techniques for quantum dot fabrication.

The researchers decided then to implement the obtained phosphine-free quantum dots to fabricate

a simple laboratory scale photodetector on the common standard ITO (Indium Tin Oxide)-coated glass substrate to characterize the devices and measure its properties. "Those lab-scale devices are operated with shining light from the bottom. For CMOS integrated CQD stacks, light comes from the top, whereas the bottom part of the device is taken by the CMOS electronics", comments Yongjie Wang, postdoc researcher at ICFO and first author of the study. "So, the first challenge we had to overcome was reverting the device setup. A process that in theory sounds simple, but in reality proved to be a challenging task".

Initially, the photodiode exhibited a low performance in sensing SWIR light, prompting a redesign that incorporated a buffer layer. This adjustment significantly enhanced the photodetector performance, resulting in a SWIR photodiode exhibiting a spectral range from 350nm to 1600nm, a linear dynamic range exceeding 118 dB, a -3dB bandwidth surpassing 110 kHz and a room temperature detectivity of the order 1012 Jones.

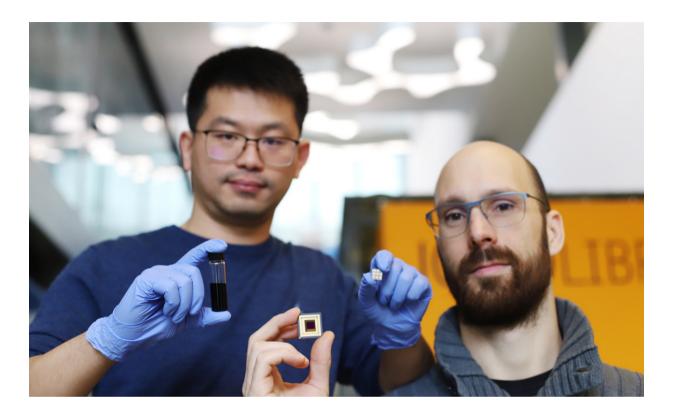
"To the best of our knowledge, the photodiodes reported here have for the first time realized solution processed, non-toxic shortwave infrared photodiodes with figures of merit on par with other heavy-metal containing counterparts", Gerasimos Konstantatos, ICREA Prof. at ICFO and leading author of the study mentions. "These results further support the fact that Ag<sub>2</sub>Te quantum dots emerge as a promising RoHS-compliant material for low-cost, high-performance SWIR photodetectors applications".

With the successful development of this heavymetal-free quantum dot based photodetector, the researchers went further and teamed up with Qurv, an ICFO spin-off, to demonstrate its potential by constructing a SWIR image sensor as a case study. The team integrated the new photodiode with a CMOS based read-out integrated circuit (ROIC) focal plane array (FPA) demonstrating for the first time a proof-of-concept, non-toxic, room temperature-operating SWIR quantum dot based image sensor. The authors of the study tested the imager to prove its operation in the SWIR by taking several pictures of a target object. In particular, they were able to image the transmission of silicon wafers under the SWIR light as well as to visualize the content of plastic bottles that were opaque in the visible light range.

"Accessing the SWIR with a low-cost technology for consumer electronics will unleash the potential of this spectral range with a huge range of applications including improved vision systems for automotive industry (cars) enabling vision and driving under adverse weather conditions", says Gerasimos Konstantatos. "SWIR band around 1.35-1.40 micrometers, can provide an eye-safe window, free of background light under day/night condition, thus, further enable long-range light detection and ranging (LiDAR), three-dimensional imaging for automotive, augmented reality and virtual reality applications".

Now the researchers want to increase the performance of photodiodes by engineering the stack of layers that comprise the photodetector device. They also want to explore new surface

"Accessing the SWIR with a low-cost technology for consumer electronics will unleash the potential of this spectral range with a huge range of applications"



 $Yong jie\ Wang\ (ICFO)\ and\ Julien\ Schreier\ (Qurv)\ holding\ a\ sample\ of\ a\ solution\ of\ quantum\ dots,\ the\ SWIR\ photodetector\ and\ the\ image\ sensor.$ 

chemistries for the  ${\rm Ag_2Te}$  quantum dots to improve the performance and the thermal and environmental stability of the material on its way to the market.

#### Reference:

Wang, Y., Lucheng, P. Schreier, J., Bi, Y. Black, A., Malla, A. Goossens, S., Konstantatos, G. (2023) Silver telluride colloidal quantum dot infrared photodetectors and image sensors. Nature Photonics.

DOI: https://www.nature.com/articles/s41566-023-01345-3



These results further support the fact that Ag<sub>2</sub>Te quantum dots emerge as a promising RoHS-compliant material for low-cost, high-performance SWIR photodetectors applications

## Novel lithography-free method yields durable antireflective glass surfaces

A team of researchers from ICFO and Corning Incorporated has developed a new method for fabricating anti-reflective (AR) surfaces achieved through nano-structured surfaces using a lithography-free process. The innovative method, described in the journal ACS Applied Materials and Interfaces, utilizes thermally dewetted silver as an etching mask to create nanohole structures on glass surfaces, significantly reducing light reflection.

Anti-reflective (AR) surfaces are valued for their ability to minimize unwanted reflections, enhancing the efficiency of various optical devices such as laser optics, camera lenses, eyeglasses, touchscreen displays, and solar harvesting systems. Several alternative strategies to that of the traditional multilayer anti-reflective coating procedure have been developed to increase the

performance and versatility of optical devices. Using bio-inspired nano-scale structures, such as nanopillars or nanoholes, directly onto a substrate surface enables the manipulation of light paths and reduces the reflection across a broad spectrum and wide range of angles.

However, the fabrication of these nano-structured surfaces with the desired properties is rather



Scheme representing the three main steps of the new method.

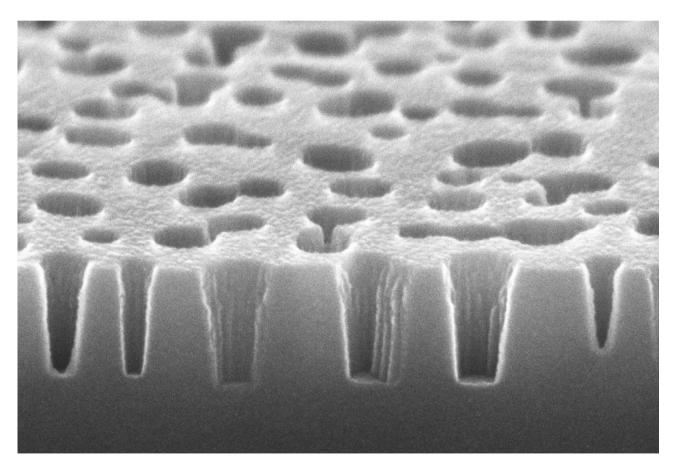
simplified method that achieves nanostructured AR surfaces. This approach uses thermally dewetted thin silver films as etching masks to generate subwavelength nanohole structures on the glass surfaces, characterized by its simplicity and cost-effectiveness by avoiding complex lithography. The results of this study have been recently published in the journal **ACS Applied Materials and Interfaces**.

complex, often involving multistep lithography methods, limiting their widespread adoption due to cost and scalability constraints.

Now, in a new study, ICFO researchers **Iliyan Karadzhov**, **Bruno Paulillo**, and **Juan Rombaut**, led by **ICREA Professor at ICFO Valerio Pruneri**, in collaboration with Corning Incorporated researchers Karl W. Koch and Prantik Mazumder, describe a

The fabrication process involves three main steps. Initially, silver nanoparticles are obtained by quickly thermally annealing an ultra-thin silver film onto a glass substrate. These particles then serve as a base for a secondary etching mask, created by depositing a thin nickel layer over the silver nanoparticles and performing selective chemical wet etching. Finally, this mask is used in a dry etching process to carve nanoholes of varying depths into the glass surface. "Nanoholes are tiny, irregularly arranged cavities on

"This process not only simplifies the fabrication of nanostructured antireflective surfaces but also enhances the mechanical resistance to abrasion"



View of the nanoholes carved on the glass substrate taken with Scanning Electron Microscope (SEM) showing their depth.

a surface that significantly reduce light reflection by smoothly transitioning the refractive index from air to substrate," explains Iliyan Karadzhov, an early-stage researcher at ICFO in the NANO-GLASS project. "They were chosen for their superior mechanical durability compared to other nanostructures like nanopillars and their ability to provide excellent AR properties with minimal light scattering," adds the first author of the study.

The final arrangement and depth of these nanoholes are determined by the initial thickness of the silver film and the duration of the dry etch process. The team fabricated several samples with varying initial masks and hole depths, testing their performance by measuring both transmittance and reflectance in the visible and near-infrared ranges. The newly developed AR surfaces exhibited a broadband omnidirectional response that achieves transmittance levels exceeding 99% in both the visible and near-infrared ranges, as well as maintaining high transmittance even at steep angles of incidence (up to 60 degrees).

The samples also demonstrated mechanical robustness and durability in abrasion tests. "One challenge was ensuring that the nanohole structures remained intact during abrasion tests while maintaining high optical performance," recalls Karl W. Koch, a researcher at Corning Incorporated. "This was overcome by optimizing the nanoholes' geometry and the fabrication process to balance the mechanical and optical properties. Another

challenge was scaling the fabrication method for large-area applications, which was addressed by leveraging scalable techniques like thermal dewetting," he adds.

"This process not only simplifies the fabrication of nanostructured antireflective surfaces but also enhances the mechanical resistance to abrasion, a critical factor for various applications," has stated Prantik Mazumder, a Corning Incorporated researcher.

"This new lithography-free method provides new possible solutions to the development of optoelectronic devices that require high transmission and durability," concluded Valerio Pruneri, the leading author of the study and NANO-GLASS project coordinator.

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Karadzhov, I., Paulillo, B., Rombaut, J., Koch, K.W., Mazumder, P., and Pruneri, V. Mechanically-durable antireflective subwavelength nanoholes on glass surfaces using lithography-free fabrication. ACS Appl. Mater. Interfaces 2024, 16, 15, 19672–19680.

DOI: http://doi.org/10.1021/acsami.3c15391

# Breaking boundaries in quantum photonics: New nanocavities unlock new frontiers in light confinement

In a significant leap forward for quantum nanophotonics, a team of European and Israeli physicists has introduced a new type of polaritonic cavities and redefined the limits of light confinement. This pioneering work, detailed in a study published in Nature Materials, demonstrates an unconventional method to confine photons, overcoming the traditional limitations in nanophotonics and simultanously achieving small volume and long lifetime photon confinement.

Physicists have long been seeking ways to force photons into increasingly small volumes. The natural length scale of the photon is the wavelength and when a photon is forced into a cavity much smaller than its wavelength, it effectively becomes more "concentrated". This concentration enhances interactions with electrons, amplifying quantum processes within the cavity.

However, despite the immense experimental success over the last decades, the effect of dissipation (optical absorption) remains a major obstacle in confining light to extremely small volumes. Photons in nanocavities are absorbed very quickly, often even before the photon reaches from one side of the cavity to the other. This dissipation limits the applicability of nanocavities to some of the most exciting applications in quantum electrodynamics.

The research group of ICREA Prof. Frank Koppens from ICFO has published a study in Nature Materials where they overcome this challenge by creating multimodal-enhanced cavities (MEC) with an unparalleled combination of subwavelength

volume and extended lifetime. These nanocavities, measuring smaller than 100x100nm² in area and only 3nm thin, confine light for significantly longer durations. The key lies in the use of hyperbolic-phonon-polaritons, unique electromagnetic excitations native to the 2D materials used to form the cavity. These hyperbolic polaritons are similar to ordinary light in most respects, but can be confined to extremely small volumes (much smaller than the wavelength cubed) in ways which defy the common intuition in optics.

#### When experiments outperformed the theoretical expectations

This discovery began with a chance observation made during a completely different project. While using a nearfield optical microscope to characterize a 2D material structure, the researchers noticed an unusually strong reflection when polaritons excited inside it hit the edge of a metallic substrate. This unexpected observation, at first sight anecdotal, turned out to be the underlying principle of a

"This paves the way to novel applications and advancements in quantum photonics, pushing the boundaries of what we thought was possible"

groundbreaking device.

The researchers figured out they could potentially use this newly discovered property to make nanocavities with high quality and small volume simultaneously, an achievement which until now eluded the nanophotonics community. The expectations were to obtain a slight improvement with respect to previous nanocavities, but when looking into the experimental measurements the team was in for a big surprise. The performance of the cavities doubled their expectations, exceeding the maximum predicted by the initial theoretical model. Even better, the nanocavities showed these relatively long lifetimes despite their reduced size (of the order of few nanometers).

"Experimental measurements are usually worse than theory would suggest, but in this case, we found the experiments outperformed the optimistic simplified theoretical predictions," said first author, Dr. Hanan Herzig Sheinfux, from Bar-Ilan University's Department of Physics. "This unexpected success paves the way to novel applications and advancements in quantum photonics, pushing the boundaries of what we thought was possible."

In fact, their MEC cavities were orders of magnitude smaller than any other optical resonator of comparable lifetime. However, their enormous achievement became their biggest challenge as well, as a theoretical explanation was still lacking. After months of study, they found out that "some really beautiful and surprisingly deep physics related to nano-ray formation and multimodal interaction was the responsible of it all", explains Dr. Herzig.

#### Multimodal-enhanced cavity of hyperbolic polaritons

The success of their nanocavities relied on a unique confinement mechanism as well as on the construction of the device. The nanocavities were crafted by drilling nanoscale holes in a gold substrate with the extreme (2-3 nanometers) precision of an He-focused ion beam microscope. After making the holes, hexagonal boron nitride (hBN), a 2D material that can support the hyperbolic phonon polaritons, was transferred on top of it. Light was meant to be confined inside the hBN in the region above the holes.

In the original model used to analyze the experiments, the confinement in the cavity can be likened to the increase in car traffic that occurs when a double lane expressway narrows down to a single lane. The incompatibility between the single and double lane traffic is forcing cars to congest, which is loosely similar to how light is reflected and confined when the substrate type changes at the edge of the hole into the gold substrate. The incompatibility between the suspended hBN and the hBN on gold acts as a "bottle neck" for polaritons, and light inside the cavity has a harder time leaking out.

However, as mentioned earlier, this simple model was unable to fully explain the experimental results. To do so, it turns out one needs to consider that hBN polaritons are a form of light-wave and that, unlike classical particles (like cars on a highway), they can be combined and interfere in complicated ways. Specifically, hBN polaritons can combine into multimodal ray-like excitations. The multimodal excitations that form above the nanoholes in

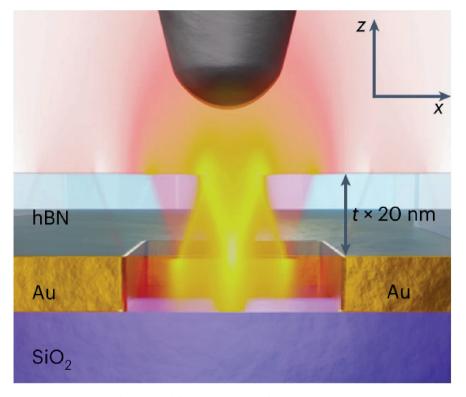
the metal are even more incompatible with the polaritons outside of the hole, leading to an even greater degree of confinement than otherwise possible.

Crucially, this method thus avoids shaping the hBN directly and preserves its pristine quality, enabling highly-confined AND long-lived photons in the cavity.

Prof. Koppens and Dr. Herzig intend to use these cavities as a novel platform for quantum light-matter interaction experiments in order to see quantum effects that were previously thought impossible, as well as to further study the intriguing and counterintuitive physics of hyperbolic phonon polariton behavior.

#### Reference:

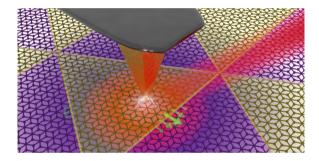
Hanan Herzig Sheinfux et al, High-quality nanocavities through multimodal confinement of hyperbolic polaritons in hexagonal boron nitride, Nature Materials (2024). DOI: https://doi.org/10.1038/s41563-023-01785-w



Schematic of the cross-section of a MEC cavity.

## A Novel One-Dimensional Superconductor

In a significant development in the field of superconductivity, researchers at the University of Manchester in collaboration with ICFO have successfully achieved robust superconductivity in high magnetic fields using a newly created one-dimensional (1D) system. This breakthrough offers a promising pathway to achieving superconductivity in the quantum Hall regime, a longstanding challenge in condensed matter physics.



Artistic view of the near-field nano-imaging technique used at ICFO to probe bilayer graphene domains and their boundaries. Credits: Matteo Ceccanti, ICFO

Superconductivity, the ability of certain materials to conduct electricity with zero resistance, holds profound potential for advancements of quantum technologies. It is for example used in key elements of future quantum computers. Notably, it was proposed that a robust superconductivity under strong magnetic fields could allow the creation of fault-tolerant quantum bits. However, achieving superconductivity under these conditions – in the so-called quantum Hall regime – has proven a mighty challenge.

The research, published in *Nature*, details an extensive work to achieve superconductivity in the quantum Hall regime led by a University of Manchester team, with the recently appointed

ICFO researcher **Dr. Julien Barrier** as its first and corresponding author, in collaboration with ICFO researcher **Dr. Roshan Krishna Kumar** and **ICREA Professor Frank Koppens** and other international institutions (the Kyung Hee University, University of Lancaster, National Institute of Materials Science and Yale University). They report on a novel method where superconductivity is supported by one-dimensional states

#### **Superconductivity with 1D electrons**

The researchers' initial efforts to induce superconductivity in high magnetic fields followed the conventional route in this community. In the proximity effect, a superconductor can induce its properties in a normal metal placed in contact with it. They intended to couple electrons propagating along device edges. To this end, the team started using a single graphene layer, cut in half with both sections kept only around 10 nanometers apart. Edge currents were expected to couple together at narrow distances, but the experiment proved otherwise: the distance between electrons was still too high.

The team built upon the acquired knowledge and followed with two graphene layers, one on top of another, misaligned by a very small angle (around 0.1°). In this situation, the sheets' structure rearranges because of important strains, which results in a very different configuration where micrometer scale domains form. These multiple regions are separated by narrow domain walls which were employed in the present study. Along these walls, the researchers proved that the electrons could propagate.

By exploiting this technique, "we fabricated superconducting junctions and observed a remarkably strong supercurrent at relatively 'balmy' temperatures (up to one Kelvin) in every single device", explains Dr. Barrier. "This was very encouraging, but we did not know the number of domain walls or where they were located. Probably, this was the biggest challenge we had to overcome".

Luckily, at that time, Dr. Roshan Krishna Kumar and Prof. Frank Koppens from ICFO had just released a technique to observe domain walls in encapsulated devices. "After discussing with Dr Krishna Kumar and Prof. Koppens, we sent a few devices to be imaged at ICFO, which allowed us to select the ones where we had certainty to have only one or two domain walls", recalls Barrier.

Thanks to these selected devices, the team was able to prove that the domain walls carried single-mode supercurrents, i.e. strictly 1D electronic states. With the study of devices incorporating a single domain wall, the research team was able to prove that their original interpretation of quantum Hall edge states forming on each side of the domain wall and coupling together to induce the superconductivity could not be correct. The domain walls carry their own one-dimensional electrons, which support more robust supercurrents at high magnetic fields than traditional quantum Hall edge states. The Manchester team also demonstrated that these states could be manipulated using gate voltages, and their superconducting properties could be influenced by the number of walls in a single device.

Overall, ICFO's imaging technique was crucial to prove that the observed superconductivity was caused by purely one-dimensional states, which allows such an effective superconductivity in the quantum Hall regime.

#### Opening the door to new physics discoveries

The discovery of single-mode 1D superconductivity shows exciting avenues for further research. These one-dimensional electron channels could be used in research outside of the field of superconductivity. High electron mobilities like the ones reported in this experiment are rare to achieve, because defects in the material tend to disrupt their motion. The ability to maintain high velocities is extremely desirable, since it can reduce heat dissipation of electronic devices, and most importantly, is a pre-requisite to induce new physics. For instance, high mobility in 2D systems allowed fascinating phenomena like the integer and fractional quantum Hall effects (Nobel Prizes in 1985 and 1998, respectively) to be observed.

Dr. Barrier concludes: "Our system introduces a novel platform for exploring physics in one-dimension. While we demonstrated its application in superconductivity, this 1D system holds promise for a vast range of technological advancements and fundamental research. The potential for our 1D system remains open-ended".

#### Reference:

J. Barrier et al., "One-dimensional proximity superconductivity in the quantum Hall regime" Nature number 628 issue 8009, (2024).

DOI: https://doi.org/10.1038/s41586-024-07271-w

Novel 2D electro-polaritonic platform for future miniaturized spectrometers

## Novel 2D electro-polaritonic platform for future miniaturized spectrometers

In a recent *Nature Communications* article, ICFO and an international team of researchers present the integration of a detector system and a polaritonic platform in the same 2D material, enabling for the first time the detection of 2D polaritonic nanoresonators with spectral resolution. The device is suitable for miniaturization and shows record levels of lateral confinement and high-quality factors simultaneously.

Polaritons are coupled excitations of electromagnetic waves with either charged particles or vibrations in the atomic lattice of a given material. They are widely used in nanophotonics because of their ability to confine light at extremely small volumes, on the order of nanometers, which is essential to enhance lightmatter interactions.

Two-dimensional materials (that is, materials only one-atom thick) are commonly used for this purpose, since the polaritons they host show even more extreme confinement, lower energy losses (resulting in longer lifetimes), and higher tunability than bulk materials.

#### Nanoresonators and polaritons for light confinement

To achieve even greater control over light confinement and enhance polaritonic properties further, nanoscale structures called nanoresonators can be employed. Moreover, when light interacts with a nanoresonator, it excites polaritons, which oscillate and resonate at

"Our platforms have exceptional quality, achieving record-breaking optical lateral confinement and high-quality factors of up to two hundreds, approximately"

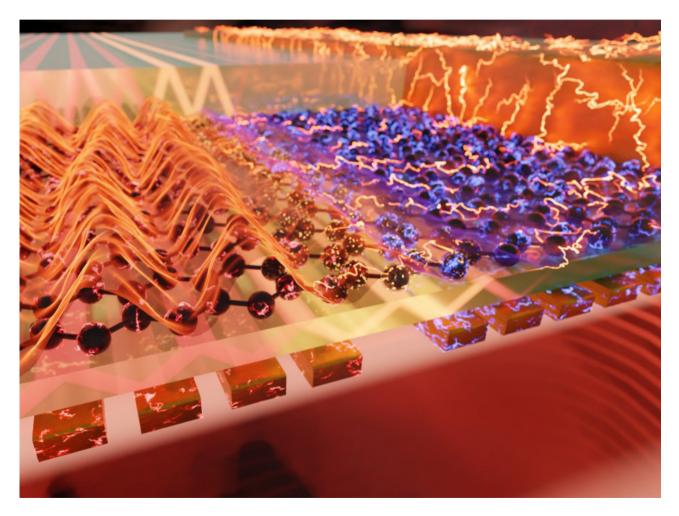
specific frequencies determined by the geometry and material properties of the resonator, enabling precise manipulation of light at the nanoscale.

While the use of polaritons for light confinement is an established practice, there is still room for improvement regarding the methods aimed at probing them. In the past years, optical measurements have become a common choice, but their bulky detectors require external equipment. This limits the miniaturization of the detection system and the signal clarity (known

as the signal-to-noise ratio) one can obtain from the measurements, which in turn hinders the application of polaritonic properties in areas where these two features are essential, such as molecular sensing.

Now, researchers from ICFO Dr. Sebastián Castilla,

Dr. Hitesh Agarwal, Dr. David Alcaraz, Dr. Adrià Grabulosa, Matteo Ceccanti, Dr. Roshan Krishna Kumar, led by ICREA Prof. Frank Koppens; the University of Ioannina; Universidade do Minho; the International Iberian Nanotechnology Laboratory; Kansas State University; the National Institute for Materials Science (Tsukuba, Japan); POLIMA



Schematic illustration of the electrical spectroscopy on the polaritonic-based graphene photodetector. Image courtesy from David Alcaraz Iranzo.

"Sensing, hyperspectral imaging, and optical spectrometry applications could benefit from this electro-polaritonic integrated platform. For instance, in the case of sensing, on-chip electrical detection of molecules and gases could become possible"

(University of Southern Denmark); and URCI (Institute of Materials Science and Computing, Ioannina) have demonstrated in a *Nature Communications* article the integration of 2D polaritons with a detection system into the same 2D material.

The integrated device enables, for the first time, spectrally resolved electrical detection of 2D polaritonic nanoresonators, and marks a significant step towards device miniaturization.

#### The novel platform presents several advantages

The team applied electrical spectroscopy to a stack of three layers of 2D materials, specifically, an hBN (hexagonal boron-nitrate) layer was placed on top of graphene, which was layered on another hBN sheet. During the experiments, researchers identified several advantages of electrical spectroscopy compared to commercial optical techniques. With the former, the spectral range covered is significantly broader (that is, it spans a wider range of frequencies, including the infrared and terahertz

ranges), the required equipment is significantly smaller, and the measurements present higher signal-to-noise ratios.

This electro-polaritonic platform represents a breakthrough in the field owing to two main features. First, an external detector for spectroscopy, required by most optical techniques, is no longer needed. A single device serves at the same time as a photodetector and a polaritonic platform, therefore enabling further miniaturization of the system. And second, while in general higher light confinement is detrimental to the quality of this confinement (for instance, shortening durations of light trapping), the integrated device successfully overcomes this limitation.

"Our platforms have exceptional quality, achieving record-breaking optical lateral confinement and high-quality factors of up to two hundreds, approximately. This exceptional level of both confinement and quality of graphene significantly enhances the photodetection efficiency", explains Dr. Sebastián Castilla, first co-author of the article.

Moreover, the electrical spectroscopy approach enables the probing of extremely small 2D polaritons (with lateral sizes of around 30 nanometers). "That was highly challenging to detect with conventional techniques due to the imposed resolution limitations", he adds.

#### **Future directions**

Castilla now reflects on what future discoveries could be unlocked by their new approach. "Sensing, hyperspectral imaging, and optical spectrometry applications could benefit from this electro-polaritonic integrated platform. For instance, in the case of sensing, on-chip electrical detection of molecules and gases could become possible", he suggests.

"I believe that our work will open the door to many applications that the bulky nature of standard commercial platforms has been inhibiting", adds the researcher.

#### Reference:

Castilla, S., Agarwal, H., Vangelidis, I. et al. Electrical spectroscopy of polaritonic nanoresonators. Nat Commun 15, 8635 (2024).

DOI: https://doi.org/10.1038/s41467-024-52838-w

The integrated device enables, for the first time, spectrally resolved electrical detection of 2D polaritonic nanoresonators, and marks a significant step towards device miniaturization

# New platforms for ultraconfined plasmons and optical coupling to external light

Researchers at ICFO tackle the problem of light confinement in nanocavities from two different perspectives. First, they successfully realize high-quality ultrathin crystalline metal structures that can support spatially compressed plasmons; and second, they demonstrate an efficient technique to couple light to confined surface plasmons.

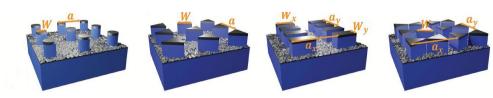
One of the biggest challenges in nanophotonics is the confinement of light inside small cavities. However, a small length scale is not the only desired property. Together with large lifetimes of the stored light and being able to work in the near-infrared frequency regime, they configure three essential features of the dreamed nanocavity that no one has simultaneously and efficiently accomplished yet.

There are many different types of materials and physics mechanisms available to build nanocavities. A promising approach is offered by the use of metals and the plasmon excitations (collective electron oscillations in the material) that they can support. Plasmons present two major advantages: they lie in the near-infrared regime, a spectral range of technological interest, and they offer an intrinsically high degree of confinement. Yet, confining photons for large lifetimes, a property generally quantified through the so-called quality factor, remains a

challenge.

One of the main reasons preventing wider exploitation of confined plasmons is their poor coupling to light. The cause relies on the disparity between the wavelength of plasmons (short because of the ultra-confinement they are being forced to) and light (larger). A conventional way to circumvent this obstacle consists in what is called "laterally structuring the material's surface". Indeed, the coupling increases but at the cost of modifying the cavity itself.

In a recent work published in *Advanced Materials* by researchers at ICFO, together with collaborators of the Materials Physics Center (CSIC-UPV/EHU), Basque Country University and Al-Azhar University, a few-atomics-layer-thick (less than 3nm) crystalline silver nanostructure was built, achieving higher quality than other cavities of similar thickness (a factor of the order of 10 compared to the



Scheme of the different geometries considered in the Advanced Materials article.

2-3 achieved by traditional techniques). Their results were obtained thanks to the new fabrication process, where they first lithographically introduced the lateral shapes on a silicon wafer and then evaporated silver films of epitaxial quality, obtaining ultrathin crystalline metal layers. This way, the team was able to reduce the detrimental effect of the imperfections.

Despite their major advances, the researchers wanted to go one step further. It seemed that the patterning process was fundamentally hindering the production of cavities with an even higher degree of quality and confinement, both simultaneously. That is when they decided to approach the problem from a different perspective. Instead of trying to reduce the imperfections introduced by the lithography, they left the surface of the cavity flat (avoiding the defects) and focused on increasing the coupling between light and plasmons.

The initial idea of ICREA Prof. at ICFO Javier García de Abajo and his group members Saad Abdullah, Dr. Eduardo Dias, Jan Krpenský and Dr. Vahagn Mkhitaryan materialized in a successful experiment, now published in ACS Photonics. In this study, they demonstrate a new method that couples light to flat surface plasmons more effectively than previous strategies.

## **Assisted light-plasmon coupling**

The experiment set-up consisted in the following: gold disks separated by a silica spacer from a planar gold surface. Plasmons lived in the latter and the goal was to couple incident light with them.

"The first approach aims at having high-quality films with lower loss and higher confinement, whereas the second one aims at optimizing parameters that allow for the maximum fraction of light coupled to plasmons"

To achieve this, a dipolar scatterer was introduced, a rather indispensable element as it assisted the otherwise inefficient light-to-plasmon coupling. The gold disks were in charge of doing this job and, so, the distance between them and the gold flat surface played a crucial role. As Saad Abdullah, the first author of the paper, says: "Pretty soon we understood that we needed a scatterer to mediate and assist the coupling of light to plasmons, but we were limited in our knowledge of where to place it".

In the end, they managed to demonstrate that there was a separation that maximized the coupling of incoming light to the plasmons underneath. However, the optimal distance varied depending on whether the disks were far apart from each other (so that interactions between them were forbidden) or placed closer (allowing those interactions). In the first case, the scatterers needed to be around 150 nanometers away from the gold surface, while in the second scenario, the best separation turned out to be five times shorter. This big difference highlights the influence of the interactions between scatterers when engineering light-to-surface coupling.

To sum up, the research group has provided two different strategies to face the same problem, both of them being an important step forward towards long-lived ultra-confinement of light. "The first

approach aims at having high-quality crystalline silver thin films that have a lower loss and allow for a high confinement, whereas the second one aims to optimize parameters that allow for the maximum fraction of the light coupled to plasmons", explains Abdullah.

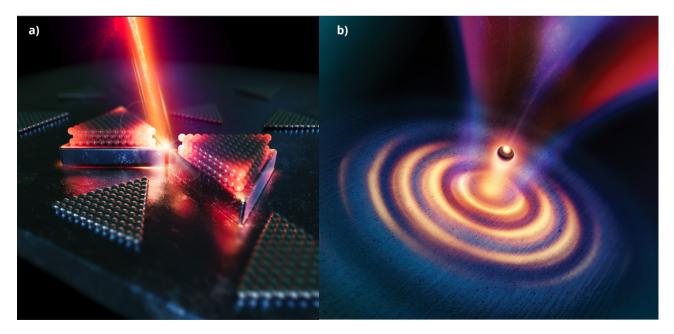
Now, the increased quality of plasmonic films they have provided may enhance the efficiency of plasmonic solar cells and photothermal detections, helping to improve diagnostics by limiting the losses associated with this equipment.

As Prof. García de Abajo finally remarks: "We have been able to successfully find new alternatives to understand light confinement in nanocavities from different perspectives. These results pose a major step forward in nanoplasmonic applications in optoelectronics, optical sensing, and the exploration of quantum-optics phenomena at the few-nanometer length scale".

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Mkhitaryan, V. et al. Ultraconfined plasmons in atomically thin crystalline silver nanostructures. Adv. Mater. 23, 25820 (2022). DOI: https://doi.org/10.1002/adma.202302520

Saad Abdullah, Eduardo J. C. Dias, Jan Krpenský, Vahagn Mkhitaryan, and F. Javier García de Abajo ACS Photonics 2024 11 (6), 2183-2193 DOI: 10.1021/acsphotonics.3c01742



a: A new fabrication method, consisting in prepatterning atomically flat silicon and epitaxially growing few-atomic-layer crystalline silver films, produce structures that support ultraconfined and relatively long-lived plasmons.

b: Coupling to confined surface plasmons is demonstrated to be boosted through dipolar scatterers prepared at a suitable distance from the surface. This concept is here implemented with gold disks acting as scatterers and separated from a gold surface by a silica spacer.

# First spatial observation of an entire second-order superlattice in twisted bilayer graphene

A team led by ICFO was able to map, for the first time, the entire spatial distribution of a secondorder superlattice within a twisted bilayer graphene device, offering a deeper fundamental understanding and revealing previously hidden features of this kind of structures.

The study shows that these structures are very sensitive to strain and to the twist angle between layers, and thus they could serve as a 'magnifying glass' to detect deviations of these parameters when engineering bilayer graphene devices.

In March of 2018, an international team led by Pablo Jarillo-Herrero from the MIT reported the discovery of superconductivity when two layers of graphene (a two-dimensional, that is, one-atom thick, layer of graphite) were stacked on top of each other with a twist angle of 1.1°. The small twist between the layers induces an interference pattern (known as moiré pattern) with a periodicity that depends on the twist angle. For the very specific 'magic angle' of 1.1°, the electronic properties are changed in such dramatic fashion that it leads to exotic physics such as the discovered superconductivity.

After that, material scientists from all over the world started to stack and twist two-dimensional materials, hoping for interesting effects -such as correlated interactions and superconductivity- to arise. As expected, slight rotations consistently gave rise to exotic physical phenomena, dramatically altering the electronic properties of the mono-layers on their own.

Nowadays, twisted bilayer devices are already quite a 'standard' practice, and the community has started to increase the number of twisted layers. This can

lead to an interference effect between the moiré lattices corresponding to different pairs of twisted bilayers. Consequently, such 'moiré superlattice of two moiré lattices' can have periodicities of hundreds of nanometers, exceeding those of the underlying moiré lattices. Due to this dramatically increased periodicity, the so-called second-order superlattice (SOSL) can be spatially observed with optical techniques. Even though some techniques (for instance, STM) have provided insights on the mechanisms taking place inside this kind of structures, they can only address a small subsection of the device, offering limited information. Instead, a direct visualization of SOSLs' entire spatial distribution across a device would provide a deeper fundamental understanding and potentially reveal undiscovered features.

The observation of the spatial distribution of a whole SOSL was still lacking until, recently, an article in *Nature Materials* came out. ICFO researchers **Dr.** Niels C. H. Hesp, Sergi Batlle-Porro, Dr. Roshan Krishna Kumar, Dr. Hitesh Agarwal, Dr. David Barcons Ruiz, Dr. Hanan Herzig Sheinfux, Dr. Petr Stepanov, led by ICREA Prof. Frank H. L. Koppens,

in collaboration with NIMS and University of Notre Dame have reported on a new type of experiment that, for the first time, maps the entire SOSL inside a twisted bilayer graphene device.

The team stacked two layers of graphene on top of a hexagonal Boron Nitrate (hBN) layer. They then performed cryogenic nanoscale photovoltage measurements (in short, cryoSNOM) and electronic transport measurements. The former combines high spatial resolution with extreme sensitivity to local electronic properties, while the latter was used to verify the twisting angles between layers and to confirm the presence of magic-angle physics. Supported by simulations, the team finally unveiled the unprecedented sensitivity of SOSLs to the strain experienced by the material and the twist angle between the layers, but the journey until arriving to these results was full of surprises.

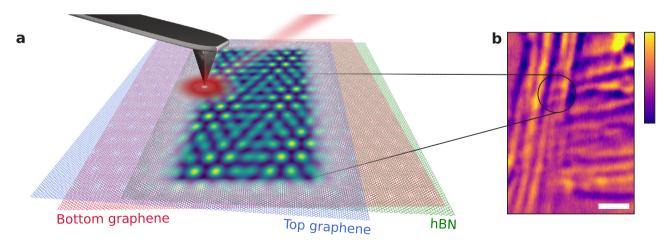
## From measurement issues to signs of a SOSL

The whole story started when the team applied

cryogenic nano-imaging and electronic transport measurements to the sample. The initial goal was to obtain hints of correlated physics and superconductivity, but throughout the process they observed some unusual patterns that no one had seen before.

Their immediate reaction was to assume that there was something wrong with the measurement system. "The cryoSNOM was facing many issues, so we suspected that the tip (the contact point of the measurement setup with the sample) was broken", explains Dr. Niels Hesp, first author of the article. But it seemed that, at least at that particular moment, the measurement system was perfectly fine.

They therefore decided to further explore these unexpected patterns, which presented a large period (of about 400 nanometers), in an attempt to discover their nature and origin. In the end, researchers realized these long-range periodicities were a clear indicative of SOSLs. "That was very extraordinary as well, because it is very unlikely to have a device prepared in this state", recalls Hesp, since "it is very hard to get the twist angles exactly right".



a: Schematic of the formation of an SOSL and the experimental design.

b: Example of a photovoltage measurement on the reported device, revealing periodic modulations that are attributed to the SOSL.

The team was not intending for this, but they embraced the opportunity, changed course of action and focused on the next step: to get proper measurements done on the sample to fully characterize it. They knew it was a challenge, as with the least voltage the device could get burnt. They needed to be extremely careful. "At some point, the cryoSNOM unexpectedly started warming up, which partially broke the sample. I was able to fix it in time, avoiding irreparable damage. Luckily, the unique device had only a little hole in the middle, leaving the second-order superlattice surprisingly unaffected", shares Dr. Petr Stepanov.

Another surprise came right after that, when researchers noticed in the simulations that the second-order superlattice manifests itself when the alignment between the graphene layers coincides exactly with the 'magic angle' of twisted bilayer graphene. Hesp, though, remarks the lack of a fundamental relation between both phenomena: "We don't see any causality between the twist angle where magic-angle physics occurs and where a SOSL occurs, and therefore it is to us a coincidence. Yet, this means that when the twist angle of the hBN layer is tuned right, the twisted bilayer graphene device not only shows magic-angle physics but also hosts a SOSL, which makes the physics of magic-angle twisted bilayer graphene even richer". Hesp also suspects that, even though the reported configuration does not modify the magic-angle

"The device not only shows magic-angle physics but also hosts a SOSL, which makes the physics of magic-angle twisted bilayer graphene even richer" physics at first sight, it will affect how some exotic phenomena (such as the anomalous Hall effect) manifest within these systems.

