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Atomically-precise texturing of hexagonal boron nitride nanostripes

Ali K, Fernández F, Kherelden MA, Makarova AA, Píš I, Bondino F, Lawrence J, de Oteyza DG, Usachov DY, Vyalikh DV, García de Abajo FJ, Abd El-Fattah ZA, Ortega JE and Schiller F Advanced Science 8, 2101455 (2021)

Monolayer hexagonal boron nitride (hBN) can be epitaxially grown on vicinal Rhodium (Rh) surfaces using a Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width. The electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since the discovery of graphene, a wide diversity of atomic-layer-thick, two-dimensional (2D) materials with varied properties have emerged. Of particular interest are those that exhibit semiconducting behaviour, such as hexagonal boron nitride (hBN). hBN is isoelectronic to graphene and has also a honeycomb lattice formed by alternating nitrogen and boron atoms, but in contrast to the semimetallic graphene, its band structure presents some characteristics that makes it particularly attractive for applications in microelectronics, either alone or in combination with other 2D materials, such as graphene. Furthermore, hBN is structurally robust and chemically inert. Although hBN flakes may be obtained by mechanical exfoliation of bulk crystals, a single hBN monolayer can be readily synthesized on metal surfaces, leading to structurally and chemically robust substrates that frequently exhibit nanoscale patterns. This makes hBN-covered metals excellent platforms to achieve functional interfaces with atoms, molecules, and aggregates, as well as to develop hybrid



2D materials, such as twisted van der Waals stacks or 2D heterostructures. The latter hold a great potential for atomically thin circuitry, such as superstructures formed with isostructural graphene, which are optimal to engineer gaps and doping, as well as to tune and enhance spin scattering.

However, this is easier said than done. Exploiting fine hBN-based nanostructures requires structural guality down to the atomic scale and precise lateral nano-structuration and integration with other twodimensional materials, which lies beyond current lithographic capabilities. The bottom-up vapour growth is the alternative, which also works for 2D hybrids, although general procedures to control shape, size, and spatial order of surface phases are still lacking.

Lateral nanopatterning of hBN through epitaxial growth. The concept of the study of vicinal hBN/Rh interfaces is presented. CVD growth of hBN induces periodic (111)/(337) faceting of the Rh substrate. The hBN monolayer uniformly coats the faceted substrate, defining an effective lateral hBN/Rh heterointerface with periodic surface potential texturing. Using commercial Rh(111) films, one could exploit such chemical and electronic modulation of hBN to explore phonon-polariton THz excitations, selective growth of optically-active molecules, and vertical stacking with other 2D materials.

Now, a team of researchers from DIPC and other institutions has found a working disruptive approach: imprinting the lateral pattern of an atomically stepped one-dimensional template into a hBN monolayer. The researchers demonstrate the bottom-up synthesis of nanostriped hBN heterostructures with atomically sharp interfaces. The idea was to follow the standard chemical vapor deposition growth route, using rhodium (Rh) vicinal surfaces as one-dimensional (1D) templates. In practice, hBN was epitaxially grown on Rh surfaces using an Rh curved crystal for a systematic exploration, which produces a periodically textured, nanostriped hBN carpet that coats Rh(111)-oriented terraces and lattice-matched Rh(337) facets with tunable width.

Thus, a 1D lateral hBN (111)/(337) heterostructure arises, featuring defect-free boundaries and significant band offsets. The resulting electronic structure reveals a nanoscale periodic modulation of the hBN atomic potential that leads to an effective lateral semiconductor multi-stripe.

Since size tunability of phases can be gained by selecting the Rh vicinal plane, a variety of new possibilities are opened by this discovery. For example, the hBN (111)/(337) faceted system could be used as a