# A 'magnifying glass' to precisely tune strain and twist angles in bilayer graphene

The holistic spatial observations that the team carried out showed that minuscule variations in the strain and twisting-angle led to drastic changes in the second-order superlattice structure. In this sense, the reported method serves as a 'magnifying glass' to spot small deviations with respect to the desired strain and twist angles. Thus, it could be used to realize quality controls in magicangle twisted bilayer graphene devices, avoiding inaccuracies during its fabrication process.

Hesp, who started this project right at the end of his PhD, is proud of how everything turned out: "If you ask me what the beauty of this work is, I would say it is not only the fascinating richness in superlattices that one can create, but also that it reveals a sizeable effect that is present in part of the twisted-bilayer graphene devices that people study without realising it".

## Reference:

Hesp, N.C.H., Batlle-Porro, S., Krishna Kumar, R. et al. Cryogenic nano-imaging of second-order moiré superlattices. Nat. Mater. (2024).

DOI: https://doi.org/10.1038/s41563-024-01993-y

# New on-chip device uses exotic light rays in 2D material to detect molecules

Researchers have developed a highly sensitive detector for identifying molecules via their infrared vibrational "fingerprint". Published in *Nature Communications*, this innovative detector converts incident infrared light into ultra-confined "nanolight" in the form of phonon polaritons within the detector's active area. This mechanism serves two crucial purposes: it boosts the overall detector's sensitivity and enhances the vibrational fingerprint of nanometer-thin molecular layer placed on top of the detector, allowing this molecular fingerprint to be more easily detected and analyzed.

The compact design and room-temperature operation of the device hold promise for developing ultra-compact platforms for molecular and gas sensing applications.

Molecules have some sort of fingerprints, unique features that can be used to differentiate them. Each type of molecule, when illuminated with the right light, vibrates at a characteristic frequency (its resonance frequency, which typically occurs at infrared frequencies) and strength. Similar to what can be done with human fingerprints, one can exploit this information to distinguish different types of molecules or gases from each other. That can also protect us from potential dangers, by identifying poisonous and dangerous substances or gases instead of criminals.

One conventional approach is infrared fingerprint spectroscopy, which uses infrared reflection or transmission spectra to identify different molecules. However, the small size of organic molecules compared to the infrared wavelength results in a weak scattering signal, making it challenging to detect small quantities of material. In recent years, this limitation has been addressed using Surface-Enhanced Infrared Absorption (SEIRA) spectroscopy. SEIRA spectroscopy leverages

infrared near-field enhancement provided by rough metal surfaces or metallic nanostructure to amplify the molecular vibrational signals. The main advantage of SEIRA spectroscopy is its ability to measure and study minute material quantities.

Recently, phonon polaritons—coupled excitations of electromagnetic waves with atomic lattice vibrations—particularly hyperbolic phonon polaritons in thin layers of hexagonal boron nitride (hBN), have emerged as promising candidates for boosting the sensitivity of SEIRA spectroscopy. "Previously, we demonstrated that phonon polaritons can be applied for SEIRA spectroscopy of nanometer-thin molecular layers and gas sensing, thanks to their long lifetimes and ultra-high field confinement," says Prof. Rainer Hillenbrand from Nanogune.

However, SEIRA spectroscopy remains a farfield technique that requires bulky equipment, such as light sources, SEIRA substrates, and typically nitrogen-cooled infrared detectors. This reliance on large instruments limits its potential for miniaturisation and on-chip applications. In parallel, "we have been investigating graphene-based infrared detectors that operate at room temperature, and we have shown that phonon polaritons can be electrically detected and can enhance detector sensitivity," adds Prof. Frank Koppens from ICFO.

By combining these two progresses, a team of researchers has now successfully demonstrated the first on-chip phononic SEIRA detection of molecular vibrations. This result was made possible through the joint experimental efforts of Nanogune and ICFO researchers, along with theoretical support from the groups of Dr. Alexey Nikitin at the Donostia International Physics Center and Prof. Luis Martín-Moreno at the Instituto de Nanociencia y Materiales de Aragón (CSIC- Universidad de Zaragoza). The researchers employed ultra-confined HPhPs to detect molecular fingerprints in nanometer-thin molecular layers directly in the photocurrent of a graphene-based detector, eliminating the need for traditional bulky IR detectors.

"One of the most exciting aspects of this approach is that this graphene-based detector opens the

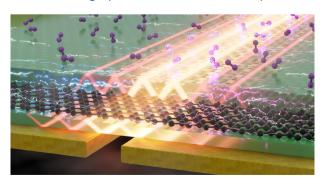


Illustration of an on-chip molecular vibration sensor based on a graphene IR detector, where phonon polaritons (bright rays) enhance the molecular fingerprint signal encoded in the photocurrent. Credit: Dr. David Alcaraz, ICFO

"We could create a true 'lab-ona-chip', capable of identifying specific molecules in small liquid samples—paving the way for medical diagnostics and environmental monitoring"

way towards miniaturisation," comments ICFO researcher Dr. Sebastián Castilla. He continues: "By integrating this detector with microfluidic channels, we could create a true 'lab-on-a-chip', capable of identifying specific molecules in small liquid samples—paving the way for medical diagnostics and environmental monitoring."

In a longer-term picture, Nanogune researcher and first author of the study, Dr. Andrei Bylinkin, believes that "on-chip infrared detectors operating at room temperature could enable rapid molecular identification, potentially integrated into smartphones or wearable electronics." He further believes that "this would offer a platform for compact sensitive, room-temperature infrared spectroscopy."

## Reference:

Bylinkin, A., Castilla, S., Slipchenko, T.M. et al. On-chip phononenhanced IR near-field detection of molecular vibrations. Nat Commun 15, 8907 (2024). Featured in the journal's Editors' Highlights

DOI: https://doi.org/10.1038/s41467-024-53182-9

# Smart sampling in time-domain spectroscopy

A team of researchers explore how time-domain spectroscopy can benefit from a well-designed sampling scheme. The proposed strategy leads to much shorter acquisition times while preserving the spectroscopic information content.

Optical spectroscopy is at the core of light-matter interaction. Modern ultrafast spectroscopy typically exploits broadband lasers with the pulse delay scanned in the time-domain. This research field, called time-domain spectroscopy, finds applications in material characterization (which, in turn, can be relevant for areas as diverse as chemistry, biology or energy), sensing or molecular classification, among others.

In general, one needs to sample a sufficient number of time steps over a long enough time range to capture the spectral response as a whole. The higher the number of samples, the more accurate reconstruction. As a downside, increasing this number requires longer data acquisition times, something that can become experimentally unfeasible, especially in more complex multidimensional spectroscopies. As surprising as it may seem, little attention to the sampling strategy has been paid within the field of spectroscopy, where generally only uniform or random distributions tend to be considered.

Now, with the aim of collecting data more effectively, ICFO researchers **Dr. Luca Bolzonello** and **Prof. ICREA Niek van Hulst**, together with Andreas Jakobsson from Lund University, have introduced a systematic approach to optimize the sampling scheme in time-domain spectroscopy experiments. The results, published in **The Journal of Chemical Physics**, show how, in stark contrast with the

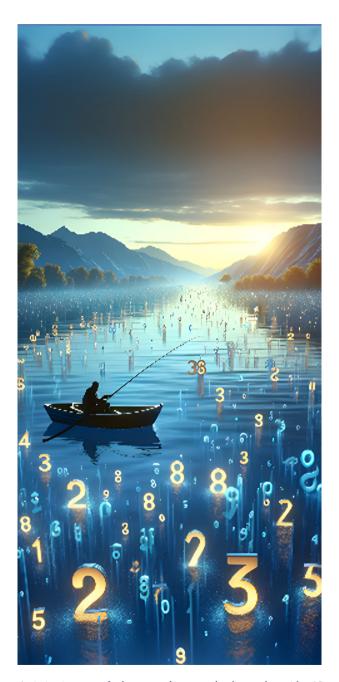
"this optimization not only saves time, but also reduces costs, minimizes sample degradation, and improves the overall efficiency"

inefficiency of traditional sampling methods, their technique can significantly reduce the acquisition time while maintaining or even enhancing the quality of the data collected.

According to Dr. Luca Bolzonello, first author of the article, "this optimization not only saves time, but also reduces costs, minimizes sample degradation, and improves the overall efficiency of experimental setups".

# Optimizing the sampling scheme

The goal of the study was to find the balance between getting the maximum possible information and carrying out the minimum number of data acquisitions. The proposed method exploits the prior knowledge of the spectroscopist performing the experiment to optimize the sampling scheme, as this foreknowledge avoids the collection of noisy data points with low information content.



Artistic image of the sampling method, made with AI (ChatGPT) by Luca Bolzonello.

More technically, researchers make use of the socalled Fisher information. Roughly speaking, the Fischer parameter matrix quantifies how much one can learn about a parameter based on the chosen sampling scheme and the noise of the experiment. "It turns out that this allows us to estimate the final uncertainty of measurements before they are even taken", explains Bolzonello. "By focusing on the most informative points, we can reduce the number of samples needed while still getting accurate and precise parameter estimates. This approach systematically enhances the quality of the data collected, making the experiments more efficient and informative".

The technique was benchmarked with several case studies, showcasing its potential to benefit the spectroscopic research. Now the team plans to implement this optimized sampling technique in a broader range of spectroscopic experiments to validate its effectiveness across different applications. In particular, classification of fluorescent signals, material characterization and the study of molecular ultrafast dynamics are the areas that will benefit the most.

## Reference:

Bolzonello L, van Hulst NF, Jakobsson A. Fisher information for smart sampling in time-domain spectroscopy. J Chem Phys. 2024 Jun 7;160(21):214110.

DOI: https://doi.org/10.1063/5.0206838

# Attosecond core-level spectroscopy reveals real-time molecular dynamics

# Attosecond core-level spectroscopy reveals real-time molecular dynamics

A team of European researchers has developed an attosecond core-level spectroscopy technique that can track the many-body molecular dynamics on its natural ultrafast timescale. Their work was benchmarked with furan, showing the power of their tool by successfully retrieving the entire history evolution of the dynamics and relaxation processes of a heterocyclic organic ring.

Chemical reactions are complex mechanisms. Many different dynamical processes are involved, affecting both the electrons and the nucleus of the present atoms. Very often the strongly coupled electron and nuclear dynamics induce radiation-less relaxation processes known as conical intersections. Such dynamics, which are at the basis of many biological and chemical relevant functions, are extremely difficult to experimentally detect.

The problem arises when one tries to simultaneously trace the nuclear and electronic motion, as their dynamics are hard to disentangle and they occur at comparable ultrafast timescales. That is why, in the past few years, capturing the molecular dynamical evolution in real-time has turned into one of the most burning challenges shared by physicists and chemists.

However, in a recent *Nature Photonics* publication, ICFO researchers **Dr. Stefano Severino**, **Dr. Maurizio Reduzzi**, **Dr. Adam Summers**, **Hung-Wei Sun**, **Ying-Hao Chien** led by the **ICREA Prof. at ICFO Jens Biegert**, together with theory support by Dr. Karl Michael Ziems and Prof. Stefanie Gräfe from the Friedrich-Schiller-Universität Jena, have

presented a powerful tool based on attosecond core-level spectroscopy to investigate molecular dynamics in real-time, which is capable of overcoming the aforementioned challenges.

They have benchmarked their method tracing the evolution of gas-phase furan, an organic molecule made of carbon, hydrogen and one oxygen arranged in a pentagonal geometry. Its cyclic structure gives this kind of species the name of chemical "ring". The choice was not arbitrary, as furan is the prototypical system for the study of heterocyclic organic rings, the essential constituents of many different day-to-day products such as fuels, pharmaceuticals or agrochemicals. Knowing their dynamics and relaxation processes is thus of huge importance.

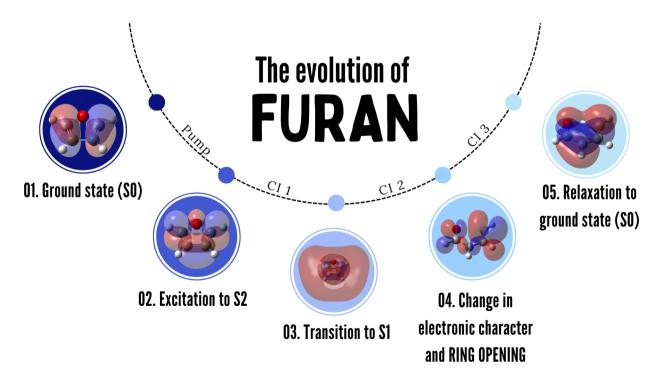
"The team was able to time-resolve the details of the entire ring-opening dynamics of furan"

# Life history of furan unlocked

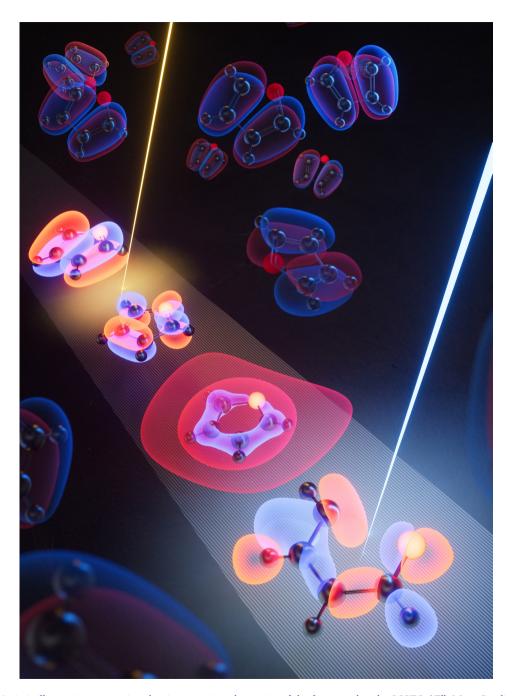
The team was able to time-resolve the details of the entire ring-opening dynamics of furan, that is, the fission of the bond between one carbon and the oxygen, which breaks its cyclic structure. To do it, they had to track the so-called conical intersections (CI), ultrafast gateways between different energy states that furan undertakes in its evolution towards ring-opening.

In their experiment, a light beam (the pump pulse) first excited the furan molecule. Then, an attosecond and much weaker pulse (the probe) was used to monitor the pump-induced changes in the sample. After the initial photoexcitation, the three expected conical intersections were located in time by analysing the changes in the absorption spectrum as a function of the delay between pump and probe. The appearance and disappearance of absorption features, as well as their oscillatory behaviour, provide signatures of the changes in the electronic state of furan.

On top of that, they could see that the passage through the first CI transition generates a quantum superposition between the initial and final electronic states, which manifested in the form of quantum beats. This ultrafast-phenomenon, which can only be explained using quantum theory, was extremely hard to identify in previous experiments. The second CI was in principle even more challenging



Schematic illustration portraying the details of the entire ring-opening dynamics of furan. ©ICFO



 $Artistic\ illustration\ portraying\ the\ ring-opening\ dynamics\ of\ the\ furan\ molecule.\ @ICFO\ /\ EllaMaru\ Studio.$ 

to capture, as the final electronic state does not emit nor absorb photons (it is an optically dark state) and thus its detection through conventional methods is extremely demanding. Nevertheless, in this case their platform performed the task as well as before

After that, the ring-opening was supposed to occur and the team's equipment was victorious again in its detection. The passage of the molecule from a closed to an open ring geometry implies a symmetry breaking that is imprinted in the absorption spectrum. The spectroscopic tool used by the researchers demonstrated to be extremely sensitive to the nuclear structure, and the ring-opening manifested itself as the appearance of new absorption peaks.

Finally, the molecule relaxed into the ground state (the lowest molecular orbital available) through the third conical intersection, whose transition was again accurately time-resolved.

# The success of attosecond core-level absorption spectroscopy

All in all, Biegert and his group have proposed and successfully reported on a new analytical methodology to unveil the complex and intricated process of molecular ring opening in its native ultrafast timescale. The combined high temporal resolution and coherent energy spectrum of their cutting-edge technique allowed them not only to track the transitions of furan across conical intersections, but also to identify electronic and nuclear coherences, quantum beats, optically dark states and symmetry changes, providing an extremely detailed picture of the whole relaxation process.

It is important to highlight that the power of attosecond core-level spectroscopy is not limited

"this new mechanism can bring to light the complex dynamics of relevant functions, such as the photoprotection mechanism of the DNA basis"

to this particular molecule, but consists in a general tool designed to be employed with other species too. Therefore, this new mechanism can bring to light the complex dynamics of relevant functions, such as the photoprotection mechanism of the DNA basis. Furthermore, the researchers identify the manipulation of efficient molecular reaction and energy relaxation dynamics as some of the most promising applications for their work.

## Reference:

Attosecond core-level absorption spectroscopy reveals the electronic and nuclear dynamics of molecular ring opening, S. Severino, K. M. Ziems, M. Reduzzi, A. Summers, H.-W. Sun, Y.-H. Chien, S. Gräfe & J. Biegert, 2024, Nature Photonics 18, pages731–737

DOI: https://doi.org/10.1038/s41566-024-01436-9





# Progress and remaining challenges in LIED, a "molecular selfie" technique

ICFO researchers review laser-induced electron diffraction (LIED), a high-resolution imaging technique that captures the structure of single gas-phase molecules using one of their own electrons, highlighting its main advantages and limitations.

Molecules constantly evolve and interact with each other, adapting their structure accordingly in the process. One of the grand challenges in science is visualizing how molecules undergo these transformations. Ideally, scientists would like to pinpoint and track over time the location of all the atoms in a molecule. This is, however, an extremely demanding task. Achieving it would require technologies with extraordinary sensitivity to detect individual molecules and unparalleled precision to map their atoms in space and time.

Laser-induced electron diffraction (LIED) makes imaging a single gas-phase molecule and locating all its atoms possible, achieving exceptional picometer (10<sup>-12</sup> meters) spatial and attosecond (10<sup>-18</sup> seconds) temporal resolution. LIED has been extensively refined and successfully applied at ICFO, resulting in numerous impactful outcomes and highlighting the institute's prominent role in driving progress in this state-of-the-art technique. ICFO researchers Dr. Katharina Chirvi and ICREA Prof. Jens Biegert have recently presented a comprehensive review of LIED in Structural Dynamics. In there, they give an overview of the technique, from its origins to the current state-of-the-art, explaining its underlying physical principles and focusing on the main strengths and limitations. The article serves as a valuable resource for understanding the current state of LIED, its methodologies, and the future potential it offers for advancing molecular dynamics research

# LIED's basic principles, strengths and weaknesses

The review explains the LIED's imaging process, which begins with a strong laser pulse focused onto a gas-phase molecule under study. The intense light ionizes the molecule, liberating an electron that is initially driven away by the laser's electric field. In a phenomenon known as recollision, the electron reverses its trajectory and returns to scatter off its parent ion. This electron scattering generates a diffraction pattern that encodes information about the molecule's interatomic distances. By analysing this data, LIED reconstructs the molecule's 3D structure with picometer and attosecond resolution—pushing the boundaries of what is physically possible in imaging.

Therefore, by employing one of the molecule's own electrons, the LIED technique achieves high-quality images, which the authors refer to as "molecular selfies". But this was not always the case. In its early stages, LIED could only image small linear and symmetric diatomic molecules. Over time, the technique evolved to retrieve 2D, and then

"by employing one of the molecule's own electrons, the LIED technique achieves high-quality images"

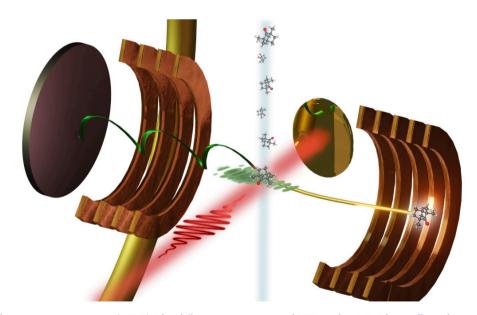
also 3D molecular structures. Today, LIED can be applied to a variety of molecular systems, including large complex structures that were previously inaccessible.

The article, though, emphasizes the importance of fulfilling several critical conditions for effective imaging, such as ensuring the electron has sufficient impact energy during recollision. The authors also describe different LIED implementations, each with its own set of advantages and limitations, which can also affect the overall performance and applicability of the technique.

Looking ahead, the researchers highlight the importance of extending the temporal observation window available for the technique, something that "would allow for a long-standing dream of scientists, namely, to produce atomic-resolution images of single molecules undergoing structural transformations."

# Reference:

K. Chirvi, J. Biegert; Laser-induced electron diffraction: Imaging of a single gas-phase molecular structure with one of its own electrons. Struct. Dyn. 1 July 2024; 11 (4): 041301. DOI: https://doi.org/10.1063/4.0000237



Scheme of a reaction microscope (REMI). The different incarnations of LIED with a REMI have allowed us to move from imaging 1D to 2D and to complex and chiral 3D molecular structures. Source: Structural Dynamics.

# **Pablo Jarillo**

Cecil and Ida Green Professor of Physics at the Massachusetts Institute of Technology and Distinguished Invited Professor at ICFO.

December 2023, ICFO

You have received many global recognitions for your demonstration of the magic angle twisted bilayer graphene. Was this a serendipitous discovery?

It's a little bit of both. There was some theoretical work about the electronic properties of magic angle twisted bilayer graphene, and we had been working in this field for about eight years before we made the discovery, so it's not something that happened randomly or accidentally. In fact, two dimensional crystalline materials came on the market around 2004 and 2005, but for many years people did not really pay too much attention to that. It was not until 2010, when several very flat, two-dimensional materials were isolated, that they started to be investigated more in detail. Then people started to change the angle between two dimensional crystalline planes. Already in 2010, my group and others started to play with changing this twist angle. And that process lasted from 2010 until 2018, when our discovery was made.

On the other hand, the type of physics we were pursuing was different from the one that we found, and no one had theoretically predicted the actual properties that we discovered. In that sense, it was a serendipitous discovery because we found something that was much bigger than what we were looking for. It's like we were looking for a small treasure and we found a big treasure.



"When I thought about taking a sabbatical, ICFO was the natural place for me to take it and the Cellex Foundation helped to make this possible."

Almost six years have passed since the famous experiment. How do you see the future of Twistronics now?

There are still many, many things to learn. In addition to graphene, several other materials have now been twisted on top of themselves and very interesting physics has been discovered, but there are hundreds of 2D materials and endless possibilities.

Now scientists are using the analog of twisting things in many other fields of physics. At ICFO and many other places, people are doing twisted photonics, for example, for photons, and others are doing twisted phononics, for classical or quantum vibrations of objects. People are doing twisted cold atom lattices. In other places people are doing twisted electrochemistry... This is expanding into many other areas of physics and neighboring fields.

That is also something very interesting, because it allows one community to learn from the other. So far, it's been mostly physicists working on this, but engineers are starting to pay attention. But, right now, we do not know how to produce these devices at large scale, how to make many of them and all of them equal. That's an impediment towards using them in applications, and also towards exploring them more, because, as I said, we have millions of combinations of materials, angles and twists; too many to be explored manually.

I joke that my PhD students are like medieval monks that are making one manuscript at a time, which takes an enormous amount of time. That manuscript is unique and cannot be easily copied or repeated. If you want a new device, you have to write another manuscript by hand. We need something similar to what happened with the printing press - the quantum press, or the twistronics press- which will enable us to, in an automated, controlled, robotic way, make thousands of devices. This could make it possible to incorporate Twistronics into applications, moving beyond science.

# You are currently on sabbatical at ICFO. What drew you here?

I have been collaborating for many years with colleagues at ICFO, mostly with the group of Frank Koppens but also with Adrian Bachtold and now with Carmen Rubio Verdú. When I thought about taking a sabbatical, ICFO was the natural place for me to take it and the Cellex Foundation helped to make this possible. I am originally from Valencia so geographically it was very appealing, but also scientifically it made great sense. To begin, I wanted to strengthen collaborative projects that we have between MIT and ICFO. I had strong collaborations and many shared papers with ICFO Pls, but now I also know the researchers in their groups and that's very rewarding and interesting. The sabbatical is an opportunity to strengthen the ties between MIT and

Spain's research community in general, with ICFO as a home base.

# You are co-leading the QTwist program at ICFO with Prof. Frank Koppens and Prof. Claudia Felser. What do you find most exciting about it?

QTwist is something of an umbrella initiative that encompasses several collaborations and a growing list of projects. Together with Claudia and Frank, as well as with Amir Yacoby from Harvard University who has also been spending part of his sabbatical here, and a number of very strong researchers from around the world who are starting to spend more time at ICFO, we are looking forward to working on some collaborative projects linking both sides of the Atlantic.

We want to work on things which few people are exploring right now. In particular, one of the things that we are quite interested in is making chiral structures. You can think of them as helical structures. DNA, for example, is a helical structure. So these structures can be right handed or left handed, similar to what happens with your hands. Twisted materials, when you put them on top of each other, can be twisted right-handed or left-handed. This is something quite interesting that we are beginning to investigate with the QTwist project.

We also aim to explore the quantum electronic properties of different twisted 2D materials, but in a more scalable way. An important component of this could be the automatic robotic exploration of 2D materials, which is something that no one in the world has accomplished yet. We think that a collaboration between ICFO, MIT, Max Planck and other leading institutions may be able to achieve it.

# QUANTUM PHYSICS

# ICFO's 2024 in Quantum Physics

In the early 21st century, we find ourselves amidst a second quantum revolution. We are now able not only to realize but also to meticulously study exotic quantum phenomena, and to harness quantum effects for technological applications. ICFO has been really active in quantum research this 2024, carrying out initiatives that are not only at the forefront of contemporary research in fundamental quantum science, but they also extend to the development of groundbreaking quantum technologies.

On the one hand, there have been numerous discoveries on fundamental quantum science. The Quantum Optics Theory group has been particularly interested in topological theories (delving into topological properties of matter and topological phase transitions), synthetic dimensions together with the Ultracold Quantum Gases group, many-body localization, and high harmonic generation, proposing analog simulators for their study and theoretically unveiling the quantumness of the emitted light, experimentally demonstrated later on with the participation of the Attoscience and Ultrafast Optics group. Regarding topology, the Quantum Nano-Optoelectronics group demonstrated, for the first time, deep subwavelength topological edge states. Moreover, the Nanophotonics Theroy group showed the interaction of low energy photons with light reveal quantum effects, the Quantum Engineering of Light gave new insights into photon coherence and distinguishability, and the Quantum Information Theory group found a new way to theoretically certify ground-state properties beyond the energy. Finally, the Attoscience and Ultrafast Optics group discovered a way to control valley polarization in bulk materials.

On the other hand, there have also been many discoveries on quantum technologies and applications. The Quantum Photonics with Solids and Atoms group transmitted entanglement in Barcelona, propagated entanglement securely and generated indistinguishable photons from dissimilar quantum nodes. Regarding the generation of photons, the Optoelectronics group developed a new photon pair quantum source. The Ultracold Quantum Gases group launched QUIONE, a strontium quantum-gas microscope that serves as a first step to construct quantum simulators; the Atomic Quantum Optics group presented a new readout method that can help to miniaturize quantum sensors; and the Theoretical Quantum-Nano Photonics demonstrated a new class of quantum optical antennas.

# Novel topological properties of matter emerge from an ultra-cold atom-cavity system

An international team of researchers reports on a new method that permits inducing symmetry-protected higher-order topology through a spontaneous symmetry-breaking mechanism in a two-dimensional system of ultra-cold bosonic atoms inside a cavity.

Topology is a field of mathematics that studies the properties of geometric objects that are preserved under continuous deformations. In physics, topology provides a framework for understanding key properties of physical systems, which has led to the discovery of new materials with unique properties.

Since the discovery of topological materials, which are distinguished by their unique non-local properties, topology has become a central area of research both in fundamental and applied physics. In recent years, substantial progress has been made in extending the existing paradigm of phases of matter to include the notion of topology and its relation to the underlying symmetries of quantum systems. This resulted in a thorough classification of npn-interacting topological systems. Nevertheless, there are still many examples of non-conventional topological phases which escape the current paradigm, presenting challenges and questions that demand new perspectives and solutions. This includes, for example, understanding the interplay of topology with interactions, or the study of higherorder topological insulators, which generalize the bulk-boundary correspondence. Currently, these phases are being proposed and discovered in a wide range of systems, including electronic systems, photonics or cold atoms in optical lattices, among others.

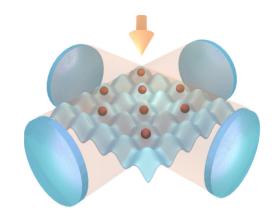
Quantum simulators made of cold atoms in optical lattices have not only been at the center of the study of topological materials because of their versatily, but are used to probe systems in which interactions between particles challenge the capabilities of available computational methods. In fact, the interplay between interactions and topology can result in interesting phenomena. For example, the combination of interaction-induced symmetry breaking and symmetry protection can give rise to delocalized fractional charges, absent in the non-interacting case. Cold atom experiments arise as perfect candidates to study interacting topological systems, but they still need to be benchmarked using advanced numerical methods.

In the recent study published in *Physical Review Letters*, ICFO researcher Joana Fraxanet, led by ICREA Prof. at ICFO Maciej Lewenstein, in collaboration with Daniel Gonzalez-Cuadra from IQOQI, Alexandre Dauphin from PASQAL and Luca Barbiero from Politecnico de Torino, report on a readily available experimental protocol to induce symmetry-protected higher-order topology through a spontaneous symmetry-breaking mechanism in an atom-cavity system.

In their study, the scientists used tensor-network based numerical techniques to investigate a system made of ultra-cold bosonic atoms coupled to two cavities. The atoms are trapped in the lowest energy band of an optical lattice, which is generated by counter-propagating laser beams. By adding two optical cavities, the scientists enhance the probability of photon-mediated interactions between the atoms, leading to effective infiniterange interactions. For the regimes of interest, these interactions induce a Peierls transition, which spontaneously breaks the translational symmetry of the system. The resulting pattern opens a topological gap, leading to a higher-order topological phase hosting corner states. The authors present a detailed protocol for the adiabatic preparation of this higher-order topological phase, which can be readily implemented using existing ultracold atom quantum simulators, therefore opening the path towards the realization of two-dimensional interaction-induced topological phases and the observation of Peierls transitions in dimensions larger than one.

As Joana Fraxanet comments, "we would like to extend the setup to include multimode cavities, allowing to generate atom-photon topological defects. These defects would generalize the topological solitons and fractionalized quasi-particles found in the Su-Schrieffer-Heeger model to two dimensions. Moreover, by exploring the regime of softcore bosons, we expect to find plaquette-ordered supersolid phases." The results

"We would like to extend the setup to include multimode cavities, allowing to generate atom-photon topological defects"



Atom-cavity experimental setup. Ultracold bosonic atoms are trapped in the lowest band of a 2D optical lattice. The atoms are coupled to two cavity modes created by two optical cavities aligned in the x and y directions, and to a laser pump aligned in the z direction. In this configuration, atoms can tunnel between nearest neighbor sites by absorbing or emitting a photon from the cavity.

presented in this study represent a step forward in understanding interacting topological phenomena, which can have important applications in quantum information processing and the discovery of novel materials. Moreover, the results are relevant to a broad community of theoretical and experimental researchers working on topological matter, ultracold atoms experiments, quantum optics and solid-state physics.

## Reference:

Higher-Order Topological Peierls Insulator in a Two-Dimensional Atom-Cavity System, Joana Fraxanet, Alexandre Dauphin, Maciej Lewenstein, Luca Barbiero, and Daniel González-Cuadra, Phys. Rev. Lett. 131, 263001 (2023). DOI: https://doi.org/10.1103/PhysRevLett.131.263001

# Researchers theoretically unveil high harmonic generation as a new source of squeezed quantum light

A team of researchers theoretically prove that the emitted light after a high harmonic generation (HHG) process is not classical, but quantum and squeezed. The study unveils the potential of HHG as a new source of bright entangled and squeezed light, two inherent quantum features with several cutting-edge applications within quantum technologies.

High harmonic generation is a highly non-linear phenomenon where a system (for example, an atom) absorbs many photons of an incoming laser and emits a single photon of much higher energy.

This process is crucial for attoscience (the science of the ultrafast processes), since it generates attosecond pulses of ultraviolet light, an essential ingredient for many applications within the field. In this regime, HHG experiments can be explained by means of semi-classical theory with great success: matter (the electrons of the atoms) is treated quantum-mechanically, while the incoming light is treated classically. According to this approach, unsurprisingly the emitted light turns out to be classical, something which was in agreement with all previous observations.

However, physicists tend to feel uncomfortable when using two different theories (quantum and classical) to describe the same phenomenon. During the last years, the efforts to understand HHG from a full quantum optical perspective have kept growing, but a more general description to show different aspects of the quantum nature of the

outgoing radiation remained an elusive milestone.

Now, ICFO researchers Philipp Stammer, Javier Rivera, Dr. Javier Argüello led by Prof. ICREA Maciei Lewenstein, together with researchers from other institutions (the Aarhus University, University of Crete, ELI-ALPS, Guadong Technion-Israel Institute of Technology) have theoretically described highharmonic generation using just quantum physics and, for the first time, they have found squeezing and entanglement features simultaneously in the emitted light. The study, published in Physical Review Letters, explains why previous classical descriptions were not in disagreement with the observations and, at the same time, unveils a new method to generate quantum optical resources with squeezing and massive entanglement in a new bright frequency regime, two features of current technological interest.

# A new method to generate entanglement and squeezing in light

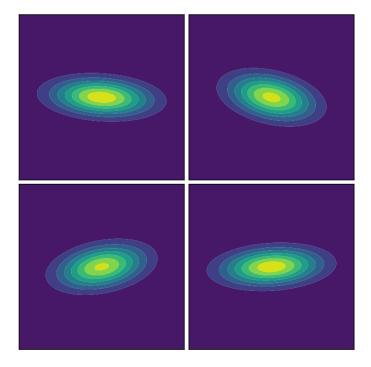
Entanglement is at the core of quantum physics,

one of its defining features. Roughly speaking, when two particles are entangled, measuring one of them influences the results that will be obtained after measuring the other. Counter-intuitively, this still holds when these particles are arbitrarily separated, which causes the so-called "non-local correlations". Nowadays, entanglement is not seen as a mere curious phenomenon. Instead, there is great consensus about its key role within quantum technologies. That is why the quantum community is seeking ways to generate entanglement, not just between two particles, but also between a higher amount of them ("multipartite entanglement").

Another defining quantum feature is the unavoidable noise when one measures some specific pairs of properties of a physical system (for example, the position and the momentum). For quasi-classical states, also called "coherent states", the amount

"The resulting final state of light turned out to be quantum in the sense that the modes are squeezed, as opposed to coherent; and that they are no longer independent, but show multipartite entanglement instead"

of uncertainty is equal for both quantities and its product is minimal. However, with squeezed states



Representation of the squeezed modes in the high harmonic generation emitted light. Source: Physical Review Letters.

"All in all, the team has proved that, under specific -but feasible- experimental conditions, one can use HHG as a source of squeezed light with multipartite entanglement"

one can decrease the noise of one property (for instance, the position) at the expense of increasing the other one (the momentum), while its product is still kept at its lowest value. This feature, which is a direct manifestation of the quantum nature of squeezed states, makes them desirable for several quantum technology applications.

Traditional theoretical quantum optical models of HHG described the modes of the resulting light beam (that is, the different frequencies at which the electromagnetic field oscillates) as coherent states without entanglement, independent from each other. In this context, the recently published paper has brought two valuable insights.

In the first place, it points out that previous studies neglected the states the electron can occupy during HHG process and that the final state of light was not showing any quantum features because of that. Even though this assumption was reasonable in most experiments, it was not providing the most general explanation of the phenomenon.

Secondly, researchers improved the whole calculation by explicitly taking into account the different states the electron can occupy. The resulting final state of light turned out to be

quantum in the sense that the modes are squeezed, as opposed to coherent; and that they are no longer independent, but show multipartite entanglement instead. ICFO researchers indicate how this situation, although not standard for attosecond experiments, could be relatively easy to engineer in the laboratory.

All in all, the team has proved that, under specific -but feasible- experimental conditions, one can use HHG as a source of squeezed light with multipartite entanglement. The first author of the paper, Philipp Stammer, explains that "massive entangled states are important for optical quantum technologies, and open a new field of research, which is generating extreme light fields with quantum properties". The applications could include quantum spectroscopy, non-linear optics or quantum metrology, where entanglement and squeezing can provide an advantage over classical lasers. Now, an experimental realization of their discovery is needed to be able to exploit this new source of quantum light in all its potential.

## Reference:

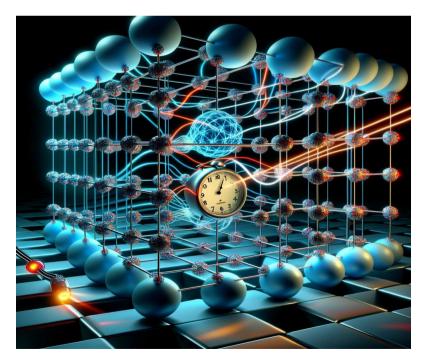
Philipp Stammer, Javier Rivera-Dean, Andrew S. Maxwell, Theocharis Lamprou, Javier Argüello-Luengo, Paraskevas Tzallas, Marcelo F. Ciappina, and Maciej Lewenstein. Phys. Rev. Lett. 132, 143603 (2024).

DOI: https://doi.org/10.1103/PhysRevLett.132.143603

# Synthetic dimensions: recent progress and future perspectives

In a review published in *Communications Physics*, researchers from ICFO, UPC, UAB, DIPC, HRI and Adam Mickiewicz University present the recent progress on utilizing synthetic dimensions of quantum matter for exploration of exotic quantum phenomena.

We live in a space with three dimensions: length, height and width. Imagining 3D objects is thus very natural to us, but there are some physics phenomena that happen in higher dimensional spaces, what makes directly observing them virtually impossible. The only way to circumvent this obstacle is to engineer artificial matter that does behave according to higher dimensional physics.



Artistic illustration of synthetic dimensions. Made with Chat GPT 4.0 by Marcin Płodzien.

"The article provides a comprehensive overview over the state-of-the-art avenues on utilizing synthetic dimension technique for studies on exotic and higher dimensional phenomena"

Then, one can access these extra dimensions, known as synthetic dimensions.

There are multiple platforms to generate the aforementioned artificial matter, which use atoms, molecules or light as their main ingredient. They are particularly useful for quantum simulation (the field that, by using quantum resources, solves specific problems that are impossible or extremely demanding for classical computers), since synthetic dimensions provide access to aspects of interacting quantum matter that otherwise would have remained in the dark.

article, published new perspective Communications Physics, reports on the recent progress on synthetic dimensions studies developed in an international collaboration between ICREA Prof. at ICFO Leticia Tarruell and ICREA Prof. at ICFO Maciej Lewenstein, with ICFO researchers Dr. Javier Argüello, Dr. Utso Bhattacharaya, Dr. Tobias Grass, Dr. Marcin Płodzién, Dr. Tymoteusz Salamon, Dr. Paolo Stornati as well as with the contribution of Universitat Politècnica de Catalunya (UPC), Universitat Autònoma de Barcelona (UAB), Adam Mickiewicz University (UAM), Donostia International Physics Center (DIPC) and Harish-Chandra Research Institute (HRI).

It is important to note that synthetic dimensions have much more practical applications than going from 3 dimensions to (quasi) 4 or even 5 dimensions. In many situations in theory or experiment, working with 1-dimensional or 2-dimensional systems is relatively easier. The synthetic dimensions approach transforms them into (quasi) 2 or (quasi) 3-dimensional systems, respectively. In this way, one can realize, for instance, 2-dimensional quantum Hall effect physics in 1 dimension, or twisted bilayer physics in 2 dimensions.

The article provides a comprehensive overview over the state-of-the-art avenues on utilizing synthetic dimension technique for studies on exotic and higher dimensional phenomena with the help of quantum random walks or time crystals, among others. Authors describe the major applications of synthetic dimensions, mainly based on atomic platforms, in fields as diverse as quantum gravity, solid-state physics or particle physics, specially focusing on what quantum simulation can bring to all these areas when it exploits synthetic dimensions.

They also detail several experiments that were either not possible using conventional 3D space realizations or for which the experimental complexity was much higher, expecting novel experimental efforts to keep shedding light on a wide variety of physics phenomena.

## Reference:

Argüello-Luengo, J., Bhattacharya, U., Celi, A. et al. Synthetic dimensions for topological and quantum phases. Commun Phys 7, 143 (2024).

DOI: https://doi.org/10.1038/s42005-024-01636-3

# The interaction of low-energy electrons with light reveals quantum effects

ICFO researchers lead a theoretical study on the interaction between low-energy electrons and light, showing for the first time the emergence of quantum and recoil effects as a consequence. The results could enhance ultrafast electron microscopy, among other potential applications.

Free electrons and light (or, more precisely, optical fields), when coupled together, play a fundamental role in state-of-the-art electron microscopy. Their synergetic relation enhances spatiotemporal and energy resolution of electron microscopes down to the picometer-attosecond-microelectronvolt range (that is, to scales of one trillionth of a meter, one quintillion of a second and one millionth of an electronvolt). This way, one can study dynamical processes and quantum phenomena in matter with a resolution reaching the atomic level and ultrafast time scales.

In general, the electron beams employed in this kind of devices have kinetic energies significantly higher than those of the optical fields. Then, the probability of a single electron interacting with a single photon becomes much smaller than unity, which in turn implies a weak electron-light coupling. In spite of the many advances that have been achieved in this regime, where the electron beam is described by a classical point-charge following a straight-line trajectory, this feature entails some fundamental limitations. In particular, the energy-momentum mismatch hinders the capabilities of these techniques for imaging atomic excitations and accessing the plethora of quantum nonlinear effects in nanostructures.

Therefore, to access such phenomena one needs to close the energy gap by lowering the electron

energies until they are comparable to the photon ones. This approach has now been tackled by ICFO researchers Adamantios P. Svnanidis and Dr. P. André D. Goncalves, led by ICREA Prof. Javier García de Abajo, together with Prof. Dr. Claus Ropers from the Max Planck Institute for Multidisciplinary Sciences and the University of Göttingen. In a **Science Advances** article, they theoretically show exotic quantum effects emerging from low-energy electron-light interactions that do not manifest in the conventional high-energy regime, such as strong electron-photon coupling at crystal surfaces, classically forbidden electron backscattering from otherwise electron-transparent surfaces, and selective strong photon absorption and emission.

Adamantios P. Synanidis, first author of the article, clarifies: "By lowering the electron energy and using an appropriate scattering surface, the electron-light coupling can be drastically increased (even diverging to infinity in special configurations), since the kinematical mismatch between the two is minimized or completely bridged".

The researchers showed that when low-energy free electrons encounter an evanescent optical field (for example, of a surface polariton) in an electron-transparent film, the electrons can backscatter. This effect, which is forbidden in the classical regime where the electron energy is much higher than that of the light, showcases the importance of recoil

# "Due to the excellent spatiotemporal control offered by electron beams, we expect several new and exciting applications to arise"

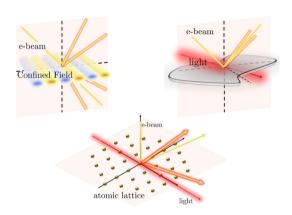
effects and the quantum character of the interaction. The team also showed the consequences of low-energy electrons diffracted by an illuminated atomic lattice, where the electron-light coupling can be selectively enhanced by correctly tuning the electron energy.

# New future directions for electron microscopy, metrology and quantum coherent control

Besides the fundamental interest that intrinsically comes with exploring electron-light-matter interactions, this study finds potential applications in ultrafast electron microscopy or metrology.

"Due to the excellent spatiotemporal control offered by electron beams, we expect several new and exciting applications to arise in the fields of ultrafast electron spectromicroscopy and quantum coherent control", further explains Synanidis. "One possible new development would be using electron beams not only as probes of physical processes in matter but also as a tool to transfer coherence to the sample by entangling with material excitations, thus introducing novel techniques with entangled beams".

In the long-term picture, these results also contribute to the future goal of building more compact electron microscopes, since low-energy electrons can greatly simplify some aspects of the current electron-microscope columns. Additionally, the use of low-energy electrons increases electron-light coupling without the need for strong light



Illustrations of the electron-light-matter interaction and recoil effects with low-energy electrons considered in the article.

fields, which enables electron-based spectroscopy of sensitive samples, such as biological ones.

## Reference:

Adamantios P. Synanidis et al., Quantum effects in the interaction of low-energy electrons with light. Sci. Adv. 10, eadp4096 (2024).

DOI: 10.1126/sciadv.adp4096

# Going beyond energy: groundstate properties unlocked in a certifiable and scalable way

A team of researchers theoretically obtain, for the first time, certifiable bounds on many-body ground-state properties beyond the energy with competitive performance. The resulting method is general and scalable.

A set of particles that interact with each other tends to minimize its energy. When the whole system actually reaches the minimum energy, its description is given by the so-called 'ground-state', or state of minimal energy. Scientists are thus very interested in discovering and analyzing its properties, which of course include -but are not limited to- the energy. For instance, magnetic and conduction properties are other worthwhile knowing features, to name just a few.

However, discovering the exact value of these ground-state properties becomes harder as the number of particles increases, reaching a point where even a supercomputer would not be able to find the solution. To circumvent this obstacle, there are two numerical methods that bound the energy of the ground state: the variational and the relaxation methods. They provide an upper and a lower bound, respectively. This means that, even though the exact ground-state energy is, strictly speaking, still uncertain, it will be for sure contained between those two values. The closer the upper and the lower bound are, the less uncertainty there will be on the energy.

Variational and relaxation methods have proven to be really effective, providing tight enough bounds to be able to infer the ground-state energy with the desired accuracy in a wide variety of physical problems. Nevertheless, when these techniques are applied to other different properties, it is not possible to know whether the obtained quantities are close to the real value, as they are no longer ensured to be upper or lower bounds. Finding non-trivial bounds would not only allow scientists to check if the information provided by variational methods was on the right path, but would also lead by itself to a certified estimation on the real value of these ground-state properties.

This issue has now been tackled by an international team in a *Physical Review X* article, with Dr. Jie Wang from the Chinese Academy of Sciences as its leading author and the participation of ICFO researchers **Dr. Jacopo Surace** and **ICREA Prof. Antonio Acín**, as well as the Perimeter Institute for Theoretical Physics, Université Grenoble Alpes, Sobbornne Université, Collège de France, ESAT, Inria Paris-Saclay, Institute Polytechnique of Paris, LAAS-CNRS and the Institute of Mathematics from Toulouse. They show how, by taking into account the variational and relaxation results for the energy, one can derive certifiable bounds on other ground-state properties in a scalable way.

# Towards the certification of any ground-state property

With their approach, consisting in a numerical method called semi-definite programming (SDP) relaxation, one can be sure that the actual value of a given ground-state property lays within the obtained range. Again, just as what happened with the energy, the ability to get the limiting bounds closer will increase the accuracy of the predictions. The novelty of the article lies in the fact that the energy bounds given by the variational and relaxation methods are now considered. The strategy leads to a significant improvement (by an order of magnitude) with respect to previous attempts, being the first time that a method exhibits competitive performance when certifying ground-state properties beyond the energy.

The team benchmarked their method with several models (Heisenberg models) that described an array of interacting particles with spin ½ (for instance, electrons). The addressed properties were the spin-spin correlation functions, which give direct information about whether the system behaves ferromagnetically or antiferromagnetically. In all the cases their SDP relaxation provided bounds in agreement with the expectations. They also successfully bounded the spin-spin correlation function of a particular system (J1 – J2 square lattice Heisenberg model for 100 spins) whose exact calculation is currently out of reach, showcasing the potential of the proposed technique.

"We are confident that our approach will become a central tool in the study of ground-state problems, a ubiquitous issue in science"



Abstract and artistic illustration representing the spin  $\frac{1}{2}$  particles.

Although SDP relaxations are just in their infancy and many improvements can be made to bring upper and lower bounds closer together, the results obtained show great promise. Moreover, their tool is completely general, so in principle it could be applied to any other observable of interest. "Our method offers deep insights into the understanding of phases of matter, how particles arrange to minimize their energy, which is essential to understand many phenomena, from chemical processes to material design", claims ICREA Prof. at ICFO Antonio Acín. "And we are confident that our approach will become a central tool in the study of ground-state problems, a ubiquitous issue in science".

## Reference:

Jie Wang, Jacopo Surace, Irénée Frérot, Benoît Legat, Marc-Olivier Renou, Victor Magron, and Antonio Acín. Certifying Ground-State Properties of Many-Body Systems. Phys. Rev. X 14, 031006 (2024). DOI: https://doi.org/10.1103/PhysRevX.14.031006

Instagram reel·



# New insights into photon coherence and distinguishability

ICFO researchers have derived and experimentally verified a new complementarity relation for quantum interference in induced coherence experiments valid for both low and high photon-flux rates, extending to the latter the applicability of quantum coherence and photon distinguishability concepts.

Quantum mechanics, a realm of surprising and counterintuitive phenomena, has fascinated scientists for decades. At its core lies quantum interference, a concept famously exemplified by the double-slit experiment, which showcases the concept of wave-particle duality. In this experiment, a quantum particle (like a photon, an electron or an atom) passes through two slits and impacts a screen, creating (after various repetitions) an interference pattern of bright and dark bands, indicative of wave-like behavior.

Being a breakthrough at the time, now we know that this phenomenon is explained by the wave-particle duality, which establishes that quantum entities exhibit particle or wave properties depending on the experimental circumstances, and that it occurs only when there is no way of knowing which slit the particle passes through.

Since then, many variations of these experiments have arisen and been demonstrated experimentally. Some of them go a step further and demonstrate a so-called complementarity principle, according to which quantum entities can go from wave-like to particle-like behavior in a continuous way.

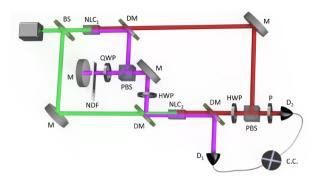
In general, the degree of quantum interference is

measured by the visibility of the interference fringes, but visibility is not always a suitable choice. That is the case, for instance, of those experiments based on the concept of induced coherence when the flux rate of the photons sent is beyond the single-photon regime. In these scenarios, new measures and complementarity relations are needed.

Now, ICFO researchers **Dr. Gerard J. Machado** (also member of the Imperial College of London), **Lluc Sendra** and **Dr. Adam Vallés**, led by **ICFO and UPC Professor Dr. Juan P. Torres** have derived a complementarity relation valid for any photon-flux rate generated in induced coherence experiments. They avoided using visibility and instead employed the concept of "first-order coherence", a parameter more convenient to measure the wave-like behavior of the photons. Their theoretical findings, experimentally verified in the low photon-flux regime, have been published in **Physical Review A**.

## **Induced coherence experiments**

The experimental setup involves two secondorder nonlinear crystals that are optically pumped by mutually coherent waves to generate a pair of photons, called signal and idler.



Sketch of the experimental setup. Source: Physical Review A.

The photons follow a particular circuit so that quantum interference occurs at the end of the signals' route. The key point is that one can tune the probability that the first crystal idler's path merges with the second crystal idler's path. When their trajectories are completely aligned, and thus indistinguishable, the origin of the idlers is unknown, and interference fringes form at the signals' output. Otherwise, the interference pattern disappears because the idler's path, and consequently its crystal of origin, can be determined.

# Complementarity relationships for low and high photon-flux rates

Previous induced coherence experiments mainly worked in the single-photon regime, where visibility is a valid indicator of its wave-like nature. There was a lack of theoretical framework and experimental realizations suitable for the high photon-flux regime though, a scarcity that the ICFO team wanted to address.

In their study, the researchers replaced visibility by the so-called 'first-order correlation' function to measure the wave coherence. "In our setup, the first-order correlation function is crucial because it allows us to measure the coherence between the two interfering photons. This coherence is directly "We have bridged the wave and the particle behavior of light, providing a unified framework that is valid across different photon-flux regimes"

related to, but in general not exactly equal to, the visibility of the interference pattern, which in turn depends on whether it is possible to distinguish the origin of the photons", explains Dr. Gerard J. Machado, first author of the article.

The researchers also introduced a new measure of distinguishability based on second-order correlation functions. By linking the coherence between two interfering photons with the updated distinguishability parameter, they were able to derive a complementarity relationship that holds for any photon-flux rate. This extends the applicability of quantum coherence and photon distinguishability beyond the single-photon regime, offering new insights into the nature of these fundamental concepts.

The team then tested their theoretically derived relationship in an induced coherence experiment in the low photon-flux regime. "We faced various obstacles during the experiment, such as maintaining and optimizing the coherence between the interfering photons and measuring coincidences between photons of different wavelengths, which required using different single-photon detectors. But through iterative improvements in our setup, we obtained the desired experimental results that matched the theoretical model", shares Dr. J. Machado.

### Foundational insights for quantum applications

Adapting the experiment to higher photon-flux rates and extending it to more complex and higher-dimensional quantum systems should be the next steps for the community. Nevertheless, this work already provides foundational insights applicable to various quantum technologies, including quantum communication, computing and metrology.

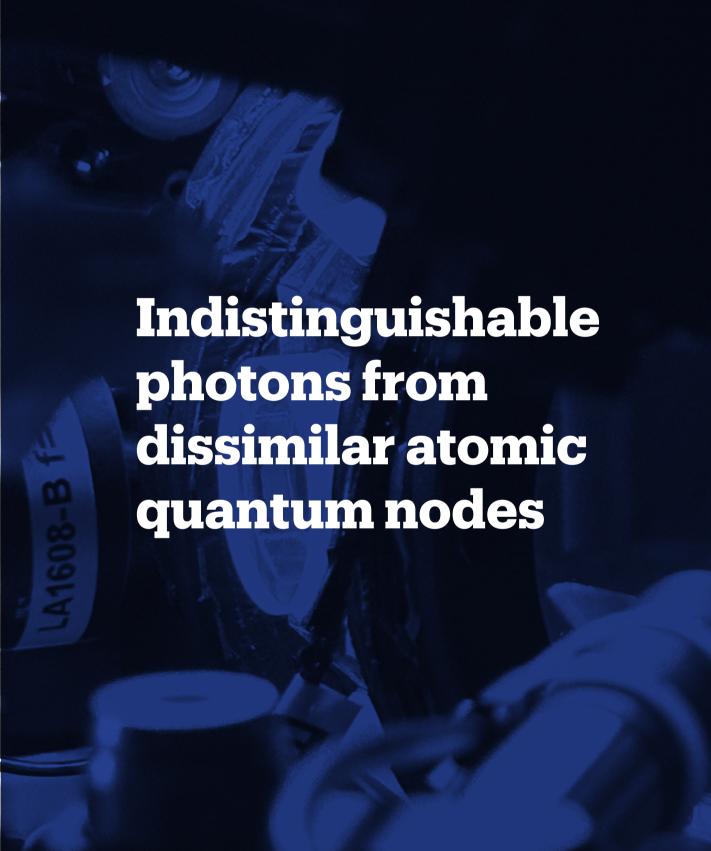
Prof. Dr. Juan P. Torres highlights the significance of their results: "We have bridged the wave behavior of light (its coherence) with its particle behavior (photon distinguishability), providing a unified framework that is valid across different photon-flux regimes, from single-photon to high parametric gain."

### Reference:

G. J. Machado, L. Sendra, A. Vallés and J. P. Torres, Complementarity relationship between coherence and path distinguishability in an interferometer based on induced coherence, Phys. Rev. A 110, 012421 (2024). DOI: 10.1103/PhysRevA.110.012421



Dr. Gerard Jiménez Machado working at ICFO in the experiment. Credit: Dr. Adam Vallés.



## Indistinguishable photons from dissimilar atomic quantum nodes

ICFO researchers have obtained a world record degree of indistinguishability between two photons coming from two dissimilar quantum nodes when no detections are discarded. These results pave the way towards future heterogeneous quantum networks.

The development of a quantum internet is a remarkable endeavor running parallel to the pursuit of practical quantum computers. This quantum network aims to facilitate the exchange of quantum bits of information (called qubits) between quantum processors, allowing for unprecedented levels of secure communication and computational power.

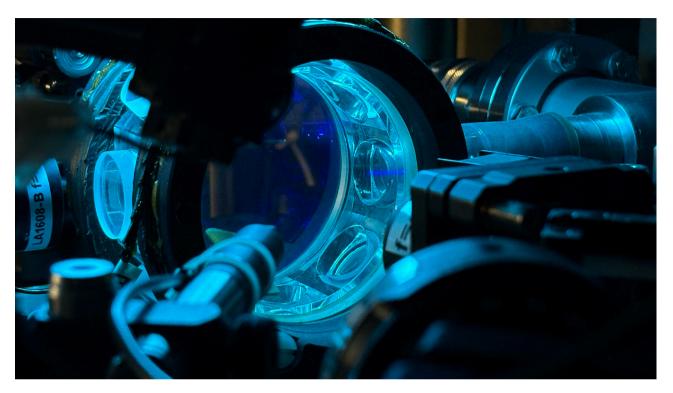
A key objective of a quantum network is to create remote entanglement between two distant processing units, which can then be utilized for specific applications. To achieve this, researchers are exploring a new technology called the quantum repeater, which facilitates the generation and transmission of entanglement between two intermediate stations, known as quantum nodes. However, the physical systems used as quantum repeaters may differ significantly from those used in quantum computers. Therefore, developing an interface between these diverse platforms is crucial.

The interface between these systems typically involves sending single photons from each and making them interfere. The quality of this quantum interference determines how effectively entanglement can be distributed

across the network. Achieving high-quality interference is challenging because the photons must be indistinguishable, and when quantum nodes are based on different technologies, making them emit indistinguishable photons is particularly difficult. A common solution to this problem is to select only a small part of the emitted photons, which increases the indistinguishability, but this comes at the expense of a strong reduction in detection rate.

"when quantum nodes are based on different technologies, making them emit indistinguishable photons is particularly difficult"

In this context, ICFO researchers **Dr. Félix Hoffet**, **Dr. Jan Lowinski**, **Dr. Lukas Heller**, **Dr. Auxiliadora Padrón-Brito** led by **ICREA Prof. Hugues de Riedmatten** have succeeded in producing highly indistinguishable photons from dissimilar quantum nodes without



Glass cell in the experimental setup. ©ICFO

discarding any detection, achieving a world record degree of indistinguishability in the field of hybrid quantum networks under such conditions. The results have recently been published in *Physical Review X Quantum*.

### How to obtain indistinguishable photons out of quantum nodes

In order to check the indistinguishability of the emitted photons, the team first needed to recreate the typical basic unit of a quantum network: two quantum nodes with different technologies. In their case the two nodes were based on cold Rubidium atoms. One of them was based on a fully blockaded cold Rydberg ensemble

(sometimes called a Rydberg superatom). This system enables quantum processing capabilities and, in this experiment, generated on-demand single photons. The other one was a quantum repeater node based on an emissive quantum memory and emitted heralded single photons.

The researchers used the quantum memory to synchronize the emission of the two photons. In the emissive memory, several generation trials are made until the detection of a photon heralds the presence of a photon in the memory. The photon is then stored in the quantum memory while a classical signal is sent to the Rydberg node, used as a trigger to generate another single photon in a quasi-deterministic fashion. Finally, the first photon is released from the

quantum memory at a precise time, and the two photons are mixed on a beam splitter where a quantum interference takes place. The quality of this quantum interference then depends on the indistinguishability between the two photons.

To achieve the reported milestone, the researchers had to develop some new techniques. First, they tailored the temporal waveforms of the emitted single photons to match each other, which is already an important result. They accomplished this by modulating the lasers used to read out the atomic excitations.

Next, since these quantum nodes operate independently, they are subject to non-correlated experimental fluctuations. This typically results in numerous problems, as it can make the photons distinguishable, thereby disrupting quantum interference within a few minutes. This issue is critical because quantum nodes need to maintain their quantum properties over extended periods, spanning several days. To address this limitation, the researchers developed new stabilization techniques. They periodically measured atomic resonances and dynamically adjusted the experiments based on the results, ensuring consistent quantum performance over tens of hours.

### One step closer to the quantum internet

This challenging experiment provided a fertile ground for observing non-linear effects that had been predicted by theory but never experimentally confirmed. Overall, this experiment demonstrates that cold atomic systems are promising candidates for scaling up quantum networks. The researchers now aim to reuse the techniques they developed and extend their experimental setup to show that distributing entanglement between hybrid

systems is feasible.

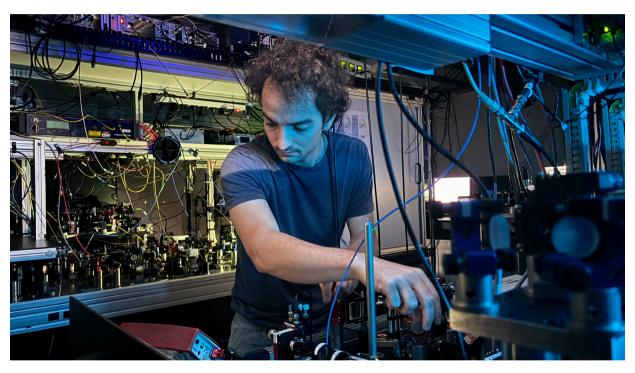
According to Dr Félix Hoffet, researcher at ICFO and first author of the study: "Cold atoms are interesting for this kind of experiments because, unlike other systems, each atom is identical. I am optimistic that this subtle distinction will prove beneficial in the long term for connecting quantum processors with quantum repeaters. Furthermore, given the rapid progress in both research fields, I believe it is now important to bridge the gap between these different platforms and consider larger-scale integration already. I am happy to contribute initial insights to this endeayour".

Hugues de Riedmatten, ICREA professor at ICFO concludes: "It is likely that future quantum networks will combine different quantum nodes made of different physical systems and with different functionalities. Creating an interface enabling the distribution of entanglement between disparate quantum systems is an outstanding challenge. Our work is a step in this direction, but there are many more challenges ahead, the first of which will be to interface quantum nodes made of different atoms."

### Reference:

Near-unity indistinguishability of single photons emitted from dissimilar and independent atomic quantum nodes, Félix Hoffet, Jan Lowinski, Lukas Heller, Auxiliadora Padrón-Brito, and Hugues de Riedmatten, PRX Quantum (2024) DOI: https://doi.org/10.1103/PRXQuantum.5.030305

"cold atomic systems are promising candidates for scaling up quantum networks"



Felix Hoffet working in the lab. ©ICFO



### The Jaynes-Cummings model: 60 years and still counting

To mark the occasion of the 60th anniversary of the Jaynes-Cummings model, the Journal of the Optical Society of America B has published a special issue on this foundational model in quantum optics, highlighting its importance in the field and the evolution of its applications.

In January of 1963, E. T. Jaynes and F. W. Cummings developed what became known as the Jaynes-Cummings model, which describes a two-level atom coupled to a single mode of the electromagnetic field. Like many of the greatest works of humanity, the model's birth went quite unnoticed. It was only in the second decade of its existence that it began to attract attention of researchers. The number of mentions of the term 'Jaynes-Cummings' has kept growing since then, showcasing the fact that it has become a deep-routed model in many different areas within quantum physics, specially in quantum optics.

The initial change of paradigm around 1973 was sparked by the signatures of coherence in the model, like the appearance of collapses and revivals of atomic inversion for an initial coherent state of light. In the decades that followed, the applications of the Jaynes-Cummings physics guickly spread.

These applications are reviewed in the special issue recently published in the *Journal of the Optical Society of America B* by the Stockholm University, ICFO researcher **Dr. Themistoklis Mavrogordatos** and colleagues from the University of Auckland, Dodd-Walls Centre for Photonic and Quantum Technologies and the University of Campinas.

The review covers some posterior generalizations of the Jaynes-Cummings model (Tavis-Cummings

and Dicke models) and its relevance with respect to a wide variety of topics, including decoherence, cavity QED, non-classical light or quantum phase transitions, among many others.

In addition to its countless applications, this model entails a fundamental importance. "As I started my first steps into quantum optics, I quickly realized that the Jaynes-Cummings model holds the key to the reappraisal of wave-particle duality, a longstanding subject since the development of the old quantum theory", explains Dr. Themistoklis Mavrogordatos.

Dr. Antonio Vidiella-Barranco, corresponding author of the article, recalls the beginnings of his scientific career as well: "I first heard about the Jaynes-Cummings model during my PhD. I was awestruck not only by its simplicity but also because it offered a nonperturbative approach, providing significant insights into the fundamentals of light-matter interaction".

### Reference:

Larson, Jonas & Mavrogordatos, Themistoklis & Parkins, Scott & Vidiella-Barranco, Antonio. (2024). The Jaynes-Cummings model: 60 years and still counting. Journal of the Optical Society of America B.

DOI: 41. 10.1364/JOSAB.536847.PhysRevX.14.031006

## Tracing topological phase transitions with X-ray absorption techniques

An international team of researchers present in *Reports on Progress in Physics Original Research* a numerical experiment that demonstrates the possibility to capture topological phase transitions via an x-ray absorption spectroscopy scheme. By overcoming previous energy resolution limitations, the method will enable further investigations on relevant systems for optoelectronics applications.

The atoms of solids, liquids, and gases exhibit very different arrangements and behavior. In solids, atoms are tightly packed in a regular pattern; in liquids, atoms are close together but randomly arranged and with some freedom to move; and in gases, atoms are further apart and can move freely. These features define the conventional phases of matter.

When one enters the quantum world, other phases of matter, which have nothing to do with atomic distribution or mobility, emerge. These are the topological phases. In this realm, some properties of the particles within a material (like atoms or electrons) can become connected through a phenomenon known as long-range entanglement. When a pair of particles is entangled, changing or measuring one of them immediately affects the other, regardless of the distance between them. These particles might be entangled in a complex pattern, spanning the entire system. Different 'entanglement patterns' of the material's electrons or other quantum particles define different topological phases. Thus, altering the way particles are entangled, rather than changing their spatial arrangement leads to a phase transition.

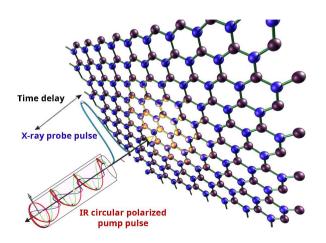
Topological states of matter offer the potential to

create exotic materials, which can be, for instance, insulators in the bulk but hold conducting states on the surface. In the last years, there has been enormous progress in the development of these modern materials. For example, some topologically non-trivial insulators could be induced by using ultrashort intense lasers. However, these light-induced topological insulators exist only while the laser pulse is on, that is, around several femtoseconds (10-15 seconds). This imposes a strong requirement to study and characterize them since an ultrafast probe in the femtosecond timescale is needed in order to capture the ultrafast topological phases.

Despite the significant progress in this direction, some challenges remain. For example, angle-resolved photoemission spectroscopy (ARPES) has proved to be effective in probing these topological systems, but it faces a drawback: the shorter the probe pulse duration (and, consequently, the closer to capturing the material's ultrafast nature), the lower the photoelectron energy resolution.

Recently, a team led by Universidad Autónoma de Madrid, with the collaboration of researchers from ICFO, **Dr. Emilio Pisanty**, **Dr. Alexandre**  "Our ultrafast scheme was very sensitive to topological phase transitions. When the topological phase changed, there was a sign imprinted in the absorption spectrum"

Dauphin and ICREA Prof. Maciej Lewenstein; M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences; King's College London; University of Salamanca; Max Planck POSTECH/KOREA Research Initiative and Condensed Matter Physics Center (IFIMAC), presented a complementary scheme to ARPES in Reports on Progress in Physics Original Research. In a numerical experiment supported by a theoretical model, the team demonstrated that X-ray absorption spectroscopy can directly capture topological phase transitions.



Sketch of the ultrafast X-ray scheme and the system under investigation. Source: Reports on Progress Physics Original Research.

The method employs ultrashort probe pulses that do not suffer from energy resolution reduction. This approach enables further studies of relevant systems for optoelectronics applications, whose investigation had so far been held back by the duration/resolution trade-off.

### Topological phase transitions leave an absorption trace

The researchers simulated the action of two ultrashort pulses, separated by a time delay, on a hexagonal boron-nitrate monolayer (hBN). One of them was a linearly-polarized x-ray pulse and the other a circularly-polarized intense infrared pulse. By changing the circular polarization of the latter from left- to right-handed, the absorption of the sample also changed. This dependence enabled them to infer the topological phase of the material.

"Our ultrafast scheme was very sensitive to topological phase transitions. When the topological phase changed, there was a sign imprinted in the absorption spectrum", explains ICREA Prof. Maciej Lewenstein. "Therefore, this method could be used to study topological phases and identify topological phase transitions within some materials. Now, we need an experimental design to be able to demonstrate it in a real-case scenario."

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Juan F P Mosquera, Giovanni Cistaro, Mikhail Malakhov, Emilio Pisanty, Alexandre Dauphin, Luis Plaja, Alexis Chacón, Maciej Lewenstein and Antonio Picon, Topological phase transitions via attosecond x-ray absorption spectroscopy, Rep. on Prog. Phys.

DOI: 10.1088/1361-6633/ad889f

## A novel framework for describing how certain quantum systems avoid equilibrium

Researchers establish a robust theoretical description of many-body localization (MBL) —a phenomenon that prevents quantum many-body systems from reaching equilibrium. This advancement enables understanding and demonstrating MBL in a wider range of quantum many-body systems.

When many quantum particles evolve over time, they typically end up arriving to an equilibrium state through a process called thermalization. Something similar happens in many classical systems. For example, if you place an ice cube in a thermos with water, the ice melts and the final (equilibrium) state is just colder water than before.

In classical physics, complex systems eventually reach equilibrium (if you wait long enough, the ice always melts). However, certain quantum many-body systems defy this norm. For them, thermalization does not occur, and the system remains out of equilibrium. That is the case of a large class of strongly disordered systems —where features like



Abstract illustration of a chain of spin ½ particles, like the one under study. Source: Abode Stock, AI generated.

### "We have shown that the physics of MBL is richer than previously thought"

particle interactions or individual energies exhibit a certain degree of randomness. This behavior is due to many-body localization (MBL), a mechanism that preserves the system's initial conditions over time.

Local integrals of motion (LIOMs) constitute a theoretical framework broadly used for the study of MBL. Nevertheless, a recent article published in *Physical Reviews Letters* led by Uniwersytet Jagielloński and with the collaboration of ICFO researchers **Dr. Piotr Sierant** and **ICREA Prof. Maciej Lewenstein** shows that LIOMs are insufficient to describe the behavior of a wide class of systems, in particular, those with more complex types of disorder. They propose a new framework, the real space renormalization group for excited states (RSRG-X), which can explain MBL in a larger amount of quantum many-body systems.

The team knew that LIOMs can capture the behavior of MBL when the disorder of the system affects properties of particles individually (on-site disorder). However, they suspected that LIOMs failed to account for systems where randomness influences the interactions between particles (bond disorder).

To test this hypothesis, researchers applied RSRG-X to a bond-disordered chain of spin particles (that is, particles that behave like tiny magnets). The results showed that, indeed, RSRG-X provides a theoretical description of MBL in such systems, where LIOMs do not even exist. Their framework uncovers new features of MBL in quantum many-body systems, including the presence of anomalously small energy level spacings, the emergence of non-

trivial entanglement structures and observable quantities that enable experimental demonstration of the phenomenon. The obtained description turned out to be qualitatively accurate and, this way, researchers demonstrated the validity of the procedure.

"We have provided a framework applicable to a wider range of systems and, thanks to that, we have shown that the physics of MBL is richer than previously thought", explains Dr. Piotr Sierant. Furthermore, the novel approach has implications which can be tested in experiments, for instance, with ultracold atom gases or superconducting qubits. Dr. Sierant adds: "Rydberg atoms are just one platform, among many others, in which the systems we have in mind could be realized. That is very convenient because, as theoreticians, we would be thrilled to see our framework implemented in a real-world scenario."

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Adith Sai Aramthottil, Piotr Sierant, Maciej Lewenstein, and Jakub Zakrzewski, Phys. Rev. Lett. 133, 196302. DOI: https://doi.org/10.1103/PhysRevLett.133.196302

## Experimental evidence of high harmonic generation producing quantum light

Researchers experimentally demonstrate that the light emitted after a high harmonic generation process in semiconductors is entangled and squeezed, two unmistakable signs of quantum light.

High harmonic generation (HHG) is a highly nonlinear phenomenon where a system (for example, an atom) absorbs many photons of a laser and emits photons of much higher energy, whose frequency is a harmonic (that is, a multiple) of the incoming laser's frequency. Historically, the theoretical description of this process was addressed from a semi-classical perspective, which treated matter (the electrons of the atoms) quantum-mechanically, but the incoming light classically. According to this approach, the emitted photons should also behave classically.

Despite this evident theoretical mismatch, the description was sufficient to carry out most of the experiments, and there was no apparent need to change the framework. Only in the last few years has the scientific community begun to explore whether the emitted light could actually exhibit a quantum behavior, which the semi-classical theory might have overlooked. Several theoretical groups, including the Quantum Optics Theory group at ICFO, have already showed that, under a full quantum description, the HHG process emits light with quantum features.

However, experimental validation of such predictions remained elusive until, recently, a team led by the Laboratoire d'Optique Appliquée (CNRS), in collaboration with ICREA Professor at ICFO Jens

**Biegert** and other multiple institutions (Institut für Quantenoptik - Leibniz Universität Hannover, Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Friedrich-Schiller-University Jena), demonstrated the quantum optical properties of high-harmonic generation in semiconductors. The results, appearing in **Physical Review X Quantum**, align with the previous theoretical predictions about HHG

In the reported experiment, the HHG source operates at room temperature using standard semiconductors and a commercial femtosecond infrared laser. This accessibility positions HHG as a highly promising platform for generating nonclassical states of light, which in turn can pave the way for more robust and scalable quantum devices that do not require complex cooling systems.

### Two unmistakable signs of quantum light

Theoreticians had already predicted that the photons emitted through an HHG process exhibit quantum behavior, which manifests itself in two defining features: entanglement and squeezing.

Entanglement occurs when two particles become interconnected, such that measuring one



Abstract illustration of two quantum entangled particles.

"Hopefully, we will be able to exploit HHG for quantum information, communication and sensing applications"

instantaneously influences the outcome after measuring the other, regardless of the distance between them. These strong correlations defy classical intuition and can only occur in the quantum world of atoms, electrons, and photons.

Squeezing, on the other hand, relates to the unavoidable uncertainty when measuring certain pairs of properties in a quantum system: increasing the measurement precision for one quantity will decrease the measurement precision for the other. Squeezed states embrace this trade-off. At the expense of increasing the noise of one property of the pair, they can reduce the noise of the complementary property.

In agreement with previous theoretical predictions, the team experimentally demonstrated the presence of both entanglement and squeezing in the emitted light. But how did they achieve it?

### **Evidencing the quantum nature of HHG**

First, the researchers directed ultrafast infrared laser pulses onto semiconductor samples —

gallium arsenide, zinc oxide, and silicon—to drive high-harmonic generation. From all the generated harmonics, they selected only two of them (the third and the fifth) using optical filters. These were then sent to a detection system capable of simultaneously analysing multiple harmonics, which was critical to reveal the quantum behavior of light.

The first sign of quantumness was related to squeezing. The equipment recorded that the variance of the photon arrival times (and, therefore, the uncertainty associated to this quantity) decreased as the laser intensity increased. This reduction could only be explained by squeezing, providing solid evidence of this feature. After that, the team turned to entanglement. To demonstrate it, they measured the correlation between the arrival times of photons from the third and fifth harmonics. Researchers consistently observed strong correlations that are prohibitive for a classical source, unmistakably indicating the presence of quantum entanglement.

These findings establish high harmonic generation as an ideal platform for producing entangled and squeezed photonic systems at room temperature. "Both features are key resources for many quantum technologies, which, for instance, rely on entanglement to transmit information or on squeezing to enhance measurement precision", explains ICREA Prof. Jens Biegert. "Neglecting the quantum optical effects was hindering the possibility of detecting nonclassical features. But, hopefully, now we will be able to exploit HHG for quantum information, communication and sensing applications in all its potential."

### Reference:

David Theidel, et. al., PRX Quantum 5, 040319 (2024). DOI: https://doi.org/10.1103/PRXQuantum.5.040319

# Researchers develop the first photon pair quantum source based on a silicon core fiber platform

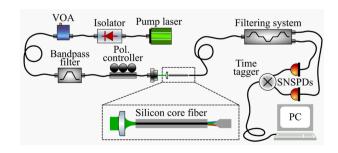
A team of researchers from ICFO and the Royal Institute of Technology (KTH) from Sweden reports on *APL Photonics* the first demonstration of a photon pair source based on a silicon core fiber. The novel platform offers a unique combination of low propagation losses, high nonlinearity and compactness making it a promising candidate for scalable quantum applications.

Quantum technologies demand photon sources with exceptional characteristics: high brightness, minimal losses and high scalability. While bulk optics and silicon photonic integrated circuits (PICs) have been the traditional choices when third-order nonlinear parametric effects are used, they often fall short in meeting all these criteria simultaneously. Silicon core fibers, however, are showing great potential as a viable platform for quantum applications, particularly in the realm of quantum communications. The highly nonlinear core material, i.e. silicon, together with the low propagation and coupling losses of the fiber structure, make silicon core fibers a compelling option for achieving the standards required by quantum technologies.

Now, ICFO researchers Davide Rizzotti, Stefano Signorini and ICREA Professor at ICFO Valerio Pruneri, together with Clarissa Harvey and Michael Fokine, researchers at the Royal Institute of Technology (KTH, Sweden), have been able to fabricate and demonstrate for the first time a quantum source of photons based on spontaneous four-wave mixing (SFWM) in a silicon core fiber.

Their achievements are described in a new study recently published in the journal *APL Photonics*. The new device combines the low loss and low cost of the fiber platform with the high nonlinearity and compactness of silicon PICs.

In their experiment, the researchers fabricated a 58 mm long silicon core fiber with a crystalline silicon core with a diameter of 1 micrometer and surrounded by a pure silica cladding. By pumping the fiber with a continuous wave laser at 1551 nm (a telecommunication standard wavelength), they



Scheme of the experimental set-up. Source: APL Photonics.

generated photon pairs through SFWM. A filtering system separated the idler and signal photons into two telecom channels and two detectors were used to detect them separately. A time tagger device measured the coincidences between the photon detectors, a standard technique to study the correlation within the generated photon pairs.

To characterize the loss performance of the silicon core fiber as a quantum light source, the team developed a new method that directly estimates the coupling and propagation losses. This novel approach allowed the estimation of losses without the need for auxiliary fibers or destructive techniques, such as the standard cutback technique.

The silicon core fiber demonstrated exceptional performance, operating at room temperature and achieving an intrinsic brightness of 570 kHz/nm/mW² and low propagation losses of approximately 0.3 dB/cm, lower than the state of the art of silicon PICs. Additionally, a measured coincidence to accidental ratio (CAR) of 133, a parameter that estimates the signal to noise ratio of photon pair sources, shows that the source fulfills the requirements for practical quantum applications.

According to the study authors, these low propagation losses "pave the way for effective fiber-based quantum sources in the telecom band." The researchers highlighted the potential of this platform "for future applications, particularly in the field of quantum communications."

"By characterizing the brightness and propagation losses of the photon pair source, we have shown how silicon core fibers can bridge the technology and application gaps between PICs and optical fibers," said Davide Rizzotti, the first author of the study. "The new sources based on silicon core fibers have great potential as a quantum source thanks to the high nonlinearity of silicon and the potential of

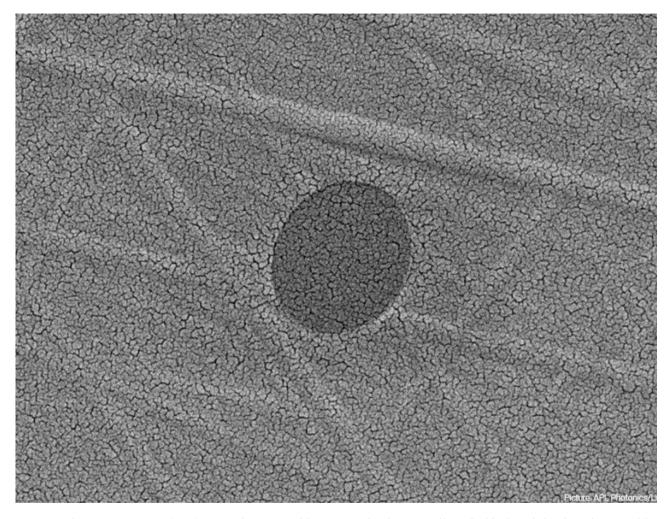
"Our study represents a significant step towards realizing the full potential of silicon core fibers in practical quantum applications"

loss-less integration with the existing optical fiber network."

"In quantum photonics is now clear that one ideal material platform does not exist, and hybrid solutions are needed to guarantee scalable and efficient devices. This study highlights the potential of the silicon core fiber as a key component in future hybrid quantum technologies," said Stefano Signorini, researcher at ICFO.

"While further developments are needed to reduce losses and improve the scalability of the platform, our study represents a significant step towards realizing the full potential of silicon core fibers in practical quantum applications, especially in the field of quantum communications," concluded Valerio Pruneri, ICREA professor at ICFO and coauthor of the study.

This research has been conducted as part of Davide Rizzotti's individual research project within the European funded NANO-GLASS project and the QSNP. Rizzotti's research is focused on the study and development of new fiber-devices for quantum communications, with the aim of reaching super low-loss devices. Indeed, low propagation and coupling loss can bring significant benefits in preserving quantum signals and increasing the efficiency of quantum communications. This research has already been conducted within the framework of the Quantum Secure Network Partnership (QSNP), an European Quantum Flagship project that aims



Scanning Electron Microscope (SEM) image of a portion of the section of a silicon core fiber. The black circle localizes the core of the fiber. (Picture: APL Photonics License: CCBY).

to develop quantum cryptography technology to secure the transmission of information over the Internet.

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Davide Rizzotti, Stefano Signorini, Clarissa Harvey, Michael Fokine and Valerio Pruneri. (2024) Silicon core fibers: a new platform for quantum light generation. APL Photonics. DOI: https://doi.org/10.1063/5.0220647

## First demonstration of deep subwavelength topological edge states

ICFO leads the first experimental demonstration of a deep subwavelength topological edge state within a nanophotonic system, a turnover in the field of topological Nanophotonics.

Topological systems are a foundational and versatile class of physical systems, ubiquitous across many fields of physics, with far-reaching implications for both fundamental research and applied technological advancements. These systems are characterized by properties that make them resilient to perturbations. In simpler terms, they possess certain qualities that are not easily affected by external factors, like disorder or changes in other physical conditions.

This resilience to perturbations is what makes topological systems so important in physics, as it means their behaviour can be very predictable and reliable under a wide range of conditions. Of particular interest are the topological edge states: states that exist at the boundary of a material and that cannot be suppressed without breaking the material's symmetry.

### Topological Nanophotonics: challenges and opportunities

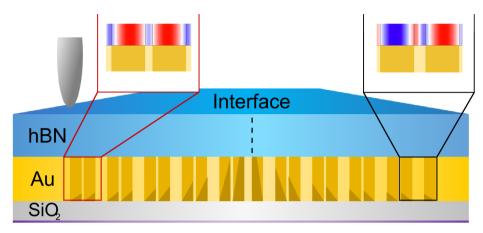
The scientific community, typically attracted by those challenges that are as complex as they are promising, sees the task of bringing topological properties down to the nanoscale as an appealing challenge. Complex because of the ultimate spatial limits of electromagnetic field manipulation that are

required; and promising because of the expected consequences, being both fundamental and applied.

To begin with, miniaturizing topological properties to such small physical scales (in the jargon, the deep subwavelength regime) would allow the scientific community to explore exotic physical phenomena (nonlinearities, non-locality, multimodal interactions...) that are expected to arise under these circumstances. On a more practical side, topological systems' inherent robustness and protection can be harnessed to develop more resilient deep subwavelength optical components, such as nanocavities or fabrication-disorder tolerant waveguides.

Despite the experimental progress towards achieving topological edge states in the deep subwavelength regime, each proposed platform exhibits some benefits but also some major drawbacks, maintaining the 'hot-topic' status in the search for the ultimate solution

An international team with ICFO researchers Lorenzo Orsini, Dr. Hanan Herzig Sheinfux, Matteo Ceccanti, Karuppasamy Soundarapandian, led by ICREA Prof. at ICFO Dr. Frank H. L. Koppens, and in collaboration with Cornell University, CNRS, University of Cambridge and Kansas State University,



Schematic of the cross-section of the 1D polaritonic nanostructure composed of two adjacent patterning distributions.

has now reported in a *Nature Nanotechnology* article a substantial advancement in this regard. For the first time, they have demonstrated a deep subwavelength topological edge state within a nanophotonic system, where the chosen platform—typically not considered by the topological Nanophotonics community— was based on the so-called hyperbolic phonon-polaritons (in short, HPhPs). Not only did they confine light into such small size scales, but they also maintained high quality factors through the whole process.

### Why hyperbolic phonon-polaritons?

Hyperbolic phonon-polaritons are a type of collective electromagnetic excitation that occurs in hyperbolic materials, where electromagnetic waves (photons) couple with the quanta of vibrations within the atomic lattice of a material (optical phonons). These HPhPs allow light to be confined and guided in very small volumes or along surfaces.

Thanks to their special features, HPhPs overcome the challenges faced by previous methods for studying topological properties at the nanoscale. These limitations include, for instance, high optical absorption —which is detrimental to reaching the deep subwavelength regime in the case of plasmon polaritons—, fabrication difficulties and the need for cryogenic temperatures —which hinder the realization of topological states in the case of graphene.

With hyperbolic phonon-polaritons these problems are minimized, since they exhibit low absorption even at room temperature and can be relatively easy to fabricate. These features, together with the fact that they allow for high volume confinement, give HPhPs excellent performance characteristics. As attractive as they may seem, HPhPs have been largely unexplored for topological applications due to their deeply complex nature, which has hindered theoretical development in this area.

Nevertheless, the team saw in the hyperbolic phonon polaritons great promise, and their ambitious goal stir them into action. "At the beginning of the project, it was uncertain how these edge states would manifest and what specific properties they would exhibit", shares Lorenzo Orsini, first author of the article. "While we anticipated their formation, finally observing them in our experiments was a fascinating confirmation of our expectations and

"taking a chance on hyperbolic phonon polaritons paid off, and now we have opened new possibilities for robust and precise control of light at the nanoscale"

an exciting development in the field".

### The experimental setup that led to success

To enable the emergence of topological edge states, the team constructed a one-dimensional polaritonic lattice platform.

First, they sharply defined rectangular holes periodically milled through a 10-nanometer gold film. On top of that, they placed a tens of nanometers thick hexagonal Boron Nitride (hBN) flake. In there, hyperbolic phonon-polaritons would be hosted. The gold layer structure was engineered such that there were two different distributions of the rectangular holes, defining two distinct regions, one next to the other. The researchers expected that, due to the presence of two different arrangements, topological edge states would form right at the boundary where both meet.

After the fabrication process, the characterization and analysis of the system took place. They used the s-SNOM spectroscopy technique to confirm the existence of a localized edge state and that it was indeed in the deep subwavelength regime.

Because of the scarcity of theoretical models, they had to rely heavily on their own experimental results, which made the need to meticulously prove and double-check each step even more crucial than

usual. This rigorous, step-by-step approach allowed them to refine the experimental design and achieve clear, reliable results, finally demonstrating deep subwavelength topological edge states within an HPhPs platform.

### The powerful potential of HPhPs platforms

In addition to the relevance inherently present in this milestone by itself, the present study also constitutes a big step forward toward the precise control of light at the nanoscale, offering an alternative platform for the realization and investigation of topological physics in nanophotonic systems. Moreover, the authors claim that their results can be extrapolated to other hyperbolic materials, something that would facilitate a broader coverage of the electromagnetic spectrum.

As Orsini concludes: "In the end, taking a chance on hyperbolic phonon polaritons paid off, and now we have opened new possibilities for robust and precise control of light at the nanoscale. A continued exploration and development in this direction could, in turn, lead to breakthroughs in areas as diverse as telecommunications, sensing technologies or quantum information processing".

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Orsini, L., Herzig Sheinfux, H., Li, Y. et al. Deep subwavelength topological edge state in a hyperbolic medium. Nat. Nanotechnol. (2024).

DOI: https://doi.org/10.1038/s41565-024-01737-8

## Atomic defects in diamond unveil a new class of efficient optical antennas

Novel optical antennas based on atomic defects in solids show up to one-million-fold intensity enhancement for the electromagnetic field emitted at close distances. The study reveals their remarkable capability to concentrate optical energy, to sense and manipulate their proximal environment.

Over a century after the invention of radio antennas by Henrich Hertz, and in the era where the miniaturization of technological devices is absolutely widespread, it is hardly surprising that a nanoscale version of regular antennas has emerged.

These optical nanoantennas, as they are called, can concentrate a large amount of radiative optical energy, massively increasing the intensity of an electromagnetic signal. This is quite analogous to how radio antennas work, but in this case operating at higher frequencies and much smaller sizes.

Nowadays, these nanoantennas face two important challenges. To start with, their miniaturization cannot achieve arbitrarily reduced dimensions, since they suffer large losses when they are made as small as a nanometer (one billionth of a meter). And moreover, the fact that the antenna is in a solid state can be detrimental to the signal: interactions with phonons (collective excitations in solids) or other fluctuations can severely limit the overall efficiency.

Now, a team led by the University of Chicago and with the contribution of Argonne National Laboratory and ICFO researchers **Dr. Francesco Andreoli** and **ICREA Prof. Darrick Chang**, has reported in **Nature Photonics** on a new optical antenna in a solid that

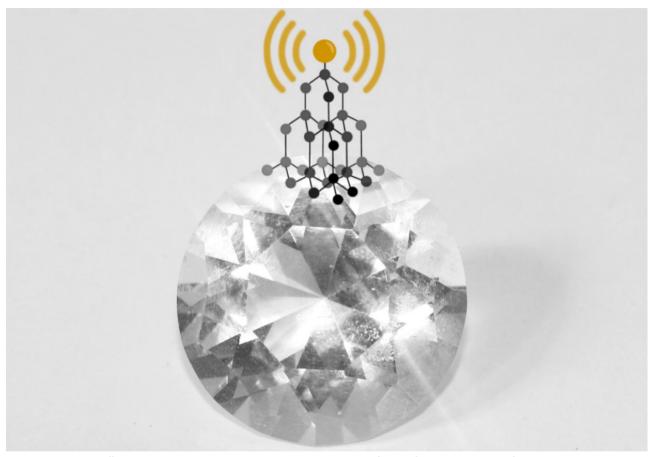
circumvents these obstacles. They propose the use of color centers in diamond, specifically Germanium-Vacancy centers (GeV), as surgically precise (both spectrally and spatially) and efficient optical papeartennas

### Germanium vacancy centers become optical nanoantennas

A color center is a defect in the regular spacing of atoms within a solid that absorbs and emits visible light of a particular color or infrared or ultraviolet radiation. A germanium-vacancy center in a diamond is a particular case of a color center, where two missing carbons are replaced by a germanium atom.

The presented study has shown both theoretically and experimentally that GeVs, when illuminated by light with a particular frequency (the resonant frequency), can function as an efficient antenna. More importantly, they show up to one-million-fold intensity enhancement in the near-field (that is, in the signal emitted or absorbed at close distances).

Furthermore, they demonstrated that GeVs can be used for both active manipulation and sensing of its proximal environment, which showcases the power



Artistic illustration portraying a germanium vacancy-centre in diamond acting as an optical nanoantenna.

of these novel nanoantennas and their unique properties.

### Shedding light into charge fluctuations in nearby vacancies

In this type of material, it can happen, by chance, that other vacancies (that is, missing carbon atoms) are created close to the GeV. Those vacancies can locally capture or release electrons from the surrounding carbon atoms that form the diamond,

changing their own charge as a consequence.

The fluctuations in the charge state of randomly created nearby vacancies alter the behavior of the GeV in a manner that is detrimental for many applications, as long as it is not controlled (for instance, for entanglement generation between solid-state qubits). One of the landmarks the team accomplished was to detect, manipulate and even induce for the first time these charge variations in the carbon vacancies.

According to Dr. Francesco Andreoli: "This detrimental effect had been already observed, but it wasn't clear up to now its cause and how to deal with it. In our study, we offer an explanation and a possible path to control this problem".

### GeVs versus traditional nanoantennas: a complementary approach

The researchers highlight how GeV nanoantennas are very different from traditional nanoantennas. On the one hand, standard nanoantennas are made of enough atoms that their optical response is dictated by that of the bulk material, while the structure of a GeV resembles that of a single atom. Consequently, a nanoantenna smaller than (roughly) ten nanometers experiences bulk absorption, causing it to drastically lose its efficiency and maximum field enhancement. On the contrary, the efficiency of a GeV as an optical antenna is given by its quantum coherence, which is effectively decoupled from its physical size. This makes the GeV perfectly compatible with nanometric distances, leading to the large field enhancements reported in the study.

On the other hand, this very same mechanism yields very different bandwidths at which each of them can operate. Traditional nanoantennas are suitable for broad bandwidths, while GeVs can only function within narrower ones. Although for some applications a large bandwidth is highly desirable (as it guarantees a broadband driving ability), GeVs' small bandwidth offers remarkable sensitivity to weak perturbations that would otherwise remain unnoticed.

### New directions for optical antennas

Given that field enhancements are often used in photochemistry, a potential application of GeV nanoantennas could be to improve the detection of "our novel perspective on color centers might open new directions for optical nanoantennas towards yet unexplored regimes"

molecules via Raman spectroscopy or other lightbased techniques. Optical sensing and quantum technologies could also benefit from them, for instance to control decoherence in solid-state qubits.

In summary, this study opens unexplored paths for optical nanoantennas, whose typical regime of operation was largely different, both at a technical level and on a more conceptual and long-term ground.

"The large near-field generated at close distances allows to concentrate massive energy in a remarkably small volume, increasing the optical efficiencies and enabling high spatial precision", emphasizes Andreoli about the demonstrated nanoantennas. "But on a broader ground, this just shows a specific example of how our novel perspective on color centers might open new directions for optical nanoantennas towards yet unexplored regimes".

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Li, Z., Guo, X., Jin, Y. et al. Atomic optical antennas in solids. Nat. Photon. (2024).

DOI: https://doi.org/10.1038/s41566-024-01456-5

Transmitting entanglement between light and matter in the metropolitan network of Barcelona



Measurement of non-classical correlations between remote locations. Map of the metropolitan area of Barcelona, with the three locations highlighted: ICFO, where the memory and SPDC source are located; CTTI, where the two optical fiber segments are connected; i2CAT, where the idler photons are detected.

# Transmitting entanglement between light and matter in the metropolitan network of Barcelona

ICFO researchers demonstrate for the first time the transmission of entanglement between matter and light over tens of kilometers through optical fiber in Barcelona.

As the efforts towards the realization of powerful quantum computers and quantum simulators continues, there is a parallel program aimed at attaining the quantum analogue to the classical internet. This new quantum network will provide ultrasecure, quantum-safe cybersecurity and, eventually, be devoted to the exchange of qubits, the unitary elements of quantum information and the language of quantum computers. It will in fact provide a net over which different quantum computers could connect, like classical processors are connected in cloud computing.

An up-front choice for the future quantum internet infrastructure is, in fact, the existing telecommunication network, which provides an almost ubiquitous channel over which light can travel very large distances with limited absorption. Because of this low absorption and its high speed, light is a great candidate as an information carrier, be it classical or quantum. Bright laser light can be readily used to transfer classical information on the internet, while the attenuation of light in optical fibers is compensated by light amplifiers placed every tens of km within these fibers. However, the transfer of quantum information, that is quantum communication, requires much

more sophisticated means.

Quantum bits are still encoded in light, specifically single photons, but this quantum encoding cannot be amplified because the rules of quantum mechanics prevent this: if you try to amplify the quantum econding, you seriously damage the information contained in the photons. Thus, the amplifiers used in classical networks cannot be used for quantum bits. This means that a radically new technology is needed to build a quantum version of the internet: the quantum repeater.

As light amplifiers ensure connectivity between distant locations, so will quantum repeaters allow for long distance communication by distributing entanglement between them. Entanglement is an exclusively quantum property of two objects which show correlations that cannot be reproduced through classical means, and it is one of the primary components for quantum communication. It can be used to transfer quantum information, for example through quantum teleportation between two nodes of a quantum repeater system.

One way of establishing remote entanglement between two nodes is through direct transmission: an entangled pair of photons can be generated, with one staying put while the other travels to the other location. This means that the latter needs to be compatible with optical fibre transmission, while the former needs to be stored in a quantum memory, leading to entanglement between light and matter.

Now, one needs a set of quantum repeaters to pair several of these nodes to achieve long-distance entanglement between quantum memories. A promising architecture for these quantum repeater nodes relies on pairing the spontaneous generation of photon pairs, a process known spontaneous parametric down conversion (SPDC), with an external quantum memory.

This is the approach that researchers at ICFO have taken. In the study published in *Optica Quantum*, Jelena Rakonjac, Samuele Grandi, Soren Wengerowsky, Dario Lago-Rivera and Felicien Appas, led by ICREA Prof. at ICFO Hugues de Riedmatten demonstrate the transmission of light-matter entanglement over tens of kilometers of optical fibre.

In their experiment, they generated pairs of photons, where one is emitted at the telecommunication wavelength of 1436nm, while the other is emitted at 606nm, compatible with the solid-state quantum memories used, realized in special crystals doped with rare-earth atoms.

They then tapped into the metropolitan network of Barcelona, connecting their system to two fibres which ran from ICFO, in Castelldefels, to the Telecommunication Centre of Catalunya (CTTI), in Hospitalet de Llobregat. By connecting both centers, they created a ring of 50km, sending the photons all the way to downtown Barcelona and back to ICFO. With this, they

"one needs a set of quantum repeaters to pair several of these nodes to achieve long-distance entanglement between quantum memories"

demonstrated that, after a full-round trip of 50 km, the light generated in the lab maintains its quantum features, without substantial decrease, showing that the photonic qubits do not manifest decoherence when traveling tens of kms in a fiber optic cable even in a metropolitan area. So, in short, quantum light left the lab, and it was ultimately detected back at its origin.

However, quantum communication requires using and verifying entanglement between remote locations, where entangled photons are detected in locations well-separated in space and time. Moving into this direction, the researchers extended their network to include a new node, this time located at the i2CAT foundation, a building in Barcelona, about 44 km from ICFO through the local optical fiber network and 17 km in straight line.

There, they installed a telecom detector to measure the arrival of photons which came through one of the fibres, while the other fibre was connected to a transducer, which turned the electrical signal of the detector into light, and sent it through the optical fiber line. This way, the information could be conveyed back to ICFO with high precision, even though the photon was detected about 17 km away. Moreover, they used the same transducers to send synchronization signals between the two nodes of this basic network, where the generation and detection

of quantum correlations were fully separated between two independent yet connected nodes.

The experiment validated the system used by the researchers to generate light-matter entanglement and has proven to be one of the pioneering candidates for the realization of a quantum repeater node, the enabling technology for long-distance quantum communication. Proof-of-principle demonstrations have already been realized in the lab, and the group is now working on improving the performance of both the memory and the source.

Moreover, the researchers have partnered with Cellnex (Xarxa obierta de Catalunya) and a new laboratory is available at the Collserola tower within the context of the QNetworks and EuroQCI Spain projects, for the realization of an entangled state of remote quantum memories. The realization of a long distance backbone for entanglement distribution between quantum memories is also one of the main goals of the Quantum Internet Alliance (QIA), the leading European effort in the realization of the quantum internet of which ICFO is a main partner.

The results of this study "namely the transmission of light-matter entanglement over fibers deployed in a metropolitan area, are the initial stepping stone towards the realization of a full-fledge quantum internet, with our source and memory quantum node at its core" as Samuele Grandi comments, researcher at ICFO and co-first author of the study.

As ICREA Prof. at ICFO Hugues de Riedmatten concludes "Light-matter entanglement is a key resource for quantum communication and was demonstrated many times in the laboratory.

Demonstrating it in the installed fiber network is a first step towards realizing a test-bed for quantum repeater technologies in the Barcelona area, preparing the ground for long distance fiber based networks".

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Transmission of Light-Matter Entanglement over a Metropolitan Network, Jelena V. Rakonjac, Samuele Grandi, Sören Wengerowsky, Dario Lago-Rivera, Félicien Appas, and Hugues de Riedmatten, Optica Quantum 1, 94-102 (2023). DOI: https://doi.org/10.1364/OPTICAQ.501048

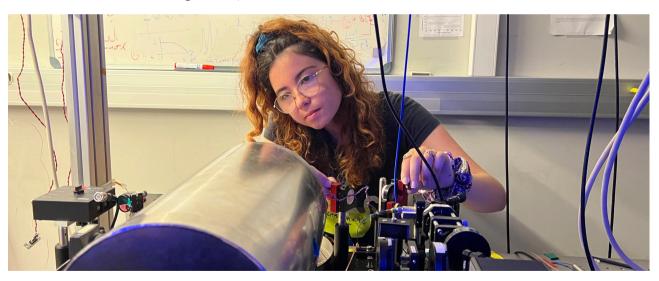
"the transmission of lightmatter entanglement over fibers deployed in a metropolitan area, are the initial stepping stone towards the realization of a full-fledge quantum internet"



### Towards the miniaturization of atomic sensors: a new readout method

ICFO researchers propose a new readout method for atomic sensors. The discovery is an important step towards the miniaturization of sensors like atomic magnetometers; a long-sought breakthrough that will enhance their spatial resolution, among other substantial improvements.

Some technological devices that aim at highprecision sensing are based on optical pumping (that is, the process in which light is used to raise —or "pump"— electrons from a lower energy level in an atom or molecule to a higher one) and atomic vapor spin physics (that is, the physics associated with the evolution and the interactions of an intrinsic magnetic property of atoms, called spin). For instance, optically pumped magnetometers



Maria Fernández manipulating the experimental set-up. Credit: ICFO

(OPMs), one of the most sensitive quantum devices to detect very weak magnetic fields, rely on these two principles. There is an important element that influences the degree of sensitivity and that, consequently, can compromise the performance of such instruments: the readout of the electronic spins' polarization (a property related to how atomic spins orient). Currently, there are state-of-the-art methods that enhance readout effectiveness, but their performance worsens as the dimensions of the sensors are reduced, holding back the miniaturization that most of the modern technologies pursue.

The issue has been recently addressed by ICFO researchers María Hernández, Yintao Ma (also member of the Xi'an Jiaotong University), Hana Medhat, Dr. Chiara Mazzinghi (also member of Instituto Nazionale di Ottica, Sesto Fiorentino) and Dr. Vito Giovanni Lucivero (also member of the Universitá degli Studi di Bari Aldo Moro), led by ICREA Professor at ICFO Morgan W. Mitchell. In a Physical Review Applied article, they have demonstrated a new nondestructive method to monitor the electron spin polarization of an atomic ensemble that, at the same time, allows for miniaturization.

### A new spin-polarization monitoring technique

In the study, the authors utilized three different components (each of them well-established on its own) and brought them all together, something that no one had ever done before.

The first ingredient was the use of an atomic vapor and the exploitation of its optical properties. In particular, they used rubidium 87, a very regular choice when dealing with sensors as they are naturally sensitive to external changes in their environment.

The second one was the use of an optical resonator. These optical elements, also known as "optical cavities", improve the spin readout by increasing the interaction length between the rubidium atoms and the infrared light, which is used to probe them. Moreover, the vapor was placed inside a so-called

"the results pave the way towards the miniaturization of atomic sensing devices that allow high spatial resolution in magnetic field detection"

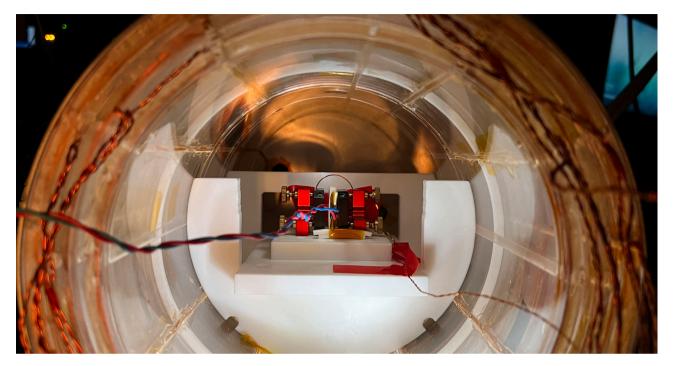
micro-electromechanical system (MEMS) vapor cell, since this kind of cell enables the miniaturization of sensing devices without this being detrimental to its quality.

And thirdly, the team performed the readout using the Pound-Drever-Hall (PDH) technique. The PDH method is widely used to measure changes in the frequency or phase of laser light with infinitesimal precision (for instance, in gravitational waves detection). In this case, by sending light into the medium and measuring the phase shift through PDH, the researchers were able to indirectly infer the atomic spin polarization (as the former depends on the latter).

In summary, the team performed PDH readout of the atomic spin polarization of a rubidium 87 vapor housed in a MEMS cell within an optical resonator. The results suggest an enhanced readout (and thus better sensitivity) even in small cells, a two-fold improvement over previous attempts.

### Benefits for future atomic sensors

The researchers claim that their method has potential to provide high efficiency readout for miniaturized atomic vapor sensing and metrology instruments. "This is an important result since it paves the way towards the miniaturization of atomic



Experimental setup for cavity-based detection of atomic polarization. Credit: ICFO.

sensing devices that allow high spatial resolution in magnetic field detection. Moreover, in principle, the method can be quantum noise limited, which will enable quantum enhanced detection in miniaturized sensors", shares María Hernández, leading author of the article.

Hernández has already started building an optical magnetometer based on this technique for microbio-magnetic applications. The miniaturization of atomic magnetometers could result in sensors with improved spatial resolution and that could also be suitable for spin squeezing, a milestone the team is looking forward to achieving.

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M. Hernández, Y. Ma, H. Medhat, C. Mazzinghi, V. Giovanni, and M. W. Mitchell. Cavity-enhanced detection of spin polarization in a microfabricated atomic vapor cell. Phys. Rev. Applied 21, 064014 (2024).

DOI: https://doi.org/10.1103/PhysRevApplied.21.064014

### Securely propagating entanglement at the push of a button

Physicists at MPQ use laser tweezers in optical resonators to create entanglement in a quantum network.

Entanglement, Einstein's "spooky action at a distance", today is THE tool of quantum information science. It is the essential resource for quantum computers and used to transmit quantum information in a future quantum network. But it is highly sensitive. It is therefore an enormous challenge to entangle resting quantum bits (qubits) with flying gubits in the form of photons "at the push of a button". However, a team led by Gerhard Rempe, Director at the Max Planck Institute of Quantum Optics in Garching, Germany, has now succeeded in doing exactly that with atoms connected in parallel. The atoms are sandwiched between two almost perfect mirrors. This setup guarantees reliable interaction with photons as flying gubits - a technique pioneered by Gerhard Rempe. Using optical tweezers, the team was able to individually control up to six atoms and entangle each with a photon. Using a multiplexing technique, the scientists demonstrated an atomphoton entanglement generation with almost 100 percent efficiency, a groundbreaking achievement for distributing entanglement over a quantum network. The work is published today in the journal Science

Interfaces between resting qubits and flying qubits come into play whenever quantum information needs to be transmitted over long distances. "One aspect is the communication of quantum information over long distances in a future quantum internet," explains **Emanuele Distante**,

who supervised the experiment as a postdoctoral researcher, and is now a researcher at ICFO in Barcelona: "The second aspect is the goal of connecting many qubits in a distributed network to form a more powerful quantum computer. Both applications require efficient interfaces between qubits at rest and qubits in motion. This is why many groups around the world are feverishly researching quantum mechanical light-matter interfaces.

Several different technical approaches are being pursued. Gerhard Rempe and his team in Garching have been working for many years on a method that uses ultracold rubidium atoms captured trapped between two almost perfect mirrors as an optical resonator. The focus is on a future quantum internet. This approach has an inherent advantage because it allows a trapped atom to interact highly efficiently with a photon, which bounces back and forth between the two mirrors about twenty thousand times like a ping-pong ball. What's more, because one of the two mirrors is slightly more transparent than the other, the photon leaves in a precisely predetermined direction. This means that it is not lost, but can be reliably coupled into an optical fiber. If this photon is entangled with the atom using a specific protocol of laser pulses, this entanglement is maintained as the photon travels.

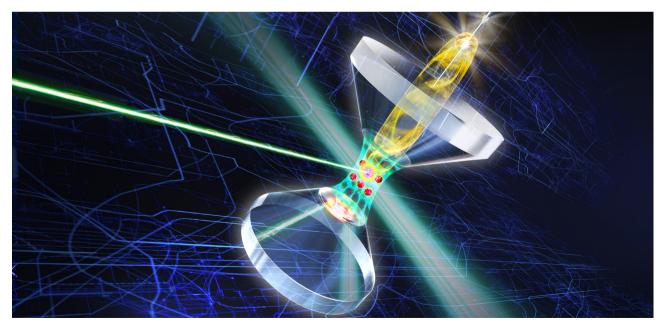
### Multiplexing to prevent transmission losses

In 2012, the Garching team succeeded in entangling an atom in one resonator with a second atom in another resonator via "photon radio" through a 60-metre-long glass fiber. With the help of the transmitted photon, they formed an extended entangled quantum object from the two atoms. However, the photon must not get lost in the glass fiber along the way, and this is precisely the problem with a longer journey. The solution, at least for medium distances of a few kilometers, is called "multiplexing". Multiplexing is a standard method used in classical information technology to make transmission more robust. Think of it as a radio link through a noisy area: If you send the radio signal along several parallel channels, the probability that it will reach the receiver via at least one channel increases

"Without multiplexing, even our current Internet would not work," explains Distante: "But transferring this method to quantum information systems is a particular challenge." Multiplexing is not only interesting for more secure transmission over longer distances in a future quantum internet, but also for a local quantum network. One example is the distributed quantum computer, which consists of several smaller processors that are connected via short optical fibers. Its resting qubits could be entangled more reliably by multiplexing with flying qubits to form a distributed, more powerful quantum computer.

### Laser tweezers for handling atoms

The challenge for the Garching team was to load several atoms into a resonator as resting qubits and to address them individually. Only if the position



Rubidium atoms are trapped in the optical resonator and are addressed individually using a highly focussed laser beam. This allows the researchers to entangle the trapped atoms with individual photons.

### "the entanglement distribution works almost deterministically, at the push of a button"

of the atoms is known can they be entangled in parallel with one photon each in order to achieve multiplexing. Hence, the team developed a technique for inserting optical tweezers into the narrow resonator. "The mirrors are only about half a millimeter apart," explains Lukas Hartung, PhD student and first author of the Science paper.

The optical tweezers consist of fine laser beams that are strong enough to capture an atom in their focus and move it precisely to the desired position. Using up to six such tweezers, the team was able to arrange a corresponding number of floating rubidium atoms in the cavity to form a neat qubit lattice. Since the atoms can easily remain in the trap for a minute – a little eternity in quantum physics – they could easily be entangled with one photon each. "This works almost one hundred per cent of the time," says Distante, emphasizing the key advantage of this technique: the entanglement distribution works almost "deterministically", i.e. at the push of a button.

### Scalable to considerably more gubits

In order to achieve this, the team used a microscope lens objective positioned above the resonator with micrometer precision in order to focus the individual beams of the light tweezers into the narrow mirror cabinet. The tweezer beams are generated via so-called acousto-optical deflectors and can therefore be controlled individually. Precise adjustment of the laser tweezers in the optics requires a great deal of dexterity. "Mastering this challenge was the

cornerstone for the success of the experiment," summarizes Stephan Welte, who helped develop the technology as part of the team and is now a researcher at FTH Zurich

The current experiment gives hope that the method can be scaled up to considerably more qubits without losses: the team estimates that up to 200 atoms could be controlled in such a resonator. As these quantum bits can be controlled very well in the resonator, this would be a huge step forward. And as the interface even feeds one hundred per cent of the entangled photons into the optical fiber, a network of many resonators, each with 200 atoms as resting qubits, would be thinkable. This would result in a powerful quantum computer. It is still a dream of the future. But with the laser tweezers, the Garching team now has a considerable part of this future firmly under control.

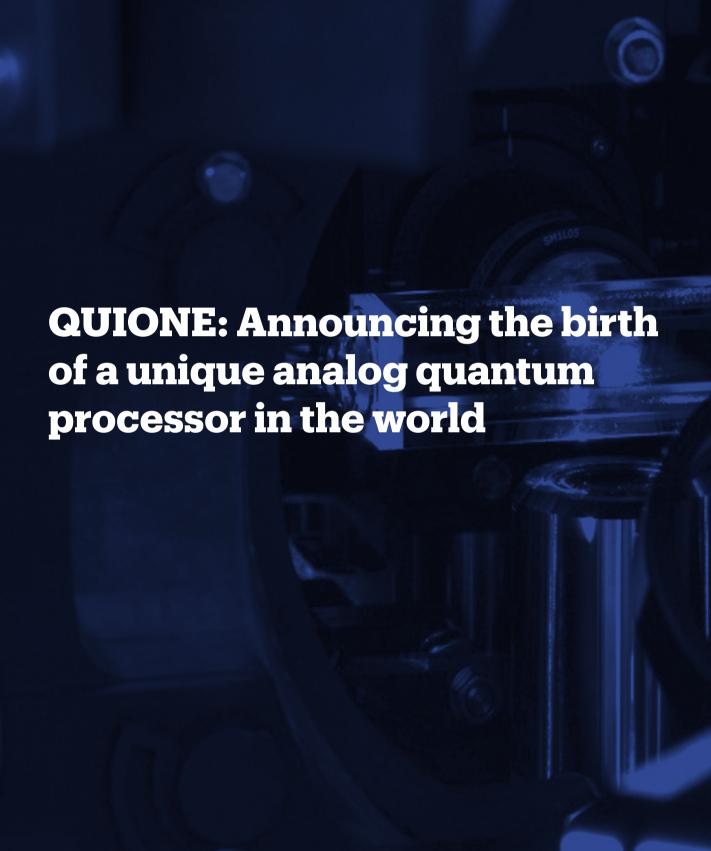
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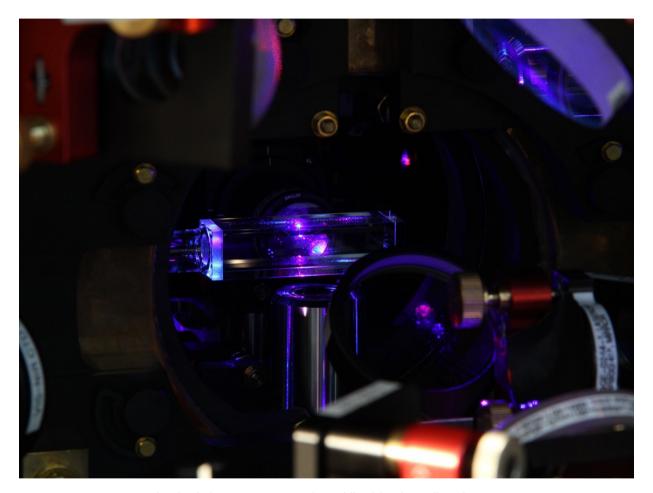
L. Hartung, M. Seubert, S. Welte, E. Distante, G. Rempe. A quantum-network register assembled with optical tweezers in an optical cavity. Science (2024).

DOI: 10.1126/science.ado6471



Emmanuele Distante, one of the authors of the article, in a lab.





The cloud of strontium atoms in the middle of the glass cell Credit: ICFO.





# QUIONE: Announcing the birth of a unique analog quantum processor in the world

ICFO researchers build QUIONE, a quantum simulator capable of observing individual atoms in a strontium quantum gas.

Quantum physics needs high-precision sensing techniques to delve deeper into the microscopic properties of materials. From the analog quantum processors that have emerged recently, the so-called quantum-gas microscopes have proven to be powerful tools for understanding quantum systems at the atomic level. These devices produce images of quantum gases with very high resolution: they allow individual atoms to be detected.

Now, ICFO researchers Sandra Buob, Jonatan Höschele, Dr. Vasiliy Makhalov and Dr. Antonio Rubio-Abadal, led by ICREA Professor at ICFO Leticia Tarruell, explain how they built their own quantum-gas microscope, named QUIONE after the Greek goddess of snow. The group's quantum-gas microscope is the only one imaging individual atoms of strontium quantum gases in the world, as well as the first of its kind in Spain. The study is published in *PRX Quantum*.

Beyond the impactful images in which individual atoms can be distinguished, the goal of QUIONE is quantum simulation. As ICREA Prof. Leticia Tarruell explains: "Quantum simulation can be used to boil down very complicated systems into simpler models to then understand open questions that current computers cannot answer, such as why some materials conduct electricity without any losses even at relatively high temperatures".

The research of the group at ICFO in this area has received support at national level (award from the Royal Spanish Society of Physics, and projects and grants from the BBVA Foundation, Ramón Areces Foundation, La Caixa Foundation and Cellex Foundation) and European level (including an ERC project). In addition, QUIONE is co-financed by the Government of Catalonia, through the Secretariat of Digital Policies of the Department of Enterprise and Work, as part of the Catalan Government's commitment to promote quantum technologies.

The singularity of this experiment lies in the fact that they have managed to bring the strontium gas to the quantum regime, place it in an optical lattice where the atoms could interact by collisions and then apply the single atom imaging techniques. These three ingredients altogether make ICFO's strontium quantum-gas microscope unique in its kind.

#### Why strontium?

Until now, these microscope setups relied on alkaline atoms, like lithium and potassium, which have simpler properties in terms of their optical spectrum compared to alkaline-earth atoms such as strontium. This means that strontium offers more ingredients to play with in these experiments.

In fact, in recent years, the unique properties of strontium have made it a very popular element for applications in the fields of quantum computing and quantum simulation. For example, a cloud of strontium atoms can be used as an atomic quantum processor, which could solve problems beyond the capabilities of current classical computers.

All in all, ICFO researchers saw great potential for quantum simulation in strontium, and they set to work to build their own quantum-gas microscope. This is how QUIONE was born.

#### QUIONE, a quantum simulator of real crystals

To this end, they first lowered the temperature of the strontium gas. Using the force of several laser beams, the speed of atoms can be reduced to a point where they remain almost motionless, barely moving, reducing their temperature to almost absolute zero in just a few milliseconds. Then, the laws of quantum mechanics rule their behavior, and the atoms display new features like quantum superposition and entanglement.

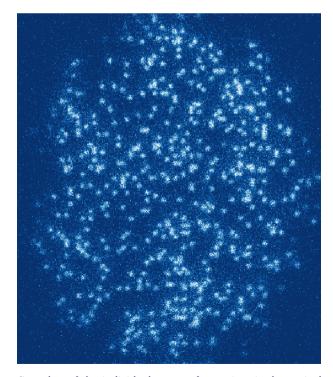
After that, with the help of special lasers, the researchers activated the optical lattice, which keeps the atoms arranged in a grid along space. "You can imagine it like an egg carton, where the individual sites are actually where you put the eggs. But instead of eggs we have atoms and instead of a carton we have the optical lattice", explains Sandra Buob, first author of the article.

The atoms in the egg cup interacted with each other, sometimes experiencing quantum tunnelling to move from one place to another. This quantum dynamics between atoms mimics that of electrons in certain materials. Therefore, the study of these systems can help understand the complex behavior of certain materials, which is the key idea of

quantum simulation.

As soon as the gas and the optical lattice were ready, the researchers took the images with their microscope and could finally observe their strontium quantum gas atom by atom. At this point, the construction of QUIONE had already been a success, but its creators wanted to get even more out of it.

Thus, in addition to the pictures, they took videos of the atoms and were able to observe that, while the atoms should remain still during the imaging, they sometimes jumped to a nearby lattice site. This can be explained by the phenomenon of quantum tunnelling. "The atoms were "hopping" from one site to another. It was something very

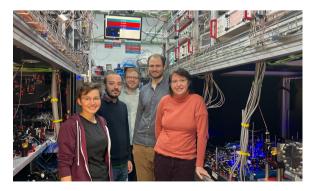


Snapshot of the individual atoms of strontium in the optical lattice. Source: PRX Quantum.

beautiful to see, as we were literally witnessing a direct manifestation of their inherent quantum behavior", shares Buob.

Finally, the research group used their quantumgas microscope to confirm that the strontium gas was a superfluid, a quantum phase of matter that flows without viscosity. "We suddenly switched off the lattice laser, so that the atoms could expand in space and interfere with each other. This generated an interference pattern, due to the wave-particle duality of the atoms in the superfluid. When our equipment captured it, we verified the presence of superfluidity in the sample", explains Dr. Antonio Rubio-Abadal.

"It is a very exciting moment for quantum simulation", shares ICREA professor Leticia Tarruell. "Now that we have added strontium to the list of available quantum-gas microscopes, we might be able to simulate more complex and exotic materials soon. Then new phases of matter are expected to arise. And we also expect to obtain much more computational power to use these machines as analog quantum computers".



The team in the lab. From left to right: Sandra Buob, Antonio Rubio-Abadal, Vasiliy Makhalov, Jonatan Höschele, and Leticia Tarruell

"Now that we have added strontium to the list of available quantum-gas microscopes, we might be able to simulate more complex and exotic materials soon"

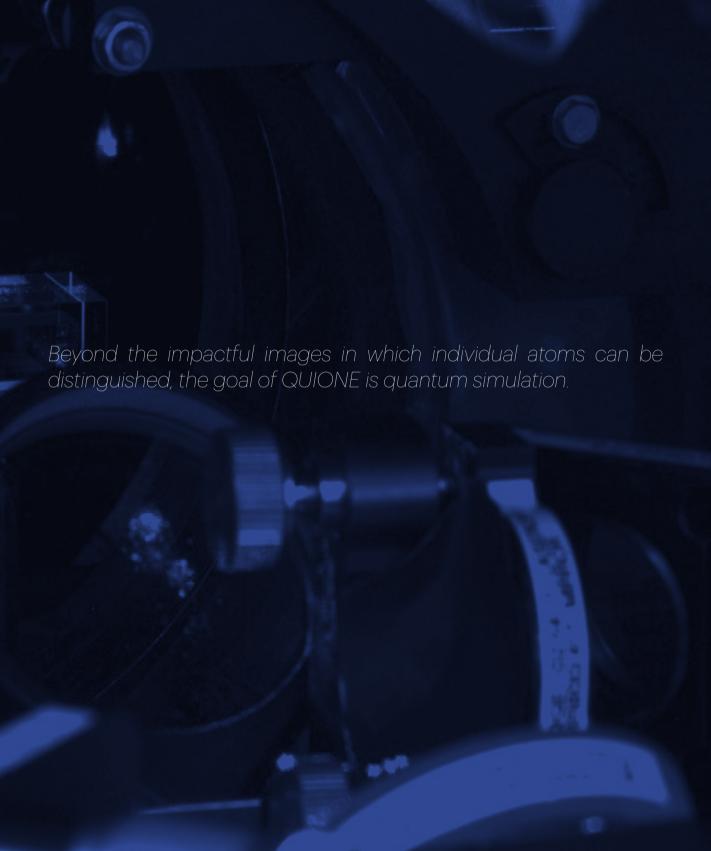
### About QUIONE and Quantum Technologies in Barcelona

QUIONE is a program created by ICFO that aims at using quantum processors based on individually controlled and detected ultracold atoms to solve problems hard for classical computers. The program includes the analog quantum processor QUIONE I, the quantum-gas microscope mentioned in the study, and a hybrid analog-digital processor named QUIONE II, which is currently under construction. QUIONE is part of the eight major programs that Government of Catalonia, through the Secretary of Digital Policies, co-finances as part of its commitment to the promotion of quantum technologies.

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S. Buob, J. Höschele, V. Makhalov, A. Rubio-Abadal and L. Tarruell, "A strontium quantum-gas microscope". PRX Quantum 5, 020316 (2024).

DOI: https://doi.org/10.1103/PRXQuantum.5.020316



# New analog simulators can facilitate the study of ultrafast dynamics processes

A team of researchers has theoretically proposed a new experimental platform based on analog simulation with atom clouds to study high-harmonic generation, an ultrafast dynamic process whose study challenges conventional computational methods. Their simulator can be adapted to approach a wide range of complex phenomena, opening the door to regimes that theory and direct experimentation are struggling to reach.

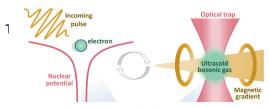
Despite all the successes in understanding electron dynamics at their natural attosecond (one quintillionth of a second) time scale, one of the fundamental processes core to this field, high-harmonic generation (HHG), raises new challenges for cold-atom simulation. It consists in a highly non-linear phenomenon where a system absorbs many photons of an incoming laser and emits a single photon of much higher energy.

The unique characteristics of HHG make it an exceptional source of extreme ultraviolet radiation and consequently of attosecond pulses of light, which has important applications to various fields such as nonlinear optics or attosecond science.

The main obstacle hindering the study of this process, apart from the ultrafast speed at which it occurs, is the high number of variables involved. In any given material, many atoms and electrons are present, so to study most of the occurring chemical processes in all its complexity would require not only to describe all these components, but also their interactions with external fields and even among themselves. This turns out to be an extremely challenging task for any current classical computer. An alternative route is to use quantum

devices, building the so-called analog simulators, whose nature allow them to better capture the complexity of the system.

Now, ICFO researchers Javier Argüello, Javier Rivera, Philipp Stammer led by the ICREA Prof. at ICFO Maciej Lewenstein and in collaboration with other institutes all over the globe (Aarhus University, University of California and Guangdong Technion-Israel Institute of Technology) have proposed, in a *Physical Review X Quantum* publication, an analog simulator to access the emission spectrum of HHG using ultracold atomic clouds. Besides showing that an accurate replication of the key characteristics HHG in atoms was possible, they also provide details on how to implement it to specific atomic targets and discuss the main sources of errors.



Schematic representation of the HHG process in atoms on the left and proposed analog simulator on the right.

An analog simulator allows scientists to study a complex quantum system (computationally challenging) through the control and manipulation of a much simpler one, which can be addressed experimentally. However, not every choice is valid, a connection between both systems must exist.

In this particular work, the complex phenomenon they chose in order to benchmark their idea was the high-harmonic generation. In there, the atomic bound electrons tunnel out the barrier formed by the atomic Coulomb potential and a laser electric field. Then, those free electrons are accelerated, causing the emission of radiation of characteristic harmonic frequencies upon recombination with their parent ions. This is the emission spectrum of the HHG that the researchers wanted to recover.

On the other hand, the connection to a much simpler quantum system was obtained by conveniently replacing certain components. Instead of an electron and a nuclear potential, they proposed to use an atomic gas that was trapped by a laser beam; and instead of the incoming light and its electric field, they suggested an external magnetic gradient that could be tuned at will. It turns out that the absorption images of this engineered system coincide with the desired emission yield.

"their method has the potential to address complex systems that otherwise could only be theoretically approximated"

Therefore, by taking absorption images of the analog simulator, the emission spectrum of the atomic high-harmonic generation can be indirectly studied.

#### A new platform for ultrafast simulation

In the end, the research group has paved the way to prove the potential of their alternative method to address complex systems that otherwise could only be theoretically approximated. They showed that state-of-the-art analog simulators are able to retrieve the HHG emission spectrum, a correspondence between the experimental and simulated parameters could be established and even an exhaustive experimental analysis was provided.

Moreover, the platform advantages are twofold. In the first place, the elements that emulate the incoming field and the nuclear potential can be easily tuned. And secondly, the simulation also provides a temporal magnification. This implies a high level of accessibility as the attosecond timescale can be avoided, allowing the scientists to work in a much slower (and thus practical) frame.

The team highlights the adaptability power of their approach, which is not restricted to simulating HHG exclusively, but could be extended to other, more exotic configurations. In particular, the simulation of ultrafast processes, such as multielectronic dynamics or the reaction of matter to non-classical light, are the ones that could benefit the most.

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Javier Argüello-Luengo, Javier Rivera-Dean, Philipp Stammer, Andrew S. Maxwell, David M. Weld, Marcelo F. Ciappina, and Maciej Lewenstein, PRX Quantum 5, 010328 (2024). DOI: https://doi.org/10.1103/PRXQuantum.5.010328

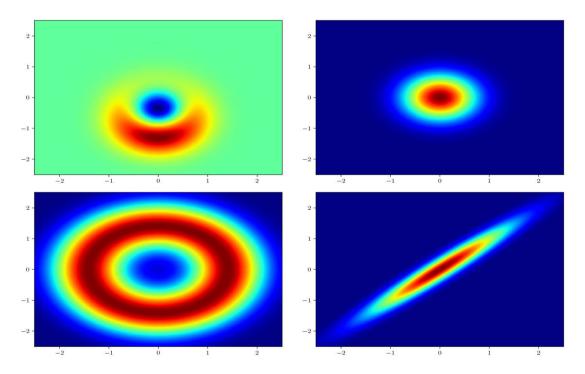
## Placing value on quantum phenomena in attosecond science

In a *Nature Reviews Physics* perspective article, researchers overview the latest advances regarding quantum phenomena within attosecond science, which are often overlooked despite their potential to influence experimental and theoretical outcomes.

Attosecond science, the field aimed at manipulating and observing phenomena with attosecond (that is, 10<sup>-18</sup> seconds) time-resolution, has opened the door to real-time observation and control in the atomic realm. For instance, it has unraveled previously unseen details of electron dynamics on their natural

time-scale or the behavior of matter under extreme conditions

On the other hand, quantum physics is a fundamental theory that describes the behavior of nature at and below the scale of atoms. One would thus expect



Examples of Wigner functions for different states considered in the quantum optical formulation of HHG. Source: Nature Reviews Physics.

"This combined field might allow conceiving novel experiments and bringing attosecond science towards optical quantum technologies"

attoscience and quantum mechanics to be closely related. Indeed, many successful applications arising from the mixture of both disciplines have kept appearing over the years, specially within the areas of quantum optics, quantum chemistry and quantum information science. Still, the 'quantumness' of many attosecond experiments has been systematically overlooked. Light is treated classically, the presence of entanglement is neglected or unexplored, signs of non-classical features of the field modes are not seen nor searched for, among others. Despite the largely spread lack of consideration, these features might strongly influence experimental and theoretical outcomes.

Now, **Philipp Stammer**, researcher at ICFO, together with researchers from the University College London, Northwestern University, Institute for Nanostructure and Solid-State Physics (University of Hamburg), have published a comprehensive perspective article in **Nature Reviews Physics** on quantum phenomena in attosecond science.

The article collects the work of different efforts aimed at unveiling the intrinsic quantum nature of attosecond science, which have evolved in separate manners. For the quantum optical approach to attosecond processes, it highlights where and how deviations from the semi-classical picture (the one using quantum mechanics to describe matter,

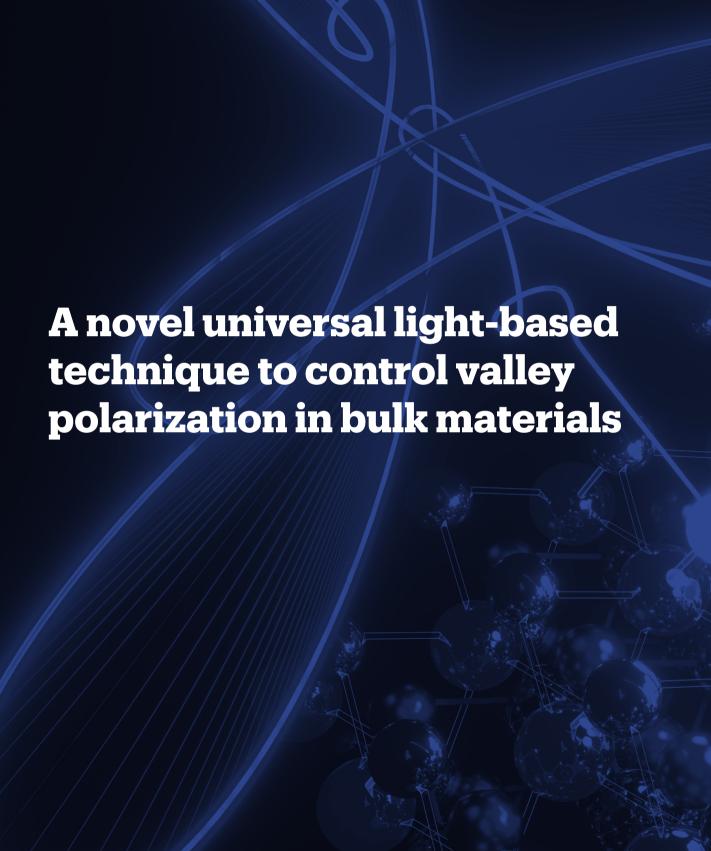
but classical mechanics to describe light) can be expected. It also provides the first unambiguous classification of quantum and classical phenomena in attosecond science, which had not been carefully defined before. For the field of quantum science, it shows that intense laser-driven processes can be used as a platform for quantum technology applications.

From the wide range of recent achievements, Philipp Stammer highlights "the full quantum optical theoretical description of the process of high harmonic generation (HHG) and above threshold ionization (ATI), showing quantum features such as squeezing and entanglement, as well as the theoretical study of driving HHG and ATI by non-classical light sources". Experimentally, he considers that "the generation of non-classical field states by means of optical Schrödinger cat states, witnessing entanglement between certain field modes or driving HHG with squeezed light" are some of the main advances.

In addition to overviewing the emerging full quantum descriptions and the increasing interest in entanglement in attosecond processes, the researchers also review some of the future perspectives. This combined field might allow conceiving novel experiments and bringing attosecond science towards optical quantum technologies by engineering quantum light or by using entanglement or quantum coherence as a resource, among other promising applications.

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Cruz-Rodriguez, L., Dey, D., Freibert, A. et al. Quantum phenomena in attosecond science. Nat Rev Phys (2024). DOI: https://doi.org/10.1038/s42254-024-00769-2



# A novel universal light-based technique to control valley polarization in bulk materials

An ICFO team, together with international collaborators, report in Nature a new method that achieves for the first time valley polarization in centrosymmetric bulk materials in a non-material-specific way.

This "universal technique" may have major applications linked to the control and analysis of different properties for 2D and 3D materials, which can in turn enable the advancement of cutting-edge fields such us information processing and quantum computing.

Electrons inside solid materials can only take certain values of energy. The allowed energy ranges are called "bands" and the space between them, the forbidden energies, are known as "band-gaps". Both of them together constitute the "band structure" of the material, which is a unique characteristic of each specific material.

When physicists plot the band structure, they usually see that the resulting curves resemble mountains and valleys. In fact, the technical term for a local energy maximum or minimum in the bands is called a "valley", and the field which studies and exploits how electrons in the material switch from one valley to the other is coined "valleytronics".

In standard semiconductor electronics, the electric charge of the electrons is the most used property exploited to encode and manipulate information. But these particles have other properties that could also be used for the same purpose, such as the valley they are in. In the past decade, the main aim of valleytronics has been to reach the control of valley population (also

known as valley polarization) in materials. Such an achievement could be used to create classical and quantum gates and bits, something that could really drive the development of computing and quantum information processing.

Previous attempts presented several drawbacks. For example, the light used to manipulate and change valley polarization had to be resonant, that is, the energy of its photons (the particles that constitute light) had to correspond exactly to the energy of the band-gap of that particular material. Any small deviation reduced the efficiency of the method so, provided that each material has their own band-gaps, generalizing the proposed mechanism seemed something out of reach. Moreover, this process had only been achieved for monolayer structures (2D materials, just one-atom-thick). This requirement hindered its practical implementation, as monolayers are usually limited in size, quality and difficult to engineer.

Now, ICFO researchers **Igor Tyulnev**, **Julita Poborska**, **Dr. Lenard Vamos**, led by **Prof. ICREA** 

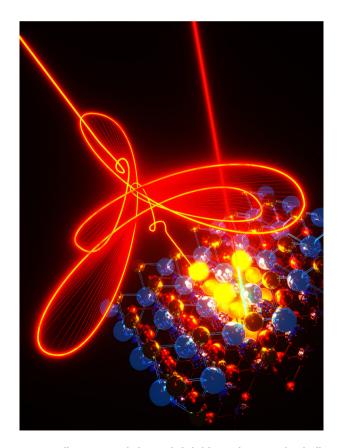
"When we started working on this project, we were told by our theory collaborators that showing valley polarization in bulk materials was rather impossible"

Jens Biegert, in collaboration with researchers from the Max-Born-Institute, the Max-Planck Institute for the Science of Light, and Instituto de Ciencia de Materiales de Madrid have found a new universal method to induce valley polarization in centrosymmetric bulk materials. The discovery, published in *Nature*, unlocks the possibility to control and manipulate valley population without being restricted by the specific chosen material. At the same time, the method can be used to obtain a more detailed characterization of crystals and 2D materials.

#### Valley polarization in bulk materials is possible

The adventure began with the experimental group led by ICREA Prof. at ICFO Jens Biegert who initially wanted to experimentally produce valley polarization using their particular method in 2D materials, following the lines of what had been theoretically proved in a previous theoretical paper by Álvaro Jiménez, Rui Silva and Misha Ivanov. To set up the experiment, the initial measurement was tried on bulk MoS<sub>2</sub> (a bulk material is made of many monolayers stacked together) with the surprising result that they saw the signature of valley polarization. "When we started working on this project, we were told by our theory collaborators that showing valley polarization in bulk materials was rather impossible", explains Julita Poborska.

The theoretical team remarks as well how, at the very beginning, their model was only suitable for single 2D layers. "At a first glance, it seemed that adding more layers would hinder the selection of specific valleys in the sample. But after the first experimental results, we adjusted the simulation to bulk materials and it validated the observations surprisingly well. We did not even try to fit anything. It is just the way it came out", adds Prof. Misha Ivanov, the theorist leader. In the end, "it turned out that yes, you can actually valley polarize bulk materials that are central symmetric, because of the symmetry conditions", concludes Poborska.



Artistic illustration of the trefoil field incident on the bulk material  ${\rm MoS}_{\scriptscriptstyle\mathcal{T}}$  @ICFO

As Igor Tyulnev, first author of the article, explains, "our experiment consisted in creating an intense light pulse with a polarization that fitted this internal structure. The result was the so-called "trefoil field", whose symmetry matched the triangular sublattices that constitute hetero-atomic hexagonal materials".

This symmetry-matched strong field breaks the space and time symmetry within the material, and, more importantly, the resulting configuration depends on the orientation of the trefoil field with respect to the material. Therefore, "by simply rotating the incident light field, we were able to modulate the valley polarization", concludes Tyulnev, a major achievement in the field and a confirmation of a novel universal technique that can control and manipulate the electron valleys in bulk materials

"by simply rotating the incident light field, we were able to modulate the valley polarization"

#### The experimental process

The experiment can be explained in three main steps: First, the synthesis of the trefoil field; then its characterization; and finally, the actual production of valley polarization.

The researchers emphasize the incredibly high precision that the characterization process required, as the trefoil field is made of not just one, but two coherently combined optical fields. One of them had to be circularly polarized in one direction, and the other needed to be the second harmonic

of the first beam, polarized with the opposite handedness. They superimposed these fields onto each other, so that the total polarization in time traced the desired trefoil shape.

Three years after the initial experimental attempts, Igor Tyulnev is thrilled by the recent *Nature* publication. The appearance in such a prestigious journal recognizes the new universal method which, as he states, "can be used not only to control the properties of a wide variety of chemical species, but also to characterize crystals and 2D materials".

As ICREA Prof. at ICFO Jens Biegert remarks: "Our method may provide an important ingredient to engineer energy efficient materials for efficient information storage and fast switching. This addresses the pressing need for low-energy consumption devices and increased computational speed. I cannot promise that what we have provided is THE solution, but it is probably one solution on this big challenge".

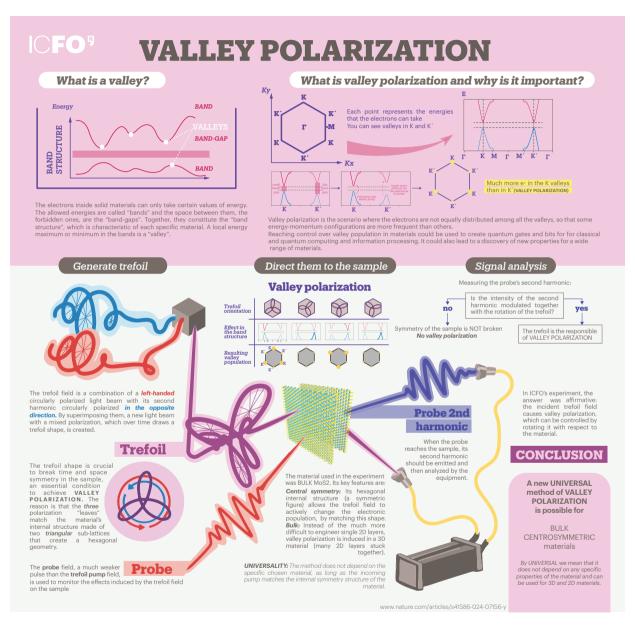
#### Reference:

Valleytronics in bulk MoS2 with a topologic optical field, Igor Tyulnev, et. al., 2024, NATURE.

DOI: https://doi.org/10.1038/s41586-024-07156-y



From left to right: Dr. Lenard Vamos, Julita Poborska, Igor Tyulnev, and ICREA Prof. Jens Biegert. ©ICFO



Schematic of the valley polarization effect, where the incident trefoil field (in purple) causes valley polarization in the bulk material MoS2. This effect can be controlled by rotating the field with respect to the material.

Youtube video:



### Donna Strickland

Professor, Department of Physics and Astronomy, University of Waterloo. Leader of the Ultrafast Laser Group. Recipient of the Nobel Prize in Physics 2018.

Donna Strickland is the 3rd woman in history to have been awarded the Nobel Prize in Physics, together with Gérard Mourou, for inventing chirped pulse amplification (CPA) - a method of making pulses of laser light of high power and short duration.

March 2024, ICFO

## Can you tell us about the Eureka moment that led to your invention of chirped pulse amplification (CPA)?

Gérard had the idea of a CPA in 1983 but it was when we went to a conference in 1984 and everybody was doing pulse compression in fibers that we realized this is how we would do it. They were already stretching the pulse in the fiber, making extra colors in the fiber so that they could make shorter pulses. They weren't trying to amplify them, simply trying to make them short.

Gérard already knew that we needed to make short pulses long so we could amplify them, so we realized that all we do was put the amplifier after the fiber before the compressor, and this would all work. That was the eureka moment, and it took a year after that for us to show that it did work.



"We thought [our discovery] would have an impact in the field, but not that it would be the huge thing that CPA turned out to be"

### The importance of the discovery isn't always clear immediately, or maybe it was in your case?

Not even close! We knew that it was the way to make a Petawatt laser, but we thought it would be in the big laser labs for the great big energy lasers, so there would have been very few lasers that could do it. We thought it would have an impact in the field, but not that it would be the huge thing that CPA turned out to be.

While we were doing our work, Peter Moulton at Lincoln Labs at MIT was doing work on a new laser material, and that allowed much shorter pulses than what we could have in a big storage energy medium. This combination allowed us to have even shorter pulses so we could get the same peak power with less energy. All academic labs could afford these lasers and that's when it became huge.

The application that CPA is known for is the eye surgery, and that came later from an accident with a student in Gérard's group. The Ti:sapphire laser reached to where your eye could just see and people were tempted to take their goggles off, easily forgetting that it was so powerful because it looked like a weak beam. Eye damage became a real problem. They took Gérard's injured student to an ophthalmologist on campus.

Typical laser damage would still be thermal and cause a tear, but this was a perfect round hole. And this ophthalmologist asked: "What kind of laser were you using that would make that kind of damage?" Now, of course, the poor students with his eye full of blood is thinking, "I don't care. That's not the question we need to answer right now!" And then it was this same ophthalmologist working with Gérard who figured out how to use CPA for ophthalmology. It is just one of these weird, quirky things in nature that lead from one thing to another.

### Can you tell us about something that you find exciting in your field today?

If I ever get my laser to work, I'm supposed to be doing low energy laser acceleration with the inventor of laser acceleration, Toshiki Tajima, a theorist. The idea is that you would go to a tumor that is one that you could get to surgically. One of the problems in removing tumors is always that you can't really tell if you've got it all, so have to choose to leave some or cut too deep. Either way it's a problem. And so Toshi has started to think, let's

let them leave the last little bit. If we could just get the laser accelerator at the end of a fiber tip, maybe then we could just radiate the last micron and the doctor can leave some, but know that the radiation will then take the rest. If I ever get my laser to work, that's what we're going to work on.

### What advice would you give ICFOnians who are looking to establish a successful career in science?

I am surprised at how many young people ask me how they can you do Nobel Prize winning graduate work. You don't want to even aim for that! If you think physics is fun, then you should do physics, and you should find the part of physics that you find most fun to do so that you actually want to do it every day. And if you want to do it every day, then you will do a really good job because you're enjoying doing it.

I didn't have a career goal. I just wanted to stay in school. I am somebody who got to do something just because I wanted to, not because I felt I had to make a paycheck, and that's something I've always felt lucky for. It's a whole different feeling when you just work for the fun of it.

## Would you like to nominate a woman in science you admire for our Women in Science we Admire campaign?

Christiane Morais Smith, University of Utrecht. She studies fractals, and I heard her give such a fabulous talk! I went up to her afterwards and told her, 'I always say Bill Phillips gives the best talks, but today I think you spoke even better than him!' In her talk she explained fractals and the fact that the dimensionality is a fraction and what that can do to help understand certain areas of science. She had beautiful videos to go along with her beautiful explanations! She is a great communicator and is one of my favorite speakers.



#### ICFO's 2024 in Energy and Environment

Humanity's current dependence on fossil fuels as a primary energy source, either for electricity, heating or transportation, has led to the unequivocal crisis of climate change, along with many other environmental problems associated with the use of natural resources that satisfy multiple human needs. Researchers at ICFO have build upon existing solutions, demonstrating new possibilities for energy consumption and environmental care.

In particular, there is a clear commitment to boost electrochemical devices. Specially within the CO<sub>2</sub> mitigation accelerated by photons and the Organic Nanostructured Photovoltaics group, who have provided several advances in this regard, enhancing fundamental studies, visible light absorption or paving the way for green hydrogen generation.

Another recurrent topic has been solar cells. The Organic Nanostructured Photovoltaics and the Functional Optoelectronic Nanomaterials group have increased the performance levels for four-terminal tandem organic solar cells and eco-friendly nanocrystal solar cells, respectively.

CO<sub>2</sub> mitigation accelerated by photons has started the ICONIC project, aimed at converting seawater pollutants into useful chemicals, while the Organic Nanostructured Photovoltaics has ended the LESGO project, which has advanced hydrogen storage with graphene-based materials.

Finally, the  $\mathrm{CO}_2$  mitigation accelerated by photons and the Thermal Photonics group jointly wrote a special issue in Photonics for Energy, and the Photon Harvesting in Plants in Biomolecules collaborated with artists to create The SOLAR SHARE, an artistic-scientific interdisciplinary initiative.

## A holistic approach to enhance electrochemical interface studies

A new review published in *Nature reviews chemistry* discusses on how the combination of photonic, electronic, chemical, and mechanical probes can help shed light on so far unresolved aspects of electrochemical interfaces (Els), one of the underlying principles of energy conversion and storage.

The electrochemical interface – typically comprising the junction between a polarized surface, a liquid (electrolyte), and dissolved reactants – is at the core of several manufacturing and energy storage technologies. These span from mature, well-established processes, such as the chloralkali electrolysis, to batteries, fuel cells, and water electrolysis for the production of solar fuels.

Els drive the atomic and molecular transformations that determine the performance in these devices. However, its predictive design – needed to enable further performance advances – is challenged by its highly dynamic character, which comes hand-in-hand. Els can drastically change during operation, from intrinsic dynamic changes related to electron and energy transfer, and the supported reactions; to extensive surface reconstruction, including changes in electronic configuration and structure.

Assessing Els at relevant working conditions (typically referred to as in situ and operando, depending on how close the conditions are to actual operation) is thus crucial to understand those principles that govern the reactions occurring at the interface and to enable its informed design.

Traditionally, Els have been studied applying different methods that could probe some specific

aspect (e.g., either structure or composition) with a given resolution, only providing partial, incomplete insights of these interfaces.

In this context, **Dr. Lu Xia** and **ICFO Prof. Dr. F. Pelayo García**, together with former ICFOnian **Dr. Ernest Pastor**, lead a multidisciplinary consortium that reviews the prospects of combining different photonic, electronic, chemical, and mechanical probes, to offer a more complete view of these Els. The review, published in **Nature reviews chemistry**, highlights the opportunities of such combinations to overcome traditional spectroscopic limitations and to bridge the existing gap between theoretical modeling, ideal systems, and working interfaces – ultimately enabling the predictive design of Els and devices with improved performance.

### From individual techniques to a complementary and theoretical approach

The study starts by acknowledging the individual analytical techniques that have been used in the past to probe electrolysis devices. It describes the properties each of them can retrieve, their advantages as well as their drawbacks. As it has been suggested before, there is a common inconvenient to all of them: each approach can only grant access

to a limited set of properties of the EI, providing just a partial picture of the whole mechanism.

In fact, Els are highly heterogeneous, intricated and dynamic, which makes single-method studies insufficient to grasp the El in all its complexity. Within the review, the researchers acknowledge the power of mixing independent approaches to better resolve different properties of the El and to prevent misleading interpretations which may not be detected by a single probe.

"Recognizing the current fragmented research efforts—often isolated within specific methodological approaches— we aimed to bridge these divides by showcasing the power of combining various analytical techniques and theoretical insights. This strategy is aimed at fostering cross-disciplinary collaboration and innovation in the field", explains Lu Xia. According to the author, addressing the complexity of the El in a holistic manner by combining multiple techniques (simultaneously or sequentially) and being theoretically informed is essential for the development of this field.

The review gives a long list of complementary approaches and details for their area of activity. For example, combining Electrochemical Impedance Spectroscopy with Surface Enhanced Raman Spectroscopy (two experimental methodologies usually applied separately) and integrating them with Density Functional Theory simulations (a theoretical description of the EI) can unlock a better understanding of several processes (charge transfer and chemical transformations) taking place at the interface. It can also predict the formation of intermediate species (transient elements that form along an electrochemical reaction), which can point out why certain interactions proceed efficiently or not. With these characteristics being revealed, a deeper knowledge of reaction mechanisms in Els is possible.

In the near future, their work can be used by other scientists to develop, optimize and guide the design of a wide range of electrochemical technologies, including fuel cells, batteries, electrolysers for hydrogen production and  $\mathrm{CO}_2$  electrochemical reduction systems. To do so, new experimental setups based on their complementarity principle need to be standardized. If implemented, this procedure could enable a broader base of researchers to contribute to this field. So far, the team has already provided a reference point that will help them to identify useful, complementary methods, suitable for probing Els in action.

#### Reference:

Pastor, E., Lian, Z., Xia, L. et al. Complementary probes for the electrochemical interface. Nat Rev Chem (2024). DOI: https://doi.org/10.1038/s41570-024-00575-5

### **nature reviews** chemistry

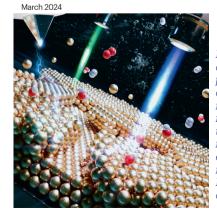


Illustration of complementary photonic, electronic, chemical, and mechanical probes in unraveling the complex mechanisms at electrochemical interfaces (EI). Nature reviews chemistry cover.

# New four-terminal tandem organic solar cell achieves 16,94% power conversion efficiency

Researchers at ICFO have fabricated a new four-terminal organic solar cell with a tandem configuration with a 16.94% power conversion efficiency (PCE). The new device is composed by a highly transparent front cell that incorporates a transparent ultrathin silver (Ag) electrode of only 7nm, which ensures its efficient operation.

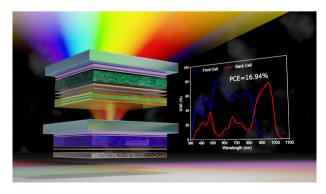
Two-terminal tandem organic solar cells (OSCs) represent one of the most promising approaches to address the transmission and thermalization losses in single-junction solar cells. These organic solar cells consist of front and rear subcells with varying bandgaps, enabling broader absorption and use of the solar spectrum. However, achieving optimal performance in such configurations demands a sufficient current balance between the two subcells. Moreover, fabricating tandem organic solar cells of these types are challenging because they need a robust interconnection layer capable of facilitating efficient charge recombination while maintaining high transparency.

The four-terminal tandem configuration has emerged as a highly efficient alternative strategy in solar cell design. Unlike the two-terminal approach, this configuration features separate electrical connections for the transparent front cell and the opaque back cell. Consequently, the issue of electrical current matching is no longer a limiting factor. This setup enables greater flexibility in selecting the bandgaps of each cell of the tandem, thereby optimizing photon absorption and enhancing the overall efficiency of solar energy production.

Now, in a new study published in the Journal Solar

**RRL**, ICFO researchers and team members of the SOREC2 European project, **Francisco Bernal-Texca**, and **Prof. Jordi Martorell** describe the fabrication of a four-terminal tandem organic solar cell that has achieved a 16.94% power conversion efficiency (PCE). Central to this achievement is the fabrication of an ultrathin transparent silver electrode, a critical component that played a pivotal role in optimizing the performance of the tandem solar cell.

To fabricate the new device, the researchers first explored the organic materials destined for the photoactive layer of both cells. They examined



Artistic illustration of the developed four-tandem organic solar cell. Image credit: ©ICFO/Francisco Bernal-Texca

the effectiveness of three distinct blends for the front cell, which is designed to harvest the high-energy photons. The blend that performed the best, named PM6:L8-BO, was finally chosen. For the back opaque cell, the researchers decided to use the PTB7-Th:O6T-4F blend, with a narrow bandgap, which makes it better suited to absorb the infrared part of the spectrum (low-energy photons).

After choosing the blends, the researchers used a numerical approach to design the four-tandem OSC's final structure. They used the matrix formalism combined with the conventional inverse problem-solving methodology to find the optimal performance and the final configuration of the solar device

The fabrication of an ultra-thin transparent silver electrode with a thickness of only 7nm was the key ingredient in the current research. This element was placed at the back of the front cell, ensuring a good light transmission to power the back cell. Conventional top Ag electrodes utilized for transparent solar cell applications typically range in thickness from 9 to 15 nm.

Its production demanded meticulous control of laboratory conditions to ensure precision and consistency. The electrode was then stacked with three dielectric layers alternating tungsten trioxide (WO<sub>3</sub>) and lithium fluoride (LiF). This photonic multilayer structure has a crucial role, because it is positioned between the two cells to facilitate efficient and uniform light distribution. "This structure exhibits a high transmission in the 750-1000 nm range and a high reflectivity in the 500-700 nm range", researchers wrote.

"The development of a transparent silver intermediate electrode is crucial for the efficient operation of the solar cell. It must present a delicate balance, being transparent enough to allow light to reach the back cell while maintaining high electrical

conductivity to ensure the optimal performance of the front cell", said Francisco Bernal, ICFO researcher and first author of the study. "Being able to fabricate an electrode of only 7nm without observing losses in the front transparent cells is a significant advancement in the field of transparent cells".

The researchers tested the photovoltaic performance of the device under 1 sun of illumination with a solar simulator and measured its quantum efficiency. The device achieved a 16,94% of power conversion efficiency which, to date, would be the highest reached for a four-terminal tandem organic cell. The authors of the study remark that the current official record in efficiency for organic tandem devices is 14,2% and that the last reported PCE for 4-terminal organic tandems is 6,5%.

"Our research holds potential applications in photoelectochemical cells (PEC), addressing crucial electrical requirements such as providing the necessary voltage to surpass established for driving water splitting or CO<sub>2</sub> reduction reactions like in SOREC2 project", explains Prof. Jordi Martorell, researcher at ICFO and SOREC2 project coordinator. "The methodology for the design and implementation of the four-terminal tandem structure could be applied to design news systems where an adequate distribution of light in the elements is crucial for the performance of a certain device".

"The development of a transparent silver intermediate electrode is crucial for the efficient operation of the solar cell" The researchers are currently directing their focus towards refining, tuning and enhancing the methodology and structural design tailored for applications such as solar fuels, where tandem devices hold widespread applicability. By optimizing the methodology and design strategies, researchers aim to unlock the full potential of these devices in harnessing solar energy for diverse and sustainable energy conversion processes, such as CO<sub>2</sub> conversion and valorization.

The SOREC2 project is a EU funded project seeking to develop a new technology to transform directly the sunlight, and CO<sub>2</sub> into added-value chemicals, enabling safe and efficient energy storage. The consortium will develop a new compact tandem

photo electrochemical cell powered by sunlight and a new hybrid catalyst system to enhance the selectivity towards C<sub>2</sub> products.

#### Reference:

Bernal-Texca, F; Martorell, J. (2024) Four-Terminal Tandem Based on a PM6:L8-BO Transparent Solar Cell and a 7nm Ag Layer Intermediate Electrode. Solar RRL. DOI: 10.1002/solr.202300728



A transparent organic solar cell developed by Francisco Bernal from the Organic Nanostructured Photovoltaics research group at ICFO. Image credit: ©ICFO/Francisco Bernal-Texca.

## ACS Photonics special issue on Photonics for Energy

The journal ACS Photonics dedicates its latest special issue to Photonics for Energy, featuring an editorial by ICFO Professors Dr. Georgia Papadakis and Dr. Pelayo García de Arquer, together with Prof. Emiliano Cortés from the Nanoinstitute Munich.

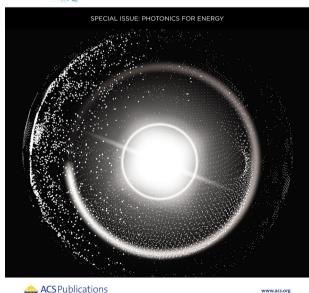
Earth is powered by sunlight, and photonic sciences are crucial in the much-needed energy transition towards finding cleaner and greener alternative energy sources. That is how ICFO professors Dr. Georgia Papadakis and Dr. Pelayo García de Arquer open the editorial of the latest ACS Photonics special issue, dedicated to Photonics for Energy, that delves into how photonics contributes to harvesting solar and thermal energy to facilitates their direct conversion into electricity and chemical fuels.

The editorial reviews advances reported in the articles that constitute the issue, explaining how photonics has enabled outstanding breakthroughs in technologies such as photovoltaics by remarkably improving their efficiency, or have promoted the finding of new ways of concentrating sunlight while reducing the economic costs of solar electricity. It also goes over recent developments in the field of thermophotovoltaic systems, which convert heat into electricity; in recycling waste heat and using smart materials; in the use of plasmonic structures to catalyse chemical reactions to convert sunlight into fuels like hydrogen, or using spectroscopies to understand the functioning of energy devices.

#### Reference:

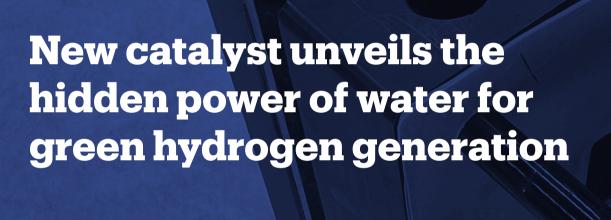
Emiliano Cortes, Georgia T. Papadakis, and F. Pelayo García de Arquer. ACS Photonics 2024 11 (4), 1360-1361 | DOI: 10.1021/acsphotonics.4c00387





Artistic representation of light and energy, with dots are evenly spaced and become smaller as they move away from the center, creating a sense of movement and energy, (C) Tomas

Charles / ICFO. Cover of ACS Photonics.



# New catalyst unveils the hidden power of water for green hydrogen generation

A team of scientists led by ICFO reports in *Science* a new milestone for sustainable green hydrogen production. Their new catalyst design harnesses water to achieve an alternative to critical raw materials for water electrolysis at industrial-relevant conditions.

Hydrogen is a promising chemical and energy vector to decarbonize our society. Unlike conventional fuels, hydrogen utilization as a fuel does not generate carbon dioxide in return. Unfortunately, today, most of the hydrogen that is produced in our society comes from methane, a fossil fuel. It does so in a process (methane reforming) that leads to substantial carbon dioxide emissions. Therefore, the production of green hydrogen requires scalable alternatives to this process.

Water electrolysis offers a path to generate green hydrogen which can be powered by renewables and clean electricity. This process needs cathode and anode catalysts to accelerate the otherwise inefficient reactions of water splitting and recombination into hydrogen and oxygen, respectively. From its early discovery in the late 18th century, the water electrolysis has matured into different technologies. One of the most promising implementations of water electrolysis is the proton-exchange-membrane (PEM), which can produce green hydrogen combining high rates and high energy efficiency.

To date, water electrolysis, and in particular PEM, has required catalysts based on scarce, rare elements, such as platinum and iridium,

among others. Only a few compounds combine the required activity and stability at the harsh chemical environment imposed by this reaction. This is specially challenging in the case of anode catalysts, which have to operate at highly corrosive acidic environments – conditions where only iridium oxides have shown stable operation at the required industrial conditions. But iridium is one of the scarcest elements on earth.

In search for solutions, a team of scientists has recently taken an important step to find alternatives to iridium catalysts. They have managed to develop a novel way to confer activity and stability to an iridium-free catalyst by harnessing so far unexplored properties of water. The new catalyst achieves, for the first time, stability in PEM water electrolysis at industrial conditions without using iridium.

This breakthrough, published in *Science*, has been carried out by ICFO researchers Ranit Ram, Dr. Lu Xia, Dr. Anku Guha, Dr. Viktoria Golovanova, Dr. Marinos Dimitropoulos, Aparna M. Das and Adrián Pinilla-Sánchez, led by Prof. at ICFO Dr. F. Pelayo García de Arquer; and includes important collaborations from ICIQ, ICN2, CNRS, Diamond Light Source and INAM.

#### Dealing with the acidity

Combining activity and stability in highly acidic environment is challenging. Metals from the catalyst tend to dissolve, as most materials are not thermodynamically stable at low pH and applied potential, in a water environment. Iridium oxides combine activity and stability at these harsh conditions, and that is why they are the prevalent choice for anodes in proton-exchange water electrolysis.

The search for alternatives to iridium is not only an important applied challenge, but a fundamental one. Intense research on the look for non-iridium catalysts has led to new insights on the reaction mechanisms and degradation, especially with the use of probes that could study the catalysts during operation combined with computational models. These led to promising results using manganese and cobalt oxide-based materials, and exploiting different structures, composition, and dopants, to modify the physicochemical properties of the catalysts.

While insightful, most of these studies were performed in fundamental not-scalable reactors and operating at softer conditions that are far from the final application, especially in terms of current density. Demonstrating activity and stability with non-iridium catalysts in PEM reactors and at PEM-relevant operating conditions (high current density) had to date remained elusive.

To overcome this, the ICFO, ICIQ, ICN2, CNRS, Diamond Light Source and INAM researchers came up with a new approach in the design of non-iridium catalysts, achieving activity and stability in acid media. Their strategy, based on cobalt (very abundant and cheap), was quite different to the common paths.

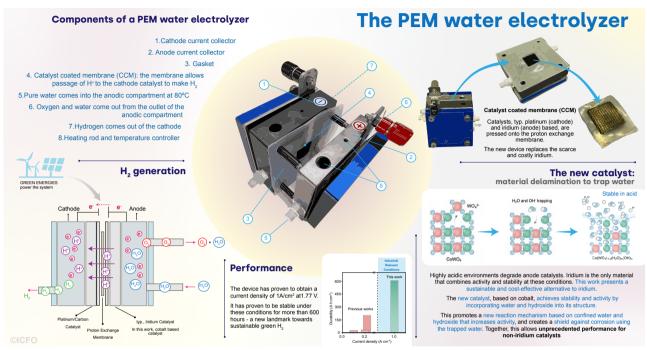
"Conventional catalyst design typically focuses on changing the composition or the structure of the employed materials. Here, we took a different approach. We designed a new material that actively involves the ingredients of the reaction (water and its fragments) in its structure. We found that the incorporation of water and water fragments into the catalyst structure can be tailored to shield the catalyst at these challenging conditions, thus enabling stable operation at the high current densities that are relevant for industrial applications", explains Professor at ICFO, García de Arquer. With their technique, consisting in a delamination process that exchanges part of the material by water, the resulting catalyst present as a viable alternative to iridium-based catalysts.

#### A new approach: the delamination process

To obtain the catalyst, the team looked into a particular cobalt oxide: cobalt-tungsten oxide (CoWO<sub>4</sub>), or in short CWO. On this starting material, they designed a delamination process using basic water solutions whereby tungsten oxides (WO<sub>4</sub><sup>2-</sup>) would be removed from the lattice and exchanged by water (H<sub>2</sub>O) and hydroxyl (OH) groups in a basic environment. This process could be tuned to



From left to right: F. Pelayo García de Arquer, Marinos Dimitropoulos, Lu Xia, Aparna M. Das, Viktoria Holovanova, Anku Guha, and Ranit Ram.



Infographic explaining the PEM water electrolyzer.

incorporate different amount of H2O and OH into the catalyst, which would then be incorporated onto the anode electrodes.

The team combined different photon-based spectroscopies to understand this new class of material during operation. Using infrared Raman and X-rays, among others, they were able to assess the presence of trapped water and hydroxyl groups, and to obtain insights on their role conferring activity and stability for water splitting in acid. "Being able to detect the trapped water was really challenging for us", continues leading co-author Dr. Guha. "Using Raman spectroscopy and other light-based techniques we finally saw that there was water in the sample. But it was not "free" water, it was confined water"; something that had a profound impact on performance.

From these insights, they started working closely with collaborators experts in catalyst modelling.

"The modeling of activated materials is challenging as large structural rearrangments take place. In this case the delamination employed in the activation treatment increases the number of active sites and changes the reaction mechanism rendering the material more active. Understanding these materials requires a detailed mapping between experimental observations and simulations", says Prof. Núria López from ICIQ. Their calculations, led by a leading co-author Dr. Benzidi, were crucial to understand how the delaminated materials, shielded by water, were active and thermodynamically protected against dissolution in highly acidic environments.

But, how is this possible? Basically, the removal of tungsten-oxide leaves a hole behind, exactly where it was previously located. Here is where the "magic" happens: water and hydroxide, which are vastly present in the medium, spontaneously fill the gap. This in turn shields the sample, as it renders

the cobalt dissolution an unfavorable process, effectively holding the catalyst components together.

Then, they assembled the delaminated catalyst into a PEM reactor. The initial performance was truly remarkable, achieving higher activity and stability than any prior art. "We increased five times the current density, arriving to 1 A/cm² – a very challenging landmark in the field. But, the key is, that we also reached more than 600 hours of stability at such high density. "So, we have reached the highest current density and also the highest stability for non-iridium catalysts", shares leading co-author Dr. Xia.

"At the beginning of the project, we were intrigued about the potential role of water itself as the elephant in the room in water electrolysis", explains Ranit Ram, first author of the study and instigator of the initial idea. "No one before had actively tailored water and interfacial water in this way". In the end, it turned out to be a real game changer.

Although the stability time is still far from industrial PEMs, this represents a big step towards making them not dependent on iridium or similar elements. Their work brings new insights for water electrolysis PEM's design, as it highlights the potential to address catalyst engineering from another perspective; by actively exploiting the properties of water.

#### Towards the industrialization

The team has seen such potential in the technique that they have already applied for a patent, with the aim of scaling it up to industry levels of production. Yet, they are aware of the non-triviality of taking this step, as Prof. García de Arquer notices: "Cobalt, being more abundant

### "we have reached the highest current density and also the highest stability for non-iridium catalysts"

than iridium, is still a very troubling material considering from where it is obtained. That is why we are working on alternatives based on manganese, nickel and many other materials. We will go through the whole the periodic table, if necessary. And we are going to explore and try with them this new strategy to design catalysts that we have reported in our study".

Despite the new challenges that will for sure arise, the team is convinced of the potential of this delamination process and they are all determined to pursue this goal. Ram, in particular, shares: "I have actually always wanted to advance renewable energies, because it will help us as a human community to fight against climate change. I believe our studies contributed one small step into the right direction".

#### Reference:

Ranit Ram et al. "Water-hydroxide trapping in cobalt tungstate for proton exchange membrane water electrolysis. Science 384,1373-1380(2024).

DOI:10.1126/science.adk9849



Youtube video







## LESGO advances hydrogen storage with graphene-based materials

After three and a half years, the LESGO team has demonstrated that graphene-based materials, such as graphene oxide, can securely store hydrogen using an energy-efficient loading process based on a flow cell electrolyzer and recover it by thermal, photon-induced and fuel-cell means.

Funded in 2020 under the European Union's Horizon 2020 research and innovation program, the project LESGO – Light to Store Energy in Reduced Graphene Oxide – finished in May. After three and a half years, the team has successfully shown that hydrogen can be securely stored in graphene-based materials, such as graphene oxide, using an energy-efficient process involving an electrolyser.

The overall goals set at the beginning of the project were to achieve an effective mechanism not only binding the hydrogen molecules to the carbon of the graphene oxide, but also achieving the desorption of the hydrogen in an alkaline fuel cell to obtain electricity.

#### **Enhancing hydrogen binding and desorption**

In the first phase, researchers successfully developed a method to enhance hydrogen binding to graphene oxide. The team created a hybrid anode using iron-nickel nanoparticles on reduced graphene oxide and nickel foam. This new anode outperformed traditional, expensive materials, maintaining high efficiency over extended use.

After building a lab-scale flow cell that effectively reduced graphene oxide to its hydrogenated form,

the team assembled the LESGO prototype in June 2023. Equipped with real-time monitoring and solar cells, the prototype allowed the demonstration of the process feasibility and the validation of the system under different irradiation and temperature conditions

In the third phase, they explored how to release hydrogen from the hydrogenated graphene oxide to generate electricity. Both theoretical calculations and experimental measurements using pulsed lasers showed promising results, indicating that the hydrogen absorption/desorption cycle would be energetically favourable. Initial tests in an alkaline fuel cell also showed potential for generating electricity, but further research is needed to optimize this process.

#### Contributing to a greener future

Throughout the project, the team also focused on building an ecosystem around the technology and gaining societal acceptance for potential reduced graphene oxide fuels, gathering direct feedback from participants in focus groups that highlighted the willingness of citizens to switch to better — and greener — alternatives.

Through these comprehensive efforts, LESGO is paving the way for advancements in hydrogen storage, with the potential to revolutionize energy systems and contribute significantly to sustainable energy solutions, especially for the electric vehicles industry, finding that it could enhance the prospects of a mobility based on the fuel cell technology.

Looking ahead, the team plans to continue exploring how to obtain an energy-dense liquid fuel from graphene oxide, and potentially bring the LESGO technology to the market.

More information at https://lesgo-project.eu/

"LESGO is paving the way for advancements in hydrogen storage, with the potential to revolutionize energy systems and contribute significantly to sustainable energy solutions"



The LESGO prototype in June 2023.

## ICFO researchers predict how mid-infrared light propagates in atmosphere

ICFO researchers have developed a numerical method, validated by experimental results, which accurately predicts that the shape of mid-infrared light pulses changes after travelling in the air, especially under high levels of humidity.

How does a light pulse propagate through the atmosphere? Although this question might seem naive, answering it requires accounting for multiple interactions with different atmospheric molecules, variable conditions across space and time, and several atmospheric parameters such as temperature, humidity and pressure. This complex interplay of factors makes it extremely difficult to find a complete solution to the question, something that has not been fully accomplished yet.

However, the scientific community is deeply interested in this problem, as the ability to predict atmospheric light propagation is key to numerous applications. These include remotely sensing atmospheric constituents for climate or weather prediction, monitoring pollutants and other harmful substances, detecting remote light sources like guide stars, and delivering energy on targets.

ICFO researchers, Christian Hensel, Dr. Lenard Vamos, Igor Tyulnev, Dr. Ugaitz Elu, led by ICREA Prof. Jens Biegert, have now made significant progress toward addressing this challenge. Focusing on mid-infrared light, the team developed a model that accurately predicts how the intensity and profile of these pulses change as they travel through the air. Experiments conducted by the researchers strongly corroborated the model's

"the pulse shape broadens during atmospheric propagation, and water vapor is identified as the main contributor"

predictions. Their findings, published in **APL Photonics**, reveal how the pulse shape broadens during atmospheric propagation, with water vapor identified as the main contributor to this effect.

#### Modelling the atmosphere: an intricate challenge

"We measured the initial electric field of an optical pulse at its origin and then applied the model to predict its propagation. We then compared the prediction with another field resolved measurement taken after propagation", says ICREA Prof. Jens Biegert, explaining in simple terms the procedure followed in the study. But the truth is that it was much a more sophisticated process. The modelling, for instance, involved using a high accuracy database of atmospheric constituents at various temperatures and humidity levels.

These constituents absorb and disperse light at thousands of different frequencies, and these frequencies change transiently during the pulse itself. "Understanding which approximations could be made in the model to reduce complexity and increase speed, while still including thousands of absorption lines, was very demanding", admits Prof. Biegert.

Moreover, air is not just oxygen and nitrogen; it contains large amounts of water as well. In particular, researchers had to account for the so-called top-hat water molecule in their simulations. This molecule has a significantly complex absorption spectrum, turning the modelling process into an even more arduous task.

### The pulse spreads out in the presence of water vapor

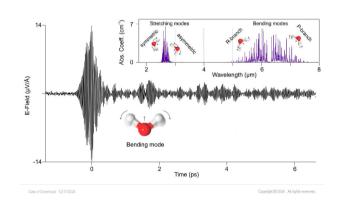
In the end, the team succeeded in incorporating all these parameters into their model. According to it, the process begins with very short and precise light pulses. As the pulses travel, they interact with atmospheric molecules, which absorb and re-emit light in random directions in a much longer decay time compared to the laser pulse. Consequently, the pulse duration increases and a long complex tail from the interference among the re-emitted light appears, degrading the initial well-defined shape. The model also showed that as humidity increases, reshaping becomes even more pronounced due to additional absorption and dispersion effects caused by excess water vapor.

Then the researchers conducted sensitive experiments in the time-domain, reproducing the predicted effects which excellent agreement, thus validating the model. "Our method is general and easy to apply for any gas compositions and pulse shapes", shares Dr. Lenard Vamos. And he adds: "This ability to predict atmospheric

propagation could enhance many technologies, where estimating pulse's features is essential for efficient designs. It could also be critical for many spectroscopic techniques, where pulse reshaping reduces temporal resolution and provides insight into the interaction process itself."

#### Reference:

Christian Hensel, Lenard Vamos, Igor Tyulnev, Ugaitz Elu, Jens Biegert; Propagation of broadband mid-infrared optical pulses in atmosphere. APL Photonics 1 August 2024; 9 (8): 080801. DOI: https://doi.org/10.1063/5.0218225



Measured mid-infrared electric field after 2.5 m of propagation in the atmosphere. The water vibrational mode is illustrated close to the induced echo. Inset: Water vibrational mode induced absorption spectrum. Source: APL Photonics, modified.

## New performance record for eco-friendly nanocrystal solar cells

ICFO researchers have developed a numerical method, validated by experimental results, which accurately predicts that the shape of mid-infrared light pulses changes after travelling in the air, especially under high levels of humidity.

In the era of climate change, renewable energies have quickly gained popularity, with solar cells being a prominent example of this shift. For instance, in 2023, installed solar photovoltaic power increased by 28% in Spain compared to the previous year, accounting for 20.3% of Spain's total energy generation pool, a trend that is similarly mirrored in most Western countries. Despite their commercialization and their unquestionable environmental benefits, solar cells still have room for improvement, as they are usually based on materials that are not fully sustainable. Ubiquitous solar harvesting - beyond solar farms - is considered the way to go to power buildings, infrastructures, IoT systems or even vehicles. That would require lightweight, low cost, flexible and eco-friendly based solar cell technology. The scientific community is thus directing its efforts toward finding sustainable alternatives that preserve (or even boost) the electricity generation efficiency, reduce costs and simplify the manufacturing efforts of current solar cells

One promising material that has emerged as an environmentally-friendly alternative is colloidal silver bismuth sulfide (AgBiS<sub>2</sub>) nanocrystal, a material that is characterized by an extremely high absorption coefficient and thus leads to ultra-thin-film absorbers for solar cells. Through a

layer-by-layer manufacturing process, solar cells with compelling performance have already been reported. But to minimize material loss, reduce costs and improve manufacturing scalability, the multi-step deposition method must be replaced by a single-step approach.

This can be realized by developing AgBiS<sub>2</sub> nanocrystal inks. Since 2020, several researches in this regard have been reported. However, the resulting AgBiS<sub>2</sub> nanocrystals have still exhibited significant surface defects accompanied by low power conversion efficiency in a solar cell, meaning that the techniques aimed at eliminating them —called surface passivation— were not sufficiently effective. The remaining surface defects trapped the electrical charge carriers generated by sunlight and triggered their recombination, reducing the device efficiency to lower levels than those achieved with a layer-by-layer manufacturing procedure.

Therefore, a simpler yet more effective passivation methodology for AgBiS<sub>2</sub> nanocrystal ink is needed to bring the efficiency of eco-friendly solar cells closer to competitive levels. Recently, ICFO researchers, Dr. Jae Taek Oh, Dr. Yongjie Wang, Dr. Carmelita Rodà, Dr. Debranjan Mandal, Dr. Gaurav Kumar, Dr. Guy Luke Whitworth, led by ICREA Prof. Gerasimos Konstantatos, have taken a significant step forward

in this direction. In an *Energy & Environmental Science* article, they have reported on a post-deposition in situ passivation (P-DIP) strategy that improves surface passivation, yielding nanocrystal ink films with enhanced optoelectronic properties. The resulting ultrathin solar cells showed higher power conversion efficiency than their multi-step deposition counterparts, setting a new performance record for eco-friendly nanocrystal solar cells.

## Post-deposition in situ passivation for improved surface passivation

ICFO researchers managed to effectively passivate surface defects present in their nanocrystal ink film. "Imagine a bumpy road that slows down cars. Surface passivation is like repaving the road, making it smoother so cars can move without getting stuck. In our case, the removal of surface defects is very important to facilitate the transportation of charge carriers created from light absorption in nanocrystal films", explains Dr. Jae Taek Oh, first author of the article. "With our P-DIP method, charge carries could move without 'bumping into so many obstacles' within the AgBiS<sub>2</sub> nanocrystals thin film", he adds.

The mitigation of defects by a proper passivation strategy translated into higher film quality and, thus, higher performance solar cells. Their efficiency of around 10% exceeded that of previous solar cells based on AgBiS<sub>2</sub> nanocrystals, involving both single-step and layer-by-layer deposition methods.

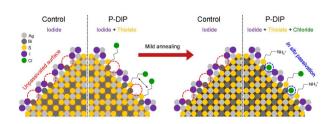
To obtain these outstanding results, the team synthesized the AgBiS<sub>2</sub> nanocrystal ink by introducing a multifunctional molecular agent containing chlorine. Its molecular structure helped stabilize the nanocrystals and disperse them evenly within the solution, two crucial factors to ensure smooth coatings. After depositing the film, they carried out additional passivation on the surfaces

### "With our P-DIP method, charge carriers could move without 'bumping into so many obstacles' "

of AgBiS<sub>2</sub> nanocrystals. This particular in situ passivation strategy extended the carrier lifetime and balanced carrier transport in the film, which are also critical aspects to enhance the efficiency of solar cells. The combination of these effects was the perfect recipe to achieve the unprecedented performance for sustainable solar cells that ICFO researchers have demonstrated in this study.

#### Reference:

J. T. Oh, Y. Wang, C. Rodà, D. Mandal, G. Kumar, G. L. Whitworth, G. Konstantatos. Energy Environ. Sci. (2024). DOI: https://doi.org/10.1039/D4EE03266G



Schematic of the post-deposition in situ passivation strategy on the AgBiS<sub>2</sub> nanocrystal. Source: EES.

## THE SOLAR SHARE: An Edible Solar Currency

The Photon Harvesting in Plants and Biomolecules group collaborates with artists through the EU's S+T+ARTS in the City Artists in residency initiative.

ICFO's Photon Harvesting in Plants and Biomolecules (PHPB) group led by **Prof. Nicoletta Liguori** is part of the Clean Planet program at ICFO, exploiting the underlying physics of light interactions with matter to develop and implement renewable, clean energy technologies that can contribute to the mitigation of climate change.

There are many pieces of this puzzle and the PHPB group utilizes experimental and computational tools to explore the regulatory mechanisms governing sunlight harvesting in photosynthetic organisms. They aim to deepen the fundamental understanding of natural photosynthesis in order to potentially uncover strategies to optimize the utilization of solar energy in photosynthetic organisms. In what they see as an urgent priority for the environment, the group is working to engineer photosynthesis for a more sustainable future, a challenge that led them to participate in the EU's



Solar currencies at Ars Electronica Festival 2024 © Disnovation.org



Eating the sun © Disnovation.org

S+T+ARTS in the CITY initiative which brings artists into research centers through a residency program with the goal of enhancing art-driven innovation. The residencies take place over 9 months, allowing time for the artists, the host institutes and local experts groups, in this case HacTe) the Barcelona Hub for Art, Science and Technology), to converge and connect, followed by reflection and the development of the artwork.

## THE CHALLENGE: Understanding and Engineering Photosynthesis for a More Sustainable Future

How does photosynthesis function at the molecular scale, and can we improve it? Unveiling the processes governing light-harvesting regulation in plants and how could we possibly improve it, could advance sustainable agriculture. The PHPB group invited artists to support the scientific challenge of making plants even stronger allies in the fight against climate change.

Artists from DISNOVATION.ORG took up the challenge, creating "THE SOLAR SHARE: An Edible Solar Currency". This project challenges prevailing economic models with insights from sunlight-harvesting organisms, crucial to the metabolism of life on Earth. Staged as a one-square-meter microalgae bioreactor, the artwork foregrounds human energy dependence on photosynthesis and proposes harvested edible microalgae as a radical economic unit: The Solar Share. This unit

is the biomass produced on one square meter of the Earth's surface that day. This edible algae unit is a photosynthetic proof of work that can be consumed, exchanged, or stored as a currency. The Solar Share is an invitation to experience firsthand a transformative economic model that reintegrates human metabolism and energy needs with the actual new energy entering the Earth system as photosynthesis. The Solar Share provocatively recenters Earth's metabolism in economics, redefining sustainability within planetary limits.

"We were motivated to launch this challenge through S+T+ARTS to inspire conversations between researchers and society, in particular with artist that could help us find ways to not only explain to large audiences the importance of fundamental science, but also to put into much larger context the type of research that we are performing in our group. It has been an amazing experience," reflects Prof. Liguori.

The first showcasing of this artwork was at the ARS Electronica Festival in Linz (Sept 4-8, 2024).



ARS Elctronica Festival in Linz (Sept 4-8, 2024) | ©HacTe.

## Pep Canadell

CSIRO Science Centre, Australia. Global Carbon Project. Executive Director Global Carbon Project and CSIRO Research Scientist.

April 2023, ICFO

## Where was the seed planted for your passion for the environment and climate change?

Since very early in my childhood I had an interest on the environment, running from school to home to make it on time for a wildlife documentary series I didn't want to miss. My interest was narrowed down when I started a bachelor's in biology at the Universitat Autònoma de Barcelona, where I quickly become interested on fire ecology in the Mediterranean and around the world, including California and Australia, where perhaps not coincidentally, are the places I have spent my last 33 years of professional life. I wanted to work on a piece of science that could help addressing an environmental issue of our times, and a great mentor suggested a few from which I picked fire. Little I knew at that time that I was going to end up working on the biggest of all environmental problems humanity faces this century: climate change.

## How did you come to lead the Global Carbon Project?

Halfway through my PhD thesis work in 1991 I left for California. I knew there was a bigger scientific world out there I had to explore. I spent a few years at San Diego State University because my research on fire, where I quickly learned about a new emerging science of climate change. There was a sense that something big was brewing and that needed attention. At this time, the Intergovernmental



"there is also the need for scientists to continue to explore where policy makers have not asked questions about"

Panel on Climate Change (IPCC), the global lead body to assess the state of the climate system and the human influence, had just been established. In addition, the UN Framework Convention on Climate Change was about to be established with 196 countries agreeing that something had to be done about the emerging issue of human-induced climate change.

The entire global scientific community had to be organized to develop a coordinated research agenda to support the many IPCC assessment cycles to come and provide the answers that the UN convention needed to pursue countries into climate action. After a few years at the University of California in Berkeley doing research on the impacts of high atmospheric CO<sub>2</sub> on terrestrial ecosystems, I took a job at Stanford University to lead a component of the Global Change and Terrestrial Ecosystems project, an international research program which later on became a predecessor of the Global Carbon Project for which I have been the

director since.

I saw an opportunity with this new type of job to bring together the power of large teams of scientists working in different countries and often in different parts of the same problem through different and independently working scientific disciplines. I saw a very individualistic science around the world which was unfit to solve the big global environmental problems we were trying to address. It seems there was more competition and ego building among scientists and countries, than collaboration: not to mention that we still had to send faxes to communicate with certain institutions and countries, not a particularly efficient way to establish and coordinate global research agendas. I clearly saw an opportunity to work towards shared and coordinated scientific goals that could make the outcomes of the effort bigger than the contributing parts and individuals.

## What transversal skills you have developed as a scientist in academia have been most useful to engage with global policy makers?

Two skills have been very important for my job. First, communication skills to be able to translate complex science into a language that can engage policy makers into a conversation. Although it is an obvious one, scientists often insist to come across as scientists, a somehow old fashion (and comfortable for scientists) view of a scientist, who needs to speak with a technical vocabulary which both prevents real communication and sometimes could even hide the lack of relevance or alignment between science and policy needs.

Second, willingness to listen from policy makers what they need and how policy making works and is developed. I found around the world that developing policy relevant science often means seating in one's office, and thinking about what science I can produce that it will be useful to policy

makers, followed by doing the science, publishing it and making sure policy makers have noticed the publication. Nothing further from the reality and how one goes about establishing the trust and developing an agreed process by which co-design and co-production guides the science and the uptake of that science all along. Scientists might often ask the wrong questions that they think are policy relevant, and even if sometimes we might get the questions right, it is not a process that will ensure uptake and impact of that science into the policy world, as it is done with a unidirectional process from scientist to policy maker.

Having said all the above, there is, of course, also the need for scientists to continue to explore where nobody has been there yet, that policy makers have not asked questions about yet, and to surface the next issue around the corner we haven't yet thought about.

## Where do you think that ICFOnians who want to contribute to the mitigation to the climate crisis can have the greatest impact?

I see the role of the upcoming generations and ICFOnians as working to resolve how we will move from a fossil fuel based economy towards one of clean and renewable energies, including how we can best harvest the power of the sun and wind. how information science and robotics will support a more efficient and less wasteful society, how we can make our food system cleaner and have a lesser impact on the environment and climate. how we will need to adapt to the changes that are unavoidable of climate change including a more aggressive climate of heatwaves, drought and floods. Interestingly, the new society and economy we need to create is one that we want with and without climate change because it is a cleaner one, more efficient, more independent energetically, more just, and smarter in the way we use energy and resources.



### ICFO's 2024 in Biophysics and Health

Fundamental and applied research in biology and medicine truly serve as the cornerstones in the ongoing quest to enhance health and well-being across society. Drawing upon the collective expertise of diverse scientific disciplines, this 2024 ICFO has continued to develop cutting-edge optical microscopy and superresolution technologies and has employed them to study biological processes.

It has been a particularly fructiferous year for bionanophotonics. The Single Molecule Biophotonics group has led diverse studies about single molecule detection, shedding light into protein sorting, developing novel nanoantennas for multicolor detection, manipulating cell membrane properties and mapping multimolecular interactions. The Atomic Quantum Optics group has followed a different approach, developing atomic sensors for monitoring molecular polarization.

On the other hand, with the aim of addressing pressing healthcare challenges, the SLN team has developed a new strategy to tackle fibrosis and scarring, the CO<sub>2</sub> mitigation accelerated by photons demonstrated a new gel to break down alcohol in the body, the Neurophotonics and Mechanical Systems Biology group has expanded the knowledge on neural circuits, and the Medical Optics group has contributed to improve renal cancer prediction, brain analysis with diffuse optics and human tyroid characterization.

Plants and photosynthetic systems have also been under the spotlight. The Molecular Nanophotonics group has presented a spectroscopic technique to probe charge separation in these systems, and the Single Molecule Biophotonics group has explained how do plant cells stay connected while dividing.

## Shedding light into protein sorting in cells

In a new study published in *eLife*, researchers provide a first experimental demonstration of the role of the protein TGN46 in the sorting process of secretory proteins, identifying the region that encodes for this function using quantitative fluorescence microscopy and mutagenesis.

Secretory proteins control various essential processes such as immunity, metabolism and cellular communication, playing a key role in many diseases such as cancer or neurological disorders. They are synthesized in the endoplasmic reticulum organelle and travel to the trans-Golgi network (TGN). This cellular compartment works like a sorting station that regulates the flow within the cell, organizing newly synthesized proteins and other molecules in different transport vehicles and directing them to their final destinations. As in a factory assembly line, each cargo molecule is processed and packaged into vesicles, that are timely and orderly guided to the correct cellular compartment or exported out of the cell, preventing congestion and ensuring proper cellular function.

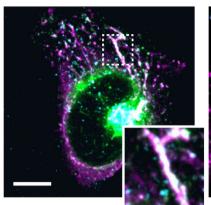
The targeting signals and molecules that participate in this sorting process, driving each protein to the correct destinations are still unclear and a subject of discussion. Previous studies have pointed out that one of the key players might be a transmembrane protein, known as the protein TGN46, that cycles quickly between the trans-Golgi network and the plasma membrane, transported to the cell surface by vesicles that also typically carry secretory proteins. However, its specific role in this sorting process had not been shown yet.

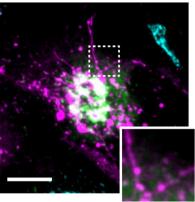
### Investigating the TGN46 role experimentally

Now, ICFO researchers Pablo Luján, Fèlix Campelo, Javier Vera and Prof. María García-Parajo, together with researchers from the Institute for Research in Biomedicine and the Center for Genomic Regulation in Barcelona, the Tokyo University of Pharmacy and Life Sciences and the Pompeu Fabra University, published a study in *eLife* showing that the protein TGN46 plays a key role in sorting the cargo proteins into their transport carriers at the TGN and that this role is described by the part of the molecule located inside the trans-Golgi network.

To investigate the function of the TGN46 protein, the team studied two types of cells, with and without the protein, and measured the amount of secretion of a specific secretory protein – named PAUF. Using immunofluorescence microscopy, they saw that the mutant cells without TGN46 secreted 75% less protein. Moreover, they used confocal fluorescence microscopy to assess how many containing vesicles were in each type of cell, seeing that the mutants had much fewer vesicles, and measured the export rate of the secretory protein with a microscopy technique named FLIP, the acronym for fluorescence loss in photobleaching microscopy.

They also observed that this secretory PAUF protein was present in the membrane tubules of the normal cells, but not in the mutant ones. All of these findings indicated that the cells without TGN46





Confocal fluorescence microscopy images of HeLa cells with and without the TGN46 protein.

"we want to understand the mechanism by which TGN46 sorts and loads these proteins into the transport carriers, because [... that] may play a role in its function"

couldn't complete the sorting and loading of the secretory proteins into their transport vesicles.

Researchers also intended to find out which parts of the TGN46 receptor were in charge of the sorting and packaging functions and found that only the luminal domain, that is the part of the receptor facing the inside of the Golgi, was necessary to complete the process.

### **Exploring the sorting mechanism further**

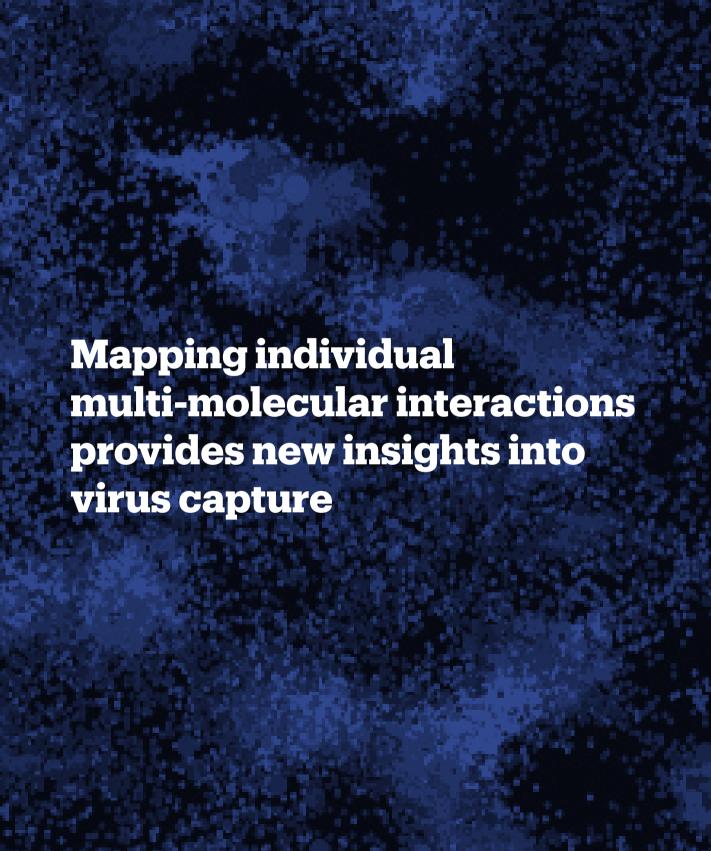
The article provides the first experimental confirmation that the protein TGN46 works as a cargo receptor, sorting secretory proteins in the trans-Golgi network, which are then packaged into

carrying vesicles, transported to the surface or secreted outside the cell.

Researchers suggest that future efforts could be placed into investigating which other secretory proteins are handled by TGN46. "The next steps we want to pursue are, first, to find the list of proteins that are secreted following this route, which could, in the long term, open new therapeutic options for diseases related to abnormalities in their secretion", points out Fèlix Campelo, ICFO researcher and one of the authors of the study. "Second, from a more biophysical perspective, we want to understand the mechanism by which TGN46 sorts and loads these proteins into the transport carriers, because preliminary evidence suggests that the ability of TGN46 to form biomolecular condensates may play a role in its function."

#### Reference:

Pablo Lujan, Carla Garcia-Cabau, et. al. (2023). Sorting of secretory proteins at the trans-Golgi network by human TGN46, eLife 12:RP91708 | DOI: https://doi.org/10.7554/eLife.91708.2



## Mapping individual multimolecular interactions provides new insights into virus capture

Researchers have provided a new and powerful single molecule methodology capable of simultaneously monitoring different molecules in living cells, a major technological breakthrough in the single molecule field.

The technique successfully uncovered individual interactions between three proteins and two different viruses, HIV-1 and SARS-CoV-2, which resulted crucial to increase their capture. These results suggest there exists a common physical mechanism that enhances viral capture, the first crucial step that ultimately leads to infection.

When a virus infects us, dendritic cells detect and capture it. They then present the virus to other immune system cells, who activate the proper immune response to, hopefully, halt the infection. However, some viruses, like HIV, have learned to take advantage from this situation, and use dendritic cells as "Trojan horses" to spread deeper into the body. Once inside, HIV inhibits the ability of dendritic cells to mature and alert the immune system. This weakens the immune response and can eventually lead to AIDS.

Understanding the early molecular events leading to viral capture and cell entry is critical for designing effective vaccines. To elucidate how a receptor in the cell membrane binds and captures a virus, information at the single molecular level is essential. However, molecules rarely act isolated; their function depends on interactions with other molecules. One can think of them as a society, where individual behavior strongly depends on the interactions with others. "You behave differently when interacting with your parents, siblings, or boss. And most of the

time, we need to interact with others to perform a better job, or simply because we cannot do it alone", explains ICREA Professor at ICFO, María García Parajo. "Exactly the same happens in a cell: interactions between individual molecules lie at the core of their function and can significantly enhance their work."

Therefore, a tool capable of tracking interactions between multiple molecules in real-time, at the single molecule level and in living cells has long been a priority in biophysics. ICFO researchers Dr. Nicolás Mateos, Dr. Enric Gutiérrez-Martínez, Dra. Jessica Angulo-Capel, Dr. Juan A. Torreno-Pina, led by ICREA Prof. María F. García-Parajo, and in collaboration with the King's College London, have recently presented in ACS Nano a technique that fulfills these conditions. The team has come up with a new and powerful single molecule methodology, which can monitor different labeled molecules simultaneously in living cells, and have used this information to construct spatiotemporal maps. These maps track the position and the interactions of several

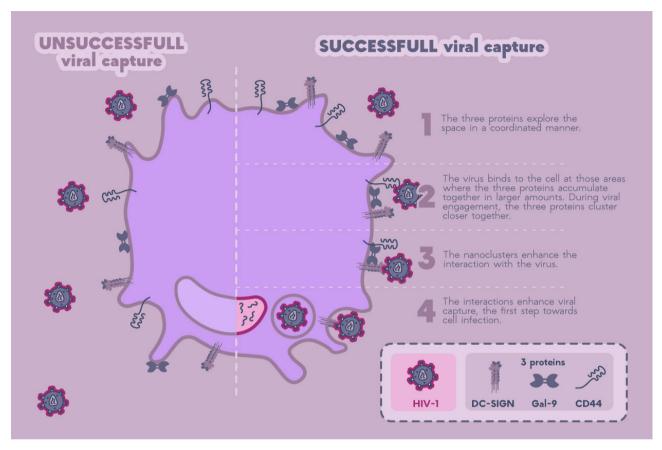


Illustration the HIV capture procedure. Credit: Isabel Santa-María.

bioparticles individually over time, something that former approaches were not able to resolve.

Using this technique, researchers captured realtime interactions between individual virus-like particles and three different proteins on the membrane of living immature dendritic cells. This mapping revealed a coordinated action of the three proteins that was crucial to capture two different viruses: HIV-1 and SARS-CoV-2.

### Multicolor HiDenMaps for visualizing molecular interactions

To study individual virus-receptor interactions and the role of other individual molecules in real-time, the team developed a multimolecular mapping technique called Multicolor High-Density Maps (HiDenMaps). To showcase it, they studied the HIV-1 virus and its interactions with three proteins (DC-SIGN, CD44 and galectin-9).

HiDenMaps were created by labelling each protein and the virus with fluorescent markers. When

"The final maps have four colors, one for each molecule. This makes it easier to 'see' where and when different molecules coincide and helps us to visualize interactions"

illuminated, each marker emitted light of a different color, enabling researchers to track their positions with nanometer precision. Data from each marker was combined into a single image, the HiDenMap. Then, the four HiDenMaps collapsed to a single multicolor map encapsulating the spatial and temporal distribution of all molecules. "The final maps have four colors, one for each molecule. This makes it easier to "see" where and when different molecules coincide and, thus, helps us to visualize interactions between them", assures Dr. Nicolás Mateos, first author of the article and main developer of the technique.

### Revealing how dendritic cells efficiently capture HIV

HiDenMaps, combined with quantitative tools, allowed researchers to follow the three proteins and the virus in real time, showing how their interactions influence viral binding and capture. For HIV-1, researchers identified four main steps. First, the three proteins explore the environment in a coordinated manner, inspecting the same or adjacent regions, like a cell patrol waiting for enemies. When the virus arrives, it is more likely to bind in areas where the three proteins accumulate in larger amounts and, during viral engagement, the three proteins cluster closer together, strengthening even more

the binding. Then, these nanoclusters enhance the interaction between the viral receptor (DC-SIGN, one of the proteins being tracked) and the virus. And, finally, the enhanced interaction increases the probability of capturing the virus —the initial step towards dendritic cell infection.

The whole process had never been observed at the single molecular level before. "We found that, while DC-SIGN can capture the virus, it needs two partners —CD44 and galectin-9— to do so efficiently", explains Dr. Mateos. "Interestingly, only when DC-SIGN interacted simultaneously with both CD44 and galectin-9, the binding and capture of the viruses were stronger, more stable and more likely to lead to infection", he adds.

### HiDenMaps: a general tool for tracking multimolecular interactions

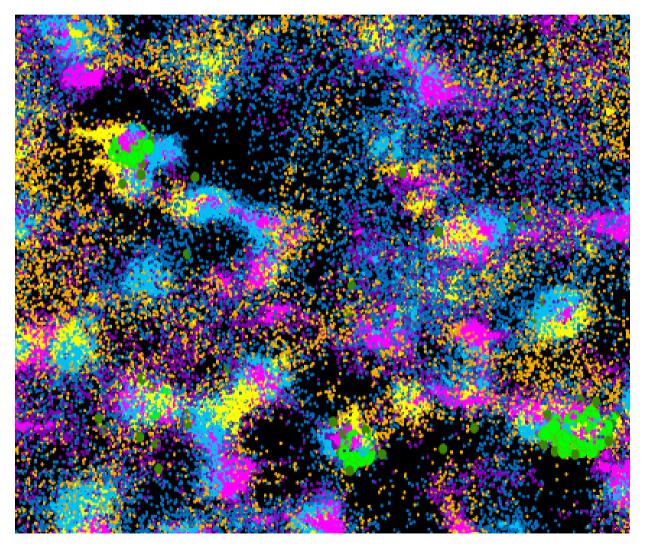
The same process was observed for SARS-CoV-2, the famous responsible for COVID-19. This suggests a potential generalized mechanism for virus capture in immature dendritic cells, where the three proteins play a central role. According to Prof. García Parajo: "This has enormous consequences for vaccine development, since preventing the early stages of viral capture by disrupting interactions between DC-SIGN and its partners could be a more effective strategy than blocking the viral receptor alone."

Even more generally, multicolor HiDenMaps could be applied to study any multimolecular interactions in living cells. Moreover, combining HiDenMaps with another existing technique called frequency multiplexing could increase the number of tracked particles. "Ideally, such a combination would result in a full rainbow-colored HiDenMap! The challenge is that, at the moment, frequency multiplexing has only been applied to fixed cells. Going to living cells is far from trivial, but certainly not impossible", shares Prof. García Parajo. This great versatility

makes HiDenMaps a major technological breakthrough for the single molecule field.

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Nicol'as Mateos, Enric Gutiárrez-Martínez, Jessica Angulo-Capel, Irene Carlon-Andres, Sergi Padilla-Parra, María F. García-Parajo, and Juan A. Torreno-Pina. ACS Nano 2024 18 (42), 28881-28893 DOI: 10.1021/acsnano.4c09085



HiDenMap of three different proteins (colored in yellow, cyan and magenta) and HIV particles (green) showing spatiotemporal coordination and virus capture. Each dot corresponds to a single molecule localization event. Source: ACS Nano.



# Novel nanoantennas enable sensitive multicolor single-molecule detection with unprecedented throughput

ICFO researchers have developed a nanoantenna platform capable of enhancing fluorescence emission across the entire visible spectrum, enabling multicolor single-molecule detection at micromolar concentrations. The proposed method can also address more than a thousand nanoantennas in parallel, speeding up data acquisition times.

Unraveling the intricacies of biological processes at the single-molecule level is crucial for capturing the heterogeneity of biological systems and expanding our knowledge of their biochemical dynamics. The complexity inherent in the biological environment, though, demands very sensitive biosensing techniques, which commonly capture the fluorescence light emitted by the desired biomolecules or their fluorescent labels. Maximizing their fluorescence brightness is essential to ensure their highly sensitive detection. To date, the investigation of the interactions between different biomolecules with single-molecule sensitivity at typical concentrations found within living organisms is a major challenge that conventional methods face.

So-called plasmonic nanoantennas can provide single-molecule sensitivity under these conditions as they can significantly increase the brightness of a nearby fluorescent molecule. However, detecting single molecules with such nanoantennas under biologically relevant conditions comes with two major challenges.

On the one hand, the detection of different molecular species that emit fluorescence light at different colors (wavelenghts), requires strong fluorescence enhancement across various spectral regions. This kind of studies, known as multicolor experiments, require nanoantennas with a spectrally wide resonance, which typically results in weak amplification of the fluorescence emission and consequently hampers the detection sensitivity.

On the other hand, biosensing applications often require single-molecule sensitivity at micromolar concentrations, the concentration level at which many biological molecules, interactions, and reactions occur. Unfortunately, at such high concentrations, the single-molecule response is obscured by the strong background signal generated by the large number of surrounding molecules.

Taking both problem areas into account, the goal becomes clear: to develop a nanoantenna design that simultaneously enhances the target molecules' fluorescence and reduces the background noise across the entire visible spectrum.

"the number of analytes to be detected could be increased by three-orders of magnitude"

Now, ICFO researchers Ediz Kaan Herkert, Lukas Lau, Roger Pons Lanau, led by ICREA Prof. María F. García-Parajo have developed a nanoantenna platform that successfully tackles these issues. It enhances fluorescence across the entire visible spectrum and at the same time reduces background fluorescence, enabling multicolor single-molecule detection at micromolar concentration. Importantly, it additionally shows a 1000-fold increase in the number of antennas that can be addressed in parallel, which facilitates a rapid screening of samples, leading in turn to high throughput (that is, the amount of information that can be processed in a given temporal window). The results have been published in ACS Applied Materials & Interfaces.

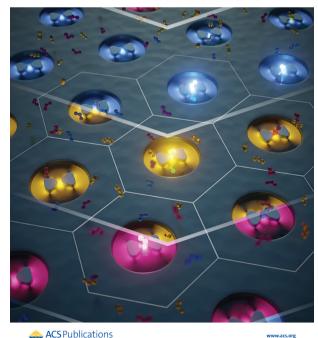
## New nanoantenna platform: High-density Hexagonal Closed-Packed Antenna-in-Box

Antenna-in-box (AiB) platforms, consisting of a nanoantenna within a nanoaperture, have been successfully applied to highly relevant biosensing tasks due to their combination of strong fluorescence background reduction and fluorescence emission enhancement.

Despite their potential for biosensing applications that has been refined throughout the years, two major challenges remain: traditional AiBs are unsuitable for multicolor experiments and their throughput is slowed down by their sequential point-by-point readout (that is, only one antenna-in-box can be measured at a time).

The design developed at ICFO overcomes these challenges by introducing high-density hexagonal closed-packed AiBs (HCP-AiBs) made of aluminum. The researchers' approach involved placing as many AiBs as close to each other as possible. In contrast to the commonly chosen square-like arrangement, a hexagonal close-packing allowed them to maximize the number of AiBs within a given space.

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Artistic illustration of aluminum hexagonal close-packed Antenna-in-Box arrays enabling sequential multicolor singlemolecule detection at micromolar analyte concentrations. Cover or ACS Applied Materials & Interfaces. "Our HCP-AiBs could be used in multicolor biosensing applications to study interactions between different proteins on the cell membrane or to monitor biomolecular binding kinetics, both with enhanced single-molecule detection sensitivity"

The high packing density significantly increased the number of AiBs that could be detected simultaneously. In the end, the team managed to address over 1000 AiBs in parallel, consequently speeding up the data acquisition times. "For biosensing applications, this means that the number of analytes to be detected could be increased by three-orders of magnitude, which is a unique accomplishment in the field", shares ICREA Prof. María F. García-Parajo.

Moreover, choosing aluminum over gold (the material traditionally employed for nanoantennas) was pivotal in achieving broadband resonances covering the entire visible range. The team then designed a custom microscope with three excitation channels, each of them successfully capturing the fluorescence emission of a different molecular species.

## Multicolor fluorescence enhancement and parallelization of the readout method unlocked

The accomplishment of multicolor fluorescence enhancement and parallelization of the readout method are unique milestones that were very hard to experimentally demonstrate in the past, but the ICFO team has now succeeded in unlocking them efficiently. "That is why I consider our results a major step forward towards true real-world applications of nanoantennas in the field of biosensing", shares Ediz Herkert, first author of the article.

But the work is not finished yet, as there is always room for improvement. "The next steps in the field should focus on developing a more time- and cost-efficient cleanroom process for producing this type of hexagonal antenna arrays, and demonstrating that the multicolor single-molecule sensitivity of HCP-AiBs can be achieved in biologically relevant conditions, including living cells", explains Herkert.

ICREA Prof. María García-Parajo sees great potential in their discovery as well: "Our HCP-AiBs could be used in multicolor biosensing applications to study interactions between different proteins on the cell membrane or to monitor biomolecular binding kinetics, both with enhanced single-molecule detection sensitivity."

#### Reference:

Ediz Kaan Herkert, Lukas Lau, Roger Pons Lanau, and Maria F. Garcia-Parajo. ACS Applied Materials & Interfaces 2024 16 (31), 41271-41280

DOI: 10.1021/acsami.4c04744

## Unlocking the ability to manipulate the properties of membranes by means of light

ICFO researchers demonstrate a new ability of the fluorescence probe Flipper to alter lipid composition, order and tension of cell membranes, unlocking the possibility to tune the biological function of membrane proteins by means of light.

In recent years, many researchers have gradually become aware of the importance of the mechanical tension of cell membranes in regulating how proteins work. Initially, however, a technique that could locally measure the tension of the membrane was missing. Scientists had no means of discovering the mechanism underlying this phenomenon and, thus, researchers from all over the globe were eager for a solution to break through the barriers in the study of membrane protein function.

Then, in 2018, researchers from Switzerland synthesized a powerful fluorescent probe called Flipper, designed to sense and report on membrane tension. It seemed to be everything the scientific community had been looking for, so everyone rushed to use it. But the initial euphoria did not last for long. Shortly after Flipper's introduction, various research groups noticed some negative effects: after applying Flipper for some minutes, cells started to die, bringing experiments to an abrupt end. It turned out that the probe was toxic to the cells.

Now, ICFO researchers **Dr. Joaquim Torra** and **Dr. Félix Campelo**, led by **ICREA Prof. María F. García-Parajo**, have turned this apparent weakness into a strength. The team has demonstrated a new ability of Flipper (previously used exclusively to

measure the tension of membranes) to alter lipid composition, order and tension of the membrane. The team further shows that, by using blue light, one can guide proteins to specific regions of the membrane. At the same time, they elucidated the mechanisms by which Flipper induces all these changes. The reported discovery has recently been published in the *Journal of the American Chemical Society*.

These findings are major results in the field because the composition and arrangement of lipids in cell membranes dramatically influence the function of proteins that are embedded on specific regions of those membranes. Thus, by using light to manipulate the properties of membranes, the team has opened the door to the possibility of tuning the biological function of membrane proteins in the near future, a long-standing goal for many researchers in the world.

### Predicting Flipper's new ability

The ICFO team was one of those groups that noticed the negative effects of Flipper in terms of toxicity while studying cell

membrane tension. This effect particularly attracted the attention of Dr. Joaquim Torra, first author of the article, when he observed it during previous experiments. But, instead of trying to get rid of it, he embraced the hurdle.

His chemical background enabled him to hypothesize that the phototoxicity of Flipper arose from the formation of reactive oxygen species, which are very toxic to cells. He then came up with an idea that would change the course of his following research projects: these species reacted in a very specific way, modifying the surrounding unsaturated lipids in a process called hydroperoxidation. He guessed (correctly, as it turned out) that these hydroperoxide lipids could increase membrane tension, trigger the separation of lipids into different regions within the membrane and drive membrane protein sorting.

## Putting theory into practice: manipulation of membrane properties achieved

After Torra's initial idea, the team set to work toward this ambitious goal. In the end, they showed that, upon controlled blue irradiation (the standard wavelength used to excite Flipper), the probe could, indeed, simultaneously induce and visualize changes in the tension, lipid composition and protein order of model and biological membranes.

The specific location of proteins on the membrane plays an important role in regulating their interactions with other molecular components and what functions they carry out (for instance, sending signals to the cell, so that in turn the cell can perform a specific action). The implications of this achievement are, therefore, highly significant.

ICREA Prof. María F. García-Parajo illustrates the concept with a down-to-earth example: "A person can be in different environments. For instance,

you could be in your home sitting in a sofa and surrounded by your family, or at work surrounded by your colleagues and in front of a computer. Depending on the environment you are, you will perform a different function. Now imagine that I can change your environment, magically transforming family into colleagues and the sofa into a computer room. Then, you would 'feel' the change of the environment and automatically change your function. This is exactly what happens in biology! The surrounding (the lipid composition, order and tension of the membrane) affects and defines the biological function of the proteins there".

The team has found in Flipper a means to achieve exactly that, making it a powerful tool to visualize and dynamically manipulate membrane heterogeneity—and therefore properties— with high precision in space and time. As a consequence, this technique offers the potential to study the interplay between membrane biophysical properties and cell functions.

### Future perspectives: bringing Flipper to living cells

"We are very excited about these results and the prospects for the future. So far, we have understood the mode of action of Flipper on model membranes and membranes extracted from living cells. Now

"If by controlling the composition of the membrane, we disturb the clustering of integrins, then we could [...] even possibly stop metastasis"

the obvious next step is to move to living cells", shares García-Parajo. The team is actively working on this right now, but first they need to overcome Flipper's inherent toxicity to cells, the main obstacle preventing further progress in this direction.

In the future, provided that Flipper works in the context of living cells, it could be possible to use the probe to reverse mechanical dysfunctionalities of membranes, helping to treat those diseases associated dysregulated mechanical with properties. "For instance, certain proteins, called integrins, are involved in the adhesion and migration of cells. It was shown that the mechanical properties of the membrane increase integrin nanoclustering and that this, in turn, can boost the migration of cancer cells, which contributes to their metastatic character", explains García-Parajo. Given their successful results, she foresees an optimistic scenario: "If by controlling the composition of the

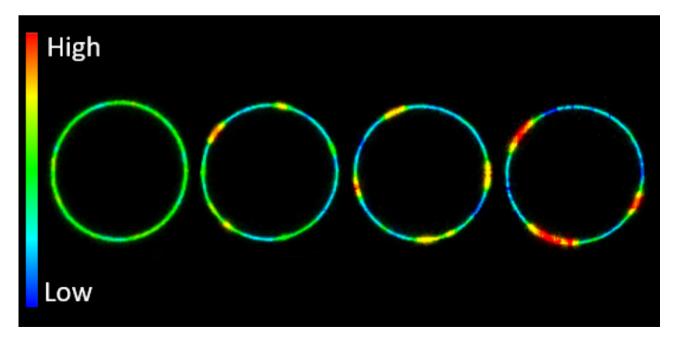
membrane, using our reported technique, we disturb the clustering of integrins, then we could affect the migrating properties of cells and even possibly stop metastasis. This is a dream that could become reality one day."

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Joaquim Torra, Felix Campelo, and Maria F. Garcia-Parajo. Journal of the American Chemical Society 2024 146 (34), 24114-24124.

DOI: 10.1021/jacs.4c08580





Photoinduced phase separation of biological membranes labeled with Flipper under prolonged FLIM imaging at 488 nm. Source: JACS.

# Ultrafast 2D spectroscopy probes charge separation in the plant photosystem

Ateam of researchers led by IBEC and ICFO has developed and validated a novel photoelectrochemical electron spectroscopy technique to probe charge separation dynamics, a crucial step for photosynthesis, in photosynthetic complexes.

Photosynthesis is the process by which some organisms (for instance, plants, algae and some bacteria) transform light energy into chemical energy. This process begins with the absorption of light (photons) by certain pigments (mainly chlorophyll) and ends with a flow of electrons that triggers the synthesis of energy carriers.

One intermediate step that has not been directly probed yet, mainly because it occurs at ultrafast timescales, is the so-called charge separation. Once the pigment absorbs a photon, an electron is excited to a higher energy level. This extra energy is then transferred to specific locations, called reaction centers, causing an electron of the chlorophyll in those centers to be again excited and transferred to another complex (the acceptor molecule). Consequently, the chlorophyll becomes positively charged, which means that charge separation has occurred. This charge difference is crucial because it sets up a flow of high-energy electrons that will drive the rest of the photosynthetic process.

To decipher photosynthetic complexes and engineer novel photosynthetic strategies, it is thus key to probe the pathways leading to charge separation. This phenomenon has recently been tackled in a joint work between IBEC and ICFO researchers **Dr. Luca Bolzonello** and **ICREA Prof. Niek F. van Hulst.** also in

collaboration with the University of Padua and Vrije Universiteit Amsterdam. The team has developed and validated a novel Photoelectrochemical Two-Dimensional Electronic Spectroscopy (PEC2DES) technique, which allows for the direct probing of charge separation dynamics in photosynthetic complexes. Their method was presented in **ACS Applied Materials and Interfaces**.

"I think our results are very significant because we have provided a new way to directly access the biologically relevant charge separation processes, which are crucial for understanding photosynthesis", remarks Dr. Luca Bolzonello, first co-author of the article.

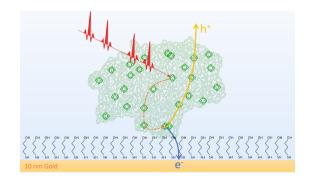
Unlike traditional optical methods, PEC2DES uniquely combines photoelectrochemical detection (PEC) with nonlinear spectroscopy (2DES), allowing for the selective investigation of the charge

"we have provided a new way to directly access charge separation processes, which are crucial for understanding photosynthesis" separation event and offering insights into the excitation and charge transfer dynamics within complex photosynthetic systems. More importantly, this technique can study the ultrafast dynamics of the excitons within the system just by reading out directly the product of the photosynthesis, that is, the electrical charges that move across the electron transport chain.

### **Combining PEC and 2DES to obtain PEC2DES**

To validate their method, researchers employed photosystem complex I-light harvesting complex I (PSI-LHCI) as model system, where light harvesting by 'antenna chlorophylls' is used to drive charge separation in the reaction center.

They first developed the photoelectrochemical setup (PEC) to measure the current generated by the PSI-LHCI complexes. Then, they integrated this setup with a two-dimensional electronic spectroscopy (2DES) system. This unprecedented combination of PEC and 2DES gave rise to the PEC2DES technique reported on their study, which for the first time identified the generated charges during charge separation.



Cartoon representation of the photoelectrochemical current response of the transparent gold electrodes of the study. Source: ACS Applied Materials and Interfaces.

"The main obstacles we encountered were the need to maintain sample stability over long periods of time, which is required by the 2DES measurements, and the difficulty to interpret the PEC2DES signal", recalls Bolzonello. "Even though we discovered that the technique is blind to some ultrafast features, we opened the path to solve the issues."

## Future perspectives: toward artificial photosynthetic systems

The team has just opened the door to tracking the ultrafast dynamics of charge separation processes with the PEC2DES technique. In the near future, they would like to refine their tool by identifying and minimizing the effects of incoherent mixing, an undesired phenomenon that contaminates the object of study, in this case, the charge separation dynamics. They also consider exploring the application of this technique to other photosynthetic complexes or aiming to artificial systems where the effect of incoherent mixing, the main limit of this new technique, is minimized.

According to the researchers, the discovery could be used in biohybrid devices and sensors that rely on the precise control and understanding of electron transfer processes within complex protein assemblies. Bolzonello further guesses that one of the promising applications of PEC2DES could be "the design and optimization of artificial photosynthetic systems, which in turn could improve solar energy conversion efficiency."

### Reference:

Manuel López-Ortiz, Luca Bolzonello, et. al. ACS Applied Materials & Interfaces 2024 16 (33), 43451-43461.

DOI: 10.1021/acsami.4c03652

# When Separation Creates Connection: How Do Plant Cells Stay Connected While Dividing?

Division and communication are prerequisites for multicellularity, but how are they coordinated? In a recent article, researchers identify the mechanisms that allow plant cells to divide while remaining connected.

Plants, like animals, are multicellular organisms composed of millions of cells organized into specialized tissues and organs. These cells are formed by cell division, a process that produces two daughter cells with identical genomes from a single parent cell. These daughter cells later differentiate into specific cell types and must communicate to coordinate development and maintain the organism's function. Intercellular communication enables cells to exchange information and molecular signals throughout their lifespan.

In plants, this communication is facilitated by nanoscopic intercellular bridges called plasmodesmata. These structures connect cells and enable the exchange of molecules like proteins, ions, hormones, and nutrients.

However, a paradox arises: how can daughter cells coordinate with each other while becoming individually autonomous? Since plasmodesmata form during cell division, how are division and connection coordinated?

## Plant Cells Bypass the Final Stage of Cell Division to Remain Connected

In plants, unlike animal cells, cell division does not lead to a clear physical separation or "abscission" between daughter cells. During cytokinesis, the final stage of cell division, a cell plate forms to separate the daughter cells. However, as this plate forms, thousands of nanoscopic openings, or "fenestrations," appear within it. Some of these fenestrations stabilize into plasmodesmata, enabling a direct cytosolic connection between cells. In this study, scientists investigated the molecular mechanisms that allow plant cells to bypass abscission to form plasmodesmata.

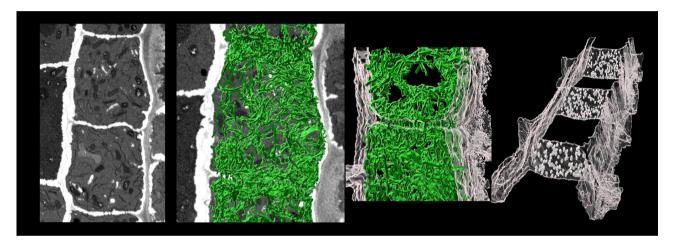
## The Endoplasmic Reticulum Has an Essential Role in Intercellular Bridge Formation

Now, CNRS and other collaborators have published a study in **Science** on the plant cells division and connection. By combining cell biology approaches, live cell fluorescence imaging, electron microscopy through close collaboration with the France-Bioimaging Bordeaux Imaging Center and biophysical modelling done by ICFO researcher **Dr. Felix Campelo**, the researchers highlighted the central role of the endoplasmic reticulum (ER) in plasmodesmata formation.

They discovered that in the model plant Arabidopsis thaliana, the formation of plasmodesmata requires the presence of the ER in the fenestrations as the cell plate expands. The ER helps stabilize the

fenestrations, which then become plasmodesmata, while its absence leads to their complete fusion and disappearance. However, the ER is a highly dynamic organelle and needs stabilization. The study identified that three members of the Multiple C2 domains and Transmembrane domain Proteins (MCTPs) family, MCTP3, 4, and 6, allow

"This research [...] reveals a central and unexpected role of the endoplasmic reticulum in orchestrating intercellular continuity"



SBF-SEM and 3D segmentation of root endodermal cells meristematic zone in Arabidopsis root meristem. The pictures show multiple plasmodesmata (magenta) across a section of cross-wall and mature wall and ER (green) cell-cell continuity. Source: Science.

for the attachment and constriction of the ER within the developing plasmodesmata, stabilizing them. Without MCTPs 3, 4, and 6, plasmodesmata formation and intercellular communication are significantly affected.

This research represents two major advances: it addresses the fundamental question of how plant cells "fail" cytokinesis to enhance communication and reveals a central and unexpected role of the endoplasmic reticulum (ER) in orchestrating intercellular continuity.

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Z.P. Li, H. Moreau, J.D. Petit, T. Souza-Moraes, M. Smokvarska, J. Perez-Sancho, M. Petrel, F. Decoeur, L. Brocard, C. Chambaud, M. Grison, A. Paterlini, M. Glavier, L. Hoornaert, A.S. Joshi, E. Gontier, W.A. Prinz, Y. Jaillais, A. Taly, F. Campelo, M.-C. Caillaud, E. M. Bayer. Plant plasmodesmata bridges form through ERdependent incomplete cytokinesis. Science, October 31, 2024,

DOI: https://doi.org/10.1126/science.adn4630

# Atomic sensors unveil hidden dynamics of molecular polarization

# Atomic sensors unveil hidden dynamics of molecular polarization

Researchers from IBEC and ICFO demonstrate the ability of atomic sensors to non-destructively monitor, measure and optimize nuclear spin hyperpolarization of some clinically relevant molecules in real-time. These features, reported in *PNAS*, could enhance and reduce costs of quality controls used in clinical magnetic resonance imaging.

Magnetic resonance imaging (MRI) has long been a cornerstone of modern medicine, providing highly detailed images of internal organs and tissues. MRI machines, those large, tubeshaped magnets commonly found in hospitals, use powerful magnets to map the densities of water and fat molecules within the body. In addition to these molecules, other substances like metabolites can also be mapped, but their concentrations are often too low to produce clear images. To overcome this, a technique known as hyperpolarization is employed to enhance the magnetic resonance signal of these substances, making them more visible during MRI scans.

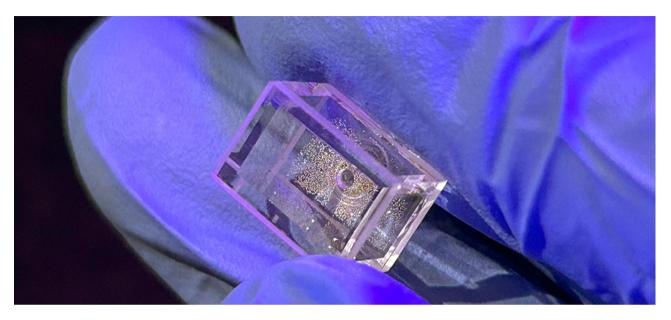
Hyperpolarization involves preparing a substance outside the body in a state where its magnetization—key to creating MRI images—is near its maximum. This process can boost the signal by thousands of times compared to its natural state. Once hyperpolarized, the substance is injected into the patient and transported to the target organ or tissue. However, before this can happen, it is crucial to confirm that the substance is adequately hyperpolarized through rigorous quality control processes.

Current quality control techniques face two significant challenges. First, these methods often

reduce the magnetization of the sample during the read-out process, thereby diminishing its ability to enhance the MRI scan. Second, the time required for measurement can be lengthy, during which the substance's magnetization naturally decays, limiting the opportunity for consecutive measurements. This results in a lack of critical data that could otherwise help maximize the efficiency of hyperpolarization. Furthermore, once the sample is hyperpolarized, there is a risk that it could lose its magnetization during transport to the MRI machine. Traditional quality control techniques, due to their time-consuming nature, may fail to detect this loss in time.

Now, a collaboration of IBEC researchers Dr. James Eills (now at Forschungszentrum Jülich, Germany) and Dr. Irene Marco Rius and ICFO researchers ICREA Prof. Morgan W. Mitchell and Dr. Michael C. D. Tayler has demonstrated how atomic sensor techniques overcome the limitations of conventional sampling when measuring the magnetization of hyperpolarized materials. This breakthrough was recently reported in the journal **PNAS**.

In particular, the team used optically-pumped atomic magnetometers (OPMs), whose operating principles differ fundamentally from traditional



A small cell containing Rubidium metal, which is the central field-sensing component within the atomic magnetometer. ©ICFO

sensors, enabling real-time detection of the fields produced by hyperpolarized molecules. OPMs' nature allowed these researchers to perform continuous, high-resolution and non-destructive observations throughout the entire experiment, including the hyperpolarization process itself.

According to the authors, if the field of hyperpolarization sensing was cinema, previous methods would be like a sequence of still photos, leaving the plot between frozen pictures open to the viewer's guess. "Instead, our technique is more

"previous methods would be like a sequence of still photos. Instead, our technique is more like a video" like a video, were you see the whole story frame by frame. Essentially, you can observe continuously and without resolution limits, so you do not miss any details!", explains Dr. Tayler, ICFO researcher and co-author of the article.

### **Unveiled behaviors during magnetization**

The team tested their OPMs by monitoring hyperpolarization in clinically relevant molecules. The atomic sensors' unprecedented resolution and real-time tracking allowed them to witness how the polarization in a metabolite compound evolved under the presence of a magnetic field.

The atomic sensors revealed 'hidden spin dynamics' that had gone unnoticed until now, offering a new path towards optimizing the hyperpolarization from the very start of the process. "Previous methods obscured subtle oscillations in the magnetization profile, which previously went undetected", remarks

Tayler. "Without the OPM, we would have achieved a suboptimal final polarization without even realizing." Beyond simple observation, the method could be used to control the polarization process in real-time and stop it at the most convenient point, for instance when the maximum polarization is attained

The study revealed another unexpected behavior when the team applied a magnetic field to repeatedly magnetize and demagnetize the hyperpolarized fumarate molecule. They expected to see the magnetization increasing to a maximum and then going back to zero over and over, transitioning smoothly every time. Contrary to these simple expectations, the molecule exhibited complex dynamics due to hidden resonances at certain magnetization-demagnetization durations and magnetic fields. "This understanding will help us detect when unwanted behavior occurs and adjust parameters (like the cycle's duration or the magnetic field intensity) to prevent it", explains Tayler.

The work represents an advancement in hyperpolarized MRI technology, thanks in large part to the collaborative efforts of IBEC's Molecular Imaging for Precision Medicine group and ICFO's Atomic Quantum Optics group. IBEC expertise in hyperpolarization methods and ICFO's expertise in OPM sensing technologies were critical in achieving the results.

"This is a beautiful example of the new science that can be achieved when researchers from different disciplines work together, and the proximity of IBEC and ICFO meant we were able to collaborate closely and achieve something truly novel", acknowledges Dr. James Eills, IBEC researcher and first author of the article.

Dr. Tayler reflects on the team's success: "The OPM measurements worked beautifully from the start.

The sensors' exquisite sensitivity revealed hidden dynamics we hadn't anticipated, as if they were meant for this purpose. The ease of use and the wealth of new information make them a powerful tool for hyperpolarization monitoring."

### Benefits for MRI and other future applications

The immediate application of this study would be to integrate portable atomic sensors into clinical sample quality control for MRI, something that is currently being implemented by the ICFO team in the Spanish Ministry Project "SEE-13-MRI". This way, one could guide molecules to the highest polarization level during hyperpolarization and reliably certify the polarization level before substances are injected into patients.

The development could significantly reduce the cost and logistical challenges of metabolic MRI. If so, this would expand its reach from the handful of specialized research centers where it is currently used, to many hospitals worldwide.

However, the potential of atomic sensors extends far beyond medical imaging. The same non-destructive, real-time tracking system using optically-pumped magnetometers (OPMs) could be applied to monitor macromolecules in chemical processes, study high-energy physics targets, or even optimize spin-based algorithms in quantum computing. According to Dr. Tayler: "The method we've developed opens up new avenues not only for improving MRI but for various fields that rely on precise magnetic sensing, and we are excited about its further development."

#### Reference:

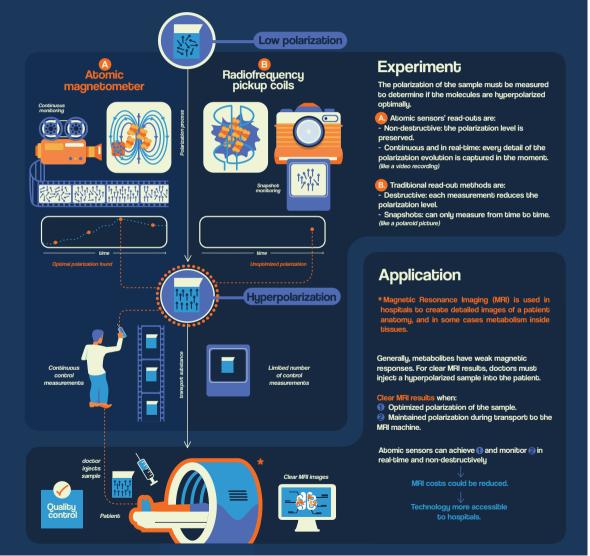
James Eills, et. al., "Live magnetic observation of parahydrogen hyperpolarization dynamics", PNAS 121 (43) (2024). DOI: https://doi.org/10.1073/pnas.2410209121

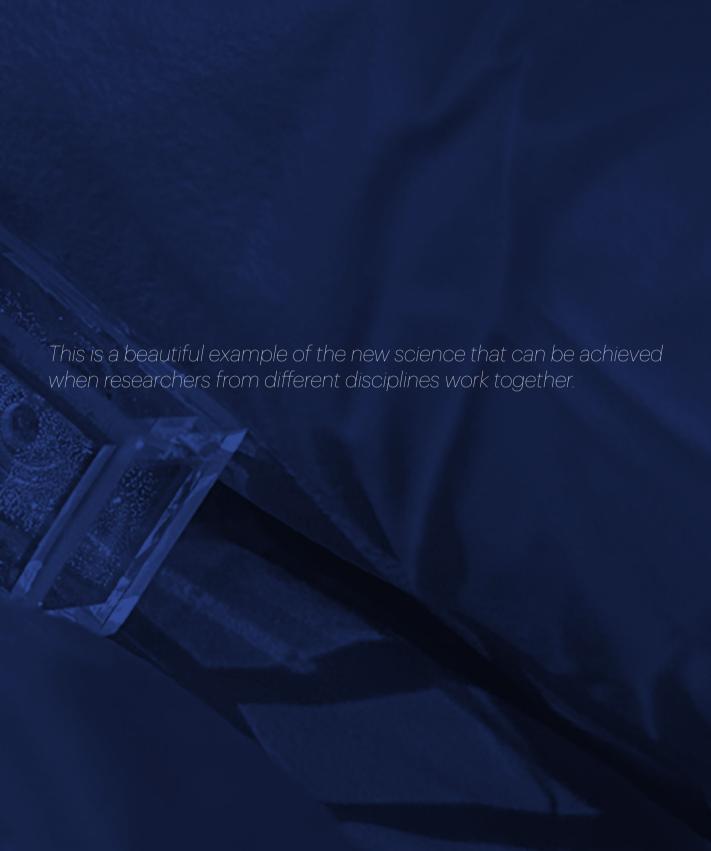
## Atomic Sensors For monitoring hyperpolarization



When molecules in a substance have their magnetic moments (like tinu arrows) pointing in the same direction, the substance is said to have high polarization, creating a significant magnetic field-similar to lining up many small magnets.

In a hyperpolarized substance, this alignment is almost 100%, resulting in a strongly enhanced magnetic field.





## New gel breaks down alcohol in the body

An international team of researchers, led by ETH Zurich scientists, has developed a protein-based gel that breaks down alcohol in the gastrointestinal tract without harming the body. In the future, people who take the gel could reduce the harmful and intoxicating effects of alcohol.

Most alcohol enters the bloodstream via the mucous membrane layer of the stomach and the intestines. These days, the consequences of this are undisputed: even small amounts of alcohol impair people's ability to concentrate and to react, increasing the risk of accidents. Drinking large quantities on a regular basis is detrimental to one's health: common consequences include liver disease, inflammation of the gastrointestinal tract and cancer. According to the World Health Organization, around 3 million people die every year from excessive alcohol consumption.

An international team of researchers led by ETH Zurich scientists has now developed a protein gel that breaks down alcohol in the gastrointestinal tract. In a study recently published in the journal **Nature Nanotechnology**, they show that in mice, the gel converts alcohol quickly, efficiently and directly into harmless acetic acid before it enters the bloodstream, where it would normally develop its intoxicating and harmful effects.

### Reducing health damage caused by alcohol

"The gel shifts the breakdown of alcohol from the liver to the digestive tract. In contrast to when alcohol is metabolised in the liver, no harmful acetaldehyde is produced as an intermediate product," explains Professor Raffaele Mezzenga from the Laboratory of Food & Soft Materials at ETH

Zurich. Acetaldehyde is toxic and is responsible for many health problems caused by excessive alcohol consumption.

In the future, the gel could be taken orally before or during alcohol consumption to prevent blood alcohol levels from rising and acetaldehyde from damaging the body. In contrast to many products available on the market, the gel combats not only the symptoms of harmful alcohol consumption but also its causes. Yet, the gel is only effective as long as there is still alcohol in the gastrointestinal tract. This means it can do very little to help with alcohol poisoning, once the alcohol has crossed into the bloodstream. Nor does it help to reduce alcohol consumption in general. "It's healthier not to drink alcohol at all. However, the gel could be of particular interest to people who don't want to give up alcohol completely, but don't want to put a strain on their bodies and aren't actively seeking the

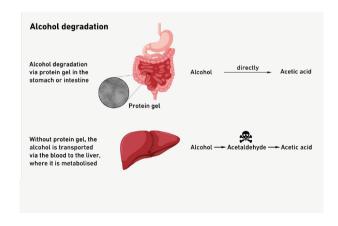
"The gel could be of particular interest to people who don't want to give up alcohol completely, but don't want to put a strain on their bodies"

effects of alcohol," Mezzenga says.

### Main ingredients: Whey, iron and gold

The researchers used ordinary whey proteins to produce the gel. They boiled them for several hours to form long, thin fibrils. Adding salt and water as a solvent then causes the fibrils to cross-link and form a gel. The advantage of a gel over other delivery systems is that it is digested very slowly. But to break down the alcohol, the gel needs several catalysts.

The researchers used individual iron atoms as the main catalyst, which they distributed evenly over the surface of the long protein fibrils. "We immersed the fibrils in an iron bath, so to speak, so that they can react effectively with the alcohol and convert it into acetic acid," says ETH researcher Jiaqi Su, the first author of the study. Tiny amounts of hydrogen peroxide are needed to trigger this reaction in the intestine. These are generated by an upstream reaction between glucose and gold nanoparticles. Gold was chosen as a catalyst for hydrogen peroxide



Alcohol degradation in the body with and without the new gel. (Visualisations: ETH Zurich / Adobe Stock).

because the precious metal is not digested and therefore stays effective for longer in the digestive tract. The researchers packed all these substances – iron, glucose and gold – into the gel. This resulted in a multi-stage cascade of enzymatic reactions that ultimately converts alcohol into acetic acid.

### Gel works in mice

The researchers tested the effectiveness of the new gel on mice that were given alcohol just once as well as on mice that were given alcohol regularly for ten days. Thirty minutes after the single dose of alcohol, the prophylactic application of the gel reduced the alcohol level in the mice by 40 percent. Five hours after alcohol intake, their blood alcohol level had dropped by as much as 56 percent compared to the control group. Harmful acetaldehyde accumulated less in these mice, and they exhibited greatly reduced stress reactions in their livers, which was reflected in better blood values.

In the mice that were given alcohol for ten days, the researchers were able to demonstrate not only a lower alcohol level but also a lasting therapeutic effect of the gel: the mice that were given the gel daily in addition to alcohol showed significantly less weight loss, less liver damage and hence better fat metabolism in the liver as well as better blood values. Other organs in the mice, such as the spleen or the intestine, as well as their tissues also showed much less damage caused by alcohol.

### Reference:

Su J, Wang P, Zhou W, Peydayesh M, Zhou J, Jin T, Donat F, Jin C, Xia L, Wang K, Ren F, Van der Meeren P, García de Arquer P, and Mezzenga R. Single-site iron-anchored amyloid hydrogels as catalytic platforms 1 for alcohol detoxification. Nature Nanotechnology.

DOI: 10.1038/s41565-024-01657-7

# Discussing photonics tools for pediatrics in the 3rd BMPN annual meeting

Gathering of experts focuses discussion on photonic techniques to improve diagnostics and treatment personalization in pediatrics.

On Wednesday 17th of April, the Barcelona Medical Photonics Network (BMPN) celebrated the third edition of its annual meeting. The BMPN formally launched in March 2021 as a platform to promote the research and development activities in photonics being carried out in the Barcelona region through long-standing collaborations between ICFO and its biomedical and clinical partners. This year's edition was co-organized with ICFO's two main medical partners in the field of Pediatrics: Sant Joan de Déu Barcelona Children's Hospital (SJD), where the event was held, and Vall Hebron University Hospital, as well as their respective research institutes.

The speakers reviewed different imaging and monitoring photonic techniques and their recent and ongoing applications in several medical fields, with special attention to brain pathologies and neurodevelopment in pediatrics. The session started with Dr. Joan Comella, director of Research, Innovation and Learning at the SJD Barcelona Children's Hospital and Director of the Institute of Research Sant Joan de Déu (IRSJD). Dr. Comella introduced the event highlighting the fundamental goal of their institution, which focuses on carrying out state-of-the-art research of rare diseases in children, and the collaborations between institutions and other hospitals as a key ingredient to achieve this goal.

### High resolution microscopy techniques for biomedical and clinical applications

Dr. Pablo Loza, Head of the SLN facility at ICFO, gave the first talk to introduce the different microscopy techniques developed by his team, reviewing a wide variety of biomedical and clinical applications. Dr. Mariona Suñol, pediatric pathologist at SJD, took over and discussed how Raman spectroscopy is a promising non-invasive tool to analyse in vivo the ocular structures affected by retinoblastomas, the most common malignant ocular tumour in children, and to evaluate the high-risk factors for its metastasis. Recently, this collaborative project between ICFO and SJD received seed financial support from the Fundació La Nineta dels Ulls, further promoting the research and knowledge of retinoblastoma disease and its treatments.

The next speaker was Dr. Cecilia Jiménez, Group Leader of the Applied Research in Neuromuscular Diseases group at IRSJD. She delved deeper into other high-resolution techniques also explored in collaboration with ICFO around neuromuscular diseases and related innovative therapies.

From a more fundamental research perspective, Prof. at ICFO Michael Krieg explained the latest advances made in his group Neurophotonics and Mechanical Systems Biology, particularly regarding



Dr. Joan Comella, director of Research, Innovation and Learning at the SJD Barcelona Children's Hospital and Director of the Institute of Research Sant Joan de Déu (IRSJD) welcomes the event.



the Photons as Synaptic Neurotransmitters (PhAST) project. As he stated, their success in optically restoring the mechanical sensitivity in worms further supports the use of light as a new non-invasive, fast and versatile neurotransmitter.

### Improving magnetoencephalography for neonates

The next two speakers tackled the current magnetoencephalographic (MEG) methods, their current status and problematics, especially for neonates, emphasizing that commercial devices have a huge size, are expensive and are not ergonomically suitable for newborn babies.

Professor Fabrice Wallois, lab Director of the GRAMFC research group and Head of the Pediatric Clinical Neurophysiology Department at the Amiens-Picardie University Hospital, addressed the MAGIC project, which targets pathologies and mechanisms of dysfunction in the brain of children and fetus, according to specific biomarkers, and directly assesses brain activity. ICREA Prof. at ICFO Morgan Mitchell, leader of the Atomic Quantum Optics group, complemented the previous

talk by sharing the Optically Pumped Magnetometers- Magnetoencephalography initiative, which is working to achieve ultraprecise atomic magnetometers in a much more manufacturable way without losing their extremely high performance.

### Non-invasive tools to monitor the baby brain

ICREA Prof. at ICFO Turgut Durduran, leader of the Medical Optics research group at ICFO, re-opened the event after the midday break. He explained the various optical tools that the group has developed over the years for non-invasive hemodynamic monitoring of infants, mainly based on the combination of two methods: near-infrared spectroscopy and diffuse optics. The hybrid resulting technique offers clinicians very useful information regarding the oxygen metabolism of tissues and the blood flow in patients, allowing doctors to make a better assessment of measures such as perfusion and intracranial pressure.



A moment during the BMPN meeting.

Putting an emphasis on these techniques, Dr. Joan Sánchez de Toledo, Chair of Pediatric Cardiology at SJD and researcher at IRSJD, and Dr. Marta Camprubí, neonatologist at SJD and researcher at IRSJD, talked about TinyBrains, an ongoing European research project coordinated by ICFO that aims at understanding the mechanisms of brain damage in neonates born with congenital heart defects through neuromonitoring. The first talk described the studies that have been carried out with animal models, while the second focused on the recent clinical studies in newborn babies, explaining how monitoring the brain through these techniques before, during and after surgery can help guide the clinical actions to be taken.

The need for electroencephalography alongside hemodynamic and metabolic monitoring was claimed to be again of huge importance for the protection of neonates and children during seizures. Dr. Carme Fonts, Head of the Neurology Service at SJD and researcher at IRSJD, centred her talk around this topic. Finally, Dr. Maria Antònia Poca, Clinical Head of Neurosurgery and responsible for the Pediatric Neurosurgery Unit at the Vall Hebron University Hospital, presented the recent photonic tools for monitoring the intracranial pressure in a non-invasive manner, as opposed to current highly invasive methods, such as the one that the SafelCP project is developing.

The annual meeting ended with Dr. Chiara Santolin, researcher at IRSJD and the UPF Center for Brain and Cognition who presented her forthcoming studies on the mechanisms of language acquisition using optical imaging.

### A fruitful ongoing collaboration

Overall, the 3rd BMPN edition showed the importance of the interconnection between photonics and medical research, highlighting and placing a special interest in how neuromonitoring tools can improve patient management in pediatrics.

Ariadna Martínez, ICFO Light for Health program coordinator, concludes: "It is our honour to see a full room each year for our annual meeting, with a mix of professional profiles that goes from technology developers to clinicians through to innovation managers, both from inside and outside the Network. Multidisciplinary endeavours thrive on collaborative ambiences like this, and while it is not an easy task (because it demands diverse perspectives, effective communication, and mutual trust) the results are very enriching".

"Multidisciplinary endeavours thrive on collaborative ambiences like this, and [...] the results are very enriching"



### **Exploring photonics for neuroscience**

ICFO recently hosted the "Hands-on course on MINDLAB", bringing together students and experts to explore advanced photonics technologies aiming to train the next generation of neuroscience researchers.

The course, organized by five research groups at ICFO, provided a comprehensive look at brain research. Designed to train the next generation of neuroscience researchers, it gave an interdisciplinary approach to brain science, spanning molecular to systemic levels. The event featured lectures by ICFO group leaders and invited speakers, paired with hands-on lab sessions. Participants joined one of the organizing research groups and attended master classes during the week. They explored ICFO's state-of-the-art labs, working with super-resolution microscopes and neurophotonics devices.

"It was an exciting event with top international speakers and students, and a successful kick-off for future workshops and initiatives at ICFO covering the molecules and the mind", comments Prof. at ICFO Michael Krieg.

Attendees included students, PhD candidates, and postdoctoral researchers from national and international institutions, all with diverse scientific backgrounds. Maddi Olaetxea, a fourth-year Biochemistry and Molecular Biology student at the University of the Basque Country, says she wasn't sure what to expect but was not disappointed. "There were certain concepts that I thought I understood, yet they were limited to a mere concept or theoretical level. This experience has given me the opportunity to put these contents into practice."

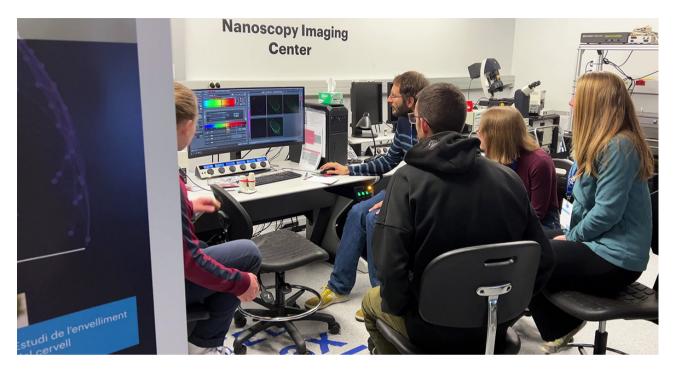
"We have been able to see first-hand the capabilities of this equipment in studying neuronal activity in in-vivo models, and these tools will be useful in my work"

"Working with the researchers at the SLN facility has been a fantastic experience", says Núria Camarero, a postdoctoral researcher at IBEC. "We have been able to see first-hand the capabilities of this equipment in studying neuronal activity in invivo models, and these tools will be useful in my work, especially for analysing the data".

#### Monitoring the brain of neonates

A highlight of the course was the TinyBrains workshop, a European project developing a non-invasive device to monitor the brains of babies with congenital heart defects.

At the opening session Jennifer Lynch, a neonatal cardiologist, discussed how innovative optical techniques can improve outcomes, emphasizing the need for better neuromonitoring tools, as



Students at the Nanoscopy laboratory ©ICFO

current methods cannot predict brain injury risks effectively. Prof. Martin Lauritzen presented his team's research on neuromodulator transport and transport of neurotherapeutics across the bloodbrain barrier, explaining how they use advanced imaging techniques in mice to understand these mechanisms.

One of the course sponsors, the proof-of-concept LowLightScope, is also focused on bioluminescence imaging. The project is developing a light-efficient microscope for fast volumetric imaging of photon-starved samples.

#### Inspiring the next generation of researchers

The course also featured a sponsor's exhibition, where companies showcased their products and

engaged with attendees. During the talk session, the companies Hamamatsu Photonics, Izasa and Pionirs gave more details about their work. The two ICFO-led initiatives TinyBrains and the Barcelona Medical Photonics Network also presented their advancements.

"The most valuable thing this experience has given me is motivation. As a final-year student, it has helped me explore and discover different fields, which has encouraged and motivated me to continue studying", says Olaetxea, recommending the experience to university students. "I wish I had the chance to attend a workshop like this when I was studying Pharmacy!" concludes Camarero.



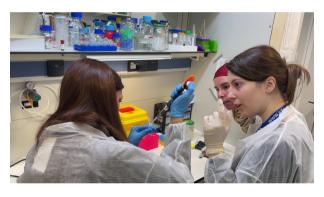
Participants working at the Biolab. ©ICFO



Participants testing the Medical Optics devices. ©ICFO



Attendees at the Photon Harvesting in Plants and Biomolecules lab. ©ICFO



Participants working at the Neurophotonics and Mechanical Systems Biology lab. @ICFO



Group picture at the MindLab. ©ICFO



# Blocking the Collagen Floodgates: New Strategy to Tackle Fibrosis and Scarring

## Blocking the Collagen Floodgates: New Strategy to Tackle Fibrosis and Scarring

Collagen hypersecretion can lead to scarring and in some cases, fibrosis, yet few strategies exist to control the response. A new experimental strategy tackles the problem at the cellular level.

Researchers at the Centre for Genomic Regulation in Barcelona and the University of Cologne in Germany, in collaboration with ICFO researchers and collaborators from the Institut Jacques Monod in France, EMBL Barcelona, the Institute for Stem Cell Science and Regenerative Medicine (inStem) in India, and the Max Planck Institute for Biology of Aging in Germany, have developed a new experimental strategy to tackle scarring and fibrosis. Experiments with patient-derived human cells and animal models showed the strategy was effective, non-toxic and its effects reversible. The findings are published today in the journal **Nature Communications**.

Scarring occurs from the secretion and accumulation of various components – primarily proteins known as collagens – into the space between individual cells, usually occurring as a response to injury or damage. Excessive collagen secretion can also cause the buildup of fibrotic tissue, a more serious condition where excess connective tissue is formed to the extent that it compromises the function of tissues and sometimes entire organs. Around 45% of deaths in the industrialised world are attributed to some form of tissue fibrosis.

Treatment options for both scarring and fibrosis are usually limited to surgery. Outside the body, scar tissue is often beneath the outer layer of the skin. Since most topical creams are not able to penetrate deeply enough to reach the affected areas effectively, their ability to remodel or heal the tissue is limited. Inside the body, scarring and fibrosis can affect many different tissues and organs, each with its unique environment and challenges and with no one-size-fits-all treatment option.

"Existing treatment options are usually ineffective because they try and fail to mop the excessive collagen up. In this work, we tried a completely different idea: to block the floodgates at the cellular level. The strategy works at the cellular level, releasing enough collagen so that tissues don't fall apart while protecting them from excessive amounts that impairs their function," explains ICREA Research Professor Vivek Malhotra, co-corresponding author of the study and researcher at the Centre for Genomic Regulation (CRG) in Barcelona, Spain.

The researchers' new strategy involves using molecules known as peptides to block the export of collagen from inside cells. The

"The strategy works at the cellular level, releasing enough collagen so that tissues don't fall apart while protecting them from excessive amounts that impairs their function"

peptides disrupt an interaction between two proteins called TANGO1 and cTAGE5. Both proteins bind to each other and are essential for the export of collagens from their site of synthesis inside the cell to the exterior. The two proteins "sit" at the endoplasmic reticulum exit site, a place in the cell where materials like proteins are packaged and transported out the cell.

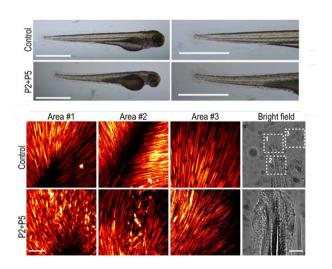
"Targeting the endoplasmic reticulum exit site has been historically considered impossible because a third of all human proteins go through it, so inhibiting its activity would likely have many off-target, toxic effects. In other words, it's been 'undruggable'. Only recently have there been indications that there is some specificity for the secretory materials. In this study we aimed to achieve this specificity by inhibiting the interface between TANGO1 and cTAGE5 with targeted precision," explains Dr. Ishier Raote, first author of the study who carried out the work at the Centre for Genomic Regulation.

Proteins are like puzzle pieces. To know how two pieces fit together, you need to see their shapes clearly. Both TANGO1 and cTAGE5 are large, complex proteins which constantly shapeshift. To date, their exact structure remains unknown, which in turn means we don't understand how they connect at the molecular level, hindering

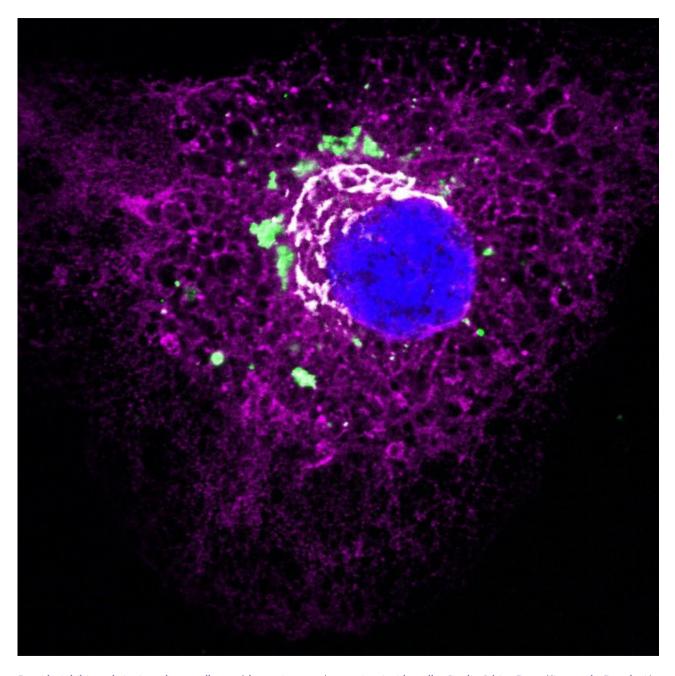
efforts to design drugs that can block the interaction.

The researchers overcame this challenge by using AlphaFold2, an artificial-intelligence program that can guess the shapes of the two proteins without needing structural data about their 3D shape. The predictions made by Al allowed the authors of the study to design peptides which can pass through a cell membrane and disrupt the interaction between TANGO1 and cTAGE5.

The researchers tested the peptides using normal human fibroblasts, the most common type of cell found in connective tissue. The peptides successfully inhibited collagen export, causing it to accumulate inside the cells. The effect was also reversible, with collagen levels increasing again after the peptides were removed within a 48-hour period.



Zebrafish larvae at 3 days post fertilization treated vs untreated (controls), and a magnified view of their tails. SHG signal from the collagen fibres in the fish fin from three different regions. Source: Nature Communications.



Peptide inhibitors bringing about collagen (shown in green) retention inside cells. Credit: Ishier Raote/Centro de Regulación Genómica.

"This [strategy's control] could range from alleviating the cosmetic effects of skin scarring to the treatment of autoimmune diseases like scleroderma, as well as to manipulate post-surgery related events associated with wound healing"

The researchers observed similar effects in experiments with fibroblasts from patients with scleroderma, a complex autoimmune disease characterized by fibrosis of the skin and internal organs. The peptides were then tested using zebrafish, a common animal model to study tissue development and wound healing.

To understand the effectiveness of the experimental strategy in reducing collagen deposition, a critical step in combating fibrosis and scarring, ICFO researchers at the Superresolution Light Microscopy & Nanoscopy Facility Marina Cunquero, Gustavo Castro and Jordi Andilla, led by Dr. Pablo Loza, and Fèlix Campelo from the Single Molecule Biophotonics group, studied the second harmonic generation signal (SHG) by shedding light on differences in collagen fibers within zebrafish fins. They saw that the strategy visibly reduced collagen deposition in wound areas, providing crucial insights into the structural changes that occur in collagen fibers.

This experiment underscores the power of cross-collaboration and interdisciplinary

research in tackling complex medical challenges, which can facilitate more targeted and effective treatments and pave the way for several potential applications, ranging from cosmetic scar treatment to addressing autoimmune diseases.

The researchers next plan to evaluate the efficacy of the peptides in pig skin because it closely resembles human skin. They will also finetune the properties of the peptides to increase their potency.

"We believe this represents a new strategy to control the effects of collagen hypersecretion. This could range from alleviating the cosmetic effects of skin scarring to the treatment of autoimmune diseases like scleroderma, as well as to manipulate post-surgery related events associated with wound healing to prevent fibrosis," concludes Dr. Malhotra.

#### Reference:

Raote, I., Rosendahl, AH., Häkkinen, HM. et al. TANGO1 inhibitors reduce collagen secretion and limit tissue scarring. Nat Commun 15, 3302 (2024). DOI: https://doi.org/10.1038/s41467-024-47004-1

This experiment underscores the power of cross-collaboration and interdisciplinary research in tackling complex medical challenges, which can facilitate more targeted and effective treatments and pave the way for several potential applications, ranging from cosmetic scar treatment to addressing autoimmune diseases.

## Towards the prediction of therapy response for renal cell cancer

Researchers find relevant biomarkers for predicting and monitoring antiangiogenic therapy outcome for a subtype of renal cell carcinoma in mice. To achieve so, the team used non-invasive diffuse optical techniques.

Clear cell renal cell carcinoma (ccRCC), characterized by its high metastasis and mortality rates, is the most prevalent subtype of renal cell carcinoma, one of the most common urinary cancers. An approach aimed at treating this kind of tumors is based on antiangiogenic drugs, that is, treatments that inhibit blood vessels formation, thus reducing nutrients and oxygen supply and, consequently, preventing further tumor growth.

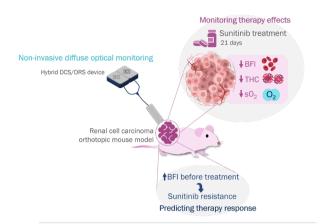
The standard first-line antiangiogenic treatment is called sunitinib. Despite being the first option in many cases, almost 30% of patients present intrinsic resistance to it or acquire resistance within the 6th to the 15th month of therapy. Choosing an ineffective treatment not only is time and energy consuming, but also can worsen cancer aggressiveness. Thus, having tools to ascertain the right diagnostic is of huge importance. While extracting predictive biomarkers of therapy resistance and response could help clinicians discriminate which patients would benefit from treatment, to date a non-invasive and practical alternative is still lacking.

ICFO researchers from the Medical Optics group led by ICREA Prof. Turgut Durduran, in collaboration the Tumor Angiogenesis group of ICO-IDIBELL led by Dr. Oriol Casanova, have obtained promising results in this regard, having recently appeared in *Biomedical Optics Express*.

"These techniques give information about the microvascular hemodynamics in a safe, non-invasive and practical way, and have already been tested on humans for other purposes"

By applying diffuse optical techniques in a ccRCC mouse model, the team has found significant biomarkers to predict the response to sunitinib treatment, both before and during therapy.

These techniques give information about the microvascular hemodynamics in a safe, non-invasive and practical way, and have already been tested on humans for other purposes. Therefore, moving from mice to humans should be feasible, researchers say. That could be a path to follow, since the results suggest that diffuse optical techniques are a suitable toolbox for predicting the therapeutic resistance of a ccRCC tumor to antiangiogenic therapy before administrating the drug and throughout the treatment.



DCS: diffuse correlation spectroscopy, DRS: diffuse reflectance spectroscopy, BFI: blood flow index, THC: total hemoglobin concentration, sO<sub>3</sub>: oxygen saturation

Illustration summarizing the main findings reported in the work by Mireles et. al. Credit: Clara Vilches.

"The provided biomarkers [...] could help medical professionals make more informed and individualized decisions"

### Towards validated biomarkers for clear cell renal cell carcinoma

In the reported experiment, some mice's tumors were treated with sunitinib and compared to the control group, where no antiangiogenic treatment was applied. Among those under sunitinib treatment, some of them responded positively and some others did not, similarly to what happens in the clinics.

Researchers applied diffuse optical techniques (diffuse correlation spectroscopy and diffuse reflection spectroscopy) to all of them and then compared the outcomes between groups. In particular, they measured three parameters: blood flow index, total hemoglobin concentration and blood oxygen saturation.

After collecting the data, researchers found that total hemoglobin concentration and specially blood flow index were potential biomarkers to determine whether the animal was inherently resistant to sunitinib before treatment. For instance, higher values of blood flow index correlated with higher chances of being resistant to sunitinib.

Moreover, they monitored in real-time the three parameters during the whole treatment protocol, and saw clear differences between therapeutic and control groups. That showcased the suitability of diffuse optical methods as tools for assessing and linking hemodynamics changes to therapeutic effects during treatment.

The provided biomarkers might allow for an early identification of intrinsic or developed resistance of these tumors to sunitinib. In turn, this could help medical professionals make more informed and individualized decisions on which drug administer to a given patient, improving therapy effects, efficiency and even avoiding worsening the disease prospects.

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Miguel Mireles, Gabriela Jiménez-Valerio, Jordi Morales-Dalmau, Johannes D. Johansson, Mar Martínez-Lozano, Ernesto E. Vidal-Rosas, Valentí Navarro-Pérez, David R. Busch, Oriol Casanovas, Turgut Durduran, and Clara Vilches, "Prediction of the response to antiangiogenic sunitinib therapy by non-invasive hybrid diffuse optics in renal cell carcinoma", Biomed. Opt. Express 15, 5773-5789 (2024).

DOI: 10.1038/s41565-024-01657-7

# Challenges and solutions for using diffuse optics in brain injury

A recent article analyzes the complexity of using diffuse optics to monitor the brain when the head structure is altered, as in the case of an injury or a stroke. The study highlights how careless measurements may lead to wrong interpretation of the data, due to limitations of current techniques and a lack of knowledge about the underlying tissue. The article proposes new guidelines to improve measurement accuracy and reliability.

Hybrid diffuse optics is a technique that uses near-infrared light to measure tissue oxygenation and blood flow, which can be used to convey information about cerebral wellbeing. However, alterations in the brain structure and tissue composition can significantly affect optical signals in ways that do not reflect the brain assessments or that provide information about other tissues' clarity instead.

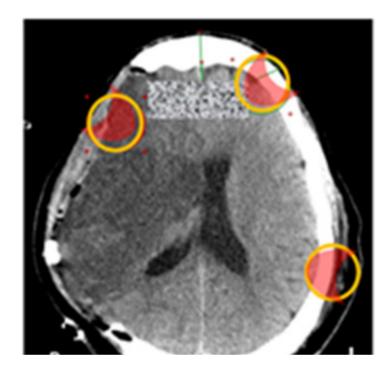
article new published recently **Neurophotonics**, ICFO researchers Susanna Tagliabue, Michal Kacprzak, Federica Maruccia and Jonas Fischer, led by ICREA Prof. Turgut **Durduran**, in collaboration with researchers from the Vall d'Hebron Hospital and Research Institute (VHIR), the team argues that heterogeneity in tissue composition, for example injuries or cerebrospinal fluid accumulations, can distort diffuse optical signals from their usual appearance on the healthy head or modify them according to its optical properties, making interpretation of results difficult. They identify the challenges of diffuse optics techniques in this difficult scenario, highlight features that can help other researchers in wiser data interpretation, and propose guidelines to improve the accuracy and reliability of measurements.

"even though the heterogeneity of the brain tissue complicates the interpretation of results, hybrid diffuse optical methods have great potential in such scenarios"

#### Investigating the signal alterations

To investigate the effects that tissue alterations have on diffuse optical signals, the authors performed measurements and computed tomography scans in three groups of patients with different pathologies, cerebral infarction, traumatic brain injuries, and brain hemorrhages, using them as case examples.

Researchers placed the probes on the patients' heads above different areas of interest that were selected using CT scans. The hybrid diffuse optical device employed in the study was built by the same researchers and comprises time-resolved spectroscopy, which measures hemoglobin concentration and tissue oxygen saturation, and



A CT scan of a brain with a stroke showing, in red, three different positions where near-infrared light interrogates the tissue, each with a different structure due to the injury.

diffuse correlation spectroscopy, which provides information on cerebral blood flow.

The article highlights the challenges of current optical methods in neuro-intensive care by detailing eight clinical case examples and analysing the diffuse optics signals quantitatively and qualitatively. Researchers conclude that even though the heterogeneity of the brain tissue complicates the interpretation of results, hybrid diffuse optical methods have great potential in such scenarios if correctly used. They propose guidelines to help improve the accuracy and reliability of measurements, including the need for stricter quality control protocols, more sophisticated devices and more advanced analysis methods, intending to promote a responsible

and effective use of diffuse optics in neurocritical care, recognizing its limitations and optimizing the techniques to obtain reliable information about brain physiology.

#### Reference:

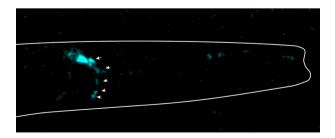
Neurophotonics, Vol. 11, Issue 4, 045005 (October 2024). DOI: https://doi.org/10.1117/1.NPh.11.4.045005

# Exploring synaptic engineering's role in understanding neural circuits

Prof. at ICFO Michael Krieg, together with Prof. Ithai Rabinowitch and Prof. Daniel Colón-Ramos have published in *Nature Reviews Neuroscience* a thorough review of synaptic engineering, an emerging approach to studying neural circuits, describing the current strategies and applications and sharing their visions about the future of the field.

The place where our behavior, memories and thoughts occur can be traced down to the microscopic gaps between the neurons, the synapses. In these spaces our neurons connect and communicate with their neighbors - or with those in farther regions of the brain-, by transmitting information from the sender, the presynaptic neuron, to the receiver, the postsynaptic neuron.

This transmission of signals allows the information to flow throughout the nervous system, forming complex circuits that are essential for all aspects of brain function and behavior. Understanding how synapses work and engineering new connections is crucial to decipher the complexities of brain



Fluorescence image with artificial synthetic connection. The arrows point towards presumptive synapses highlighted by the localization of synaptic light-generating enzymes.

and behavior, and to address various neurological conditions.

There are several methods to manipulate and study these neural circuits, but most of them often require complex hardware, invasive interventions, and high illumination intensities, potentially leading to side effects. In this context, synaptic engineering offers an alternative by focusing on single synaptic connections between neurons, without the need for real-time external monitoring or triggering. In synaptic engineering, researchers can create synthetic synaptic connections and introduce them to already existing neural circuits or, generate new circuits. By emulating a circuit, we can learn a lot more about how it works and its plasticity, explore new connections between neurons and even establish causal relations between the structure of those circuits and how they function.

Although relatively recent, synaptic engineering has seen successful development and validation especially in model organisms like the roundworm Caenorhabditis elegans, and increasingly in mammalian systems, proving itself as an effective method to study the structure and function of the neural circuits and explore new configurations.

### "optical synapses can be engineered, using light as a synthetic neurotransmitter"

#### An overview of synaptic engineering

Now **Prof. at ICFO Michael Krieg**, together with Prof. Ithai Rabinowitch from the Hebrew University of Jerusalem and Prof. Daniel Colón-Ramos from the Yale University School of Medicine, has published in **Nature Reviews Neuroscience** a thorough review of the existing synaptic engineering methods, their current applications and their visions about the future of the field. The article reviews the three main synaptic engineering strategies —electrical synapses—, chemical synapses and the neuropeptides, respectively - explaining their features and describing the differences in each one's dynamics, directionality and pre and postsynaptic signals.

The first strategy addressed is the engineering of electrical synapses, which focuses on the channels, known as gap junctions, that allow the crossing of ions and small molecules between neurons. This also constitutes the first demonstration of synthetic neuronal engineering. In vertebrates, these channels are composed mainly of a group of proteins known as connexins. By selectively expressing these proteins, researchers can manipulate and rewire the existing connections, allowing the exploration of how the information flows along the circuits.

The second approach is the engineering of optical synapses, where certain light-emitting enzymes located in the presynaptic neurons, the luciferases, are involved in the activation of specific light-sensitive ion channels in the postsynaptic neurons. Two experiments, one of which was designed by ICFO researchers, have demonstrated that these optical synapses can be engineered, using light as a synthetic neurotransmitter.

The third reviewed methodology is the introduction of foreign neuropeptides and their corresponding receptors for signalling, which allows the creation of new neuronal pathways and reconfiguring those already existing, helping to understand the process of modulation in the neural circuits.

#### **Promising potential for future applications**

Future directions for synaptic engineering include expanding the engineering methods, implementing on-off switching mechanisms, and exploring multiplexing —inserting multiple independent synthetic synapses simultaneously to reconfigure neural circuits.

article emphasizes, the engineering has a promising potential for several applications beyond constituting a useful tool to test hypotheses and address questions related to basic science. Using these methods, synthetic biology strategies could be applied to modify certain behaviors in organisms, for example, to detect and attack pathogens, or be used for treating damaged neural systems. The authors conclude by envisioning the possibility of developing large-scale synaptic engineering designs, which could contribute to a better understanding of more complex neural circuits.

#### Reference:

Rabinowitch, I., Colón-Ramos, D.A. & Krieg, M. Understanding neural circuit function through synaptic engineering. Nat. Rev. Neurosci. 25, 131–139 (2024).

DOI: https://doi.org/10.1038/s41583-023-00777-8

### **Joan Comella**

Director of Research, Innovation and Learning at the SJD Barcelona Children's Hospital and Director of the Institute of Research Sant Joan de Déu (IRSJD).

June 2024, ICFO

IRSJD is an important partnering institute in the Barcelona Medical Photonics Network (BMPN) and with a special collaboration through the Joint Lab with ICFO. What do you see as the strength of these strategic partnerships and how specifically does IRSJD's research benefit?

The Sant Joan de Déu Hospital is a reference hospital dedicated primarily to childhood diseases. In addition to basic care, we see diseases known as rare, minority, or complex, for which there is very little known and that other hospitals cannot or do not want to take on. Our vocation is to try to cure, diagnose, and understand these diseases. Although we have very good doctors and surgeons, sometimes we need new technology to understand the cause of these diseases.

In Barcelona we are lucky to have excellent research centers, like ICFO, who, precisely because of the very cutting-edge type of research they do and the technology they are developing, make excellent partners. They allow us to analyze our patients' complex cases from a new perspective, helping to generate new knowledge to understand the origins of these diseases. We agree to collaborate on topics of common interest, creating open innovation with multidisciplinary teams working towards solutions. The BMPN is a long-term alliance and it is not just important for IRSJD. At ICFO you do fantastic science that sometimes seems like magic to us. We can help this science have an impact on children's lives.



"We all need to raise awareness in society that science is important and that science changes lives, allowing us to imagine a much better future"

I understand that, as director of IRSJD, your goal is to continue and strengthen your institute's "pursuits of global excellence with a tangible impact on enhancing the diagnosis and treatment of disease in its field". How are you doing this?

It always comes down to children who have very serious rare or minority diseases for which industry is not prepared to make a large and long-term investment. These are cases where we must try to contribute through patient care and research. We belong to 95% of the European networks of pediatric hospitals and coordinate two of them. We are also collaborating with hospitals in the United States. As an international collaborative network, if there is a discovery in one of these centers, this can quickly

be incorporated into the rest of those centers. There are also increasingly some pharmaceutical companies that are betting on these therapies and we have to help them so that they can be developed through clinical research.

But I insist that when it comes down to understanding diseases to seek these diagnoses and treatments, we need alliances with the most basic research centers

Having held leadership positions in hospitals, research facilities, research-related societies, foundation and associations in Catalonia, Spain, and Europe, you are uniquely poised to assess the relative strengths of our research ecosystem here in Spain. How are we doing?

The evolution of science in Spain in the last 40 years has been a fascinating success story. We have gone from not being on the map, to systematically appearing in positions among the top 15 countries in the world. In addition to publications, Spain is a true international power doing clinical research, second in the world after the US in doing clinical trials in some cases. Catalonia has rates of attracting competitively funded projects that are among the highest in Europe. This is the good news.

Spain has proven less successful at converting good science into an economic return. We are much worse in innovation, but we have a good basis to get better, because the science is high quality. We must also be able to strengthen the private sector with the generation of spin-off companies and by demanding that large industrial companies base their growth on innovation and scientific knowledge. These aren't negative aspects, I rather see them as opportunities.

Then we have the problems, real problems that are preventable, though. The main one is bureaucracy. It is increasingly difficult for us to be able to carry

out our work due to documentation that often does not add any value. Bureaucracy and regularization are killing science. Our regulation in Spain should not be higher than that of the countries with which we must compete. We have to explain politicians that we need their support, we need them to trust us establishing mechanisms that allow us to compete on equal terms with the pioneering countries in science in the world. Otherwise, we are shooting ourselves in the foot!

You have demonstrated throughout your career that there are many roles a scientist can play to have an impact. What advice would you give to ICFOnians who would like to see research improve the lives of people.

There is an argument that says that it is not rich countries that invest in science, but rather countries that have invested in science that become rich. To convert science to wealth and therefore sustain our welfare system and future generations, we must first be able to convert science into something tangible, which changes people's lives. This can be monetized, creating jobs and will happen if we are able to explain science's role in this process to society.

Vote for political options that are committed to carrying out research and innovation, the model of economic sustainability. We all need to raise awareness in society that science is important and that science changes lives, allowing us to imagine a much better future.

#### **Trustees**





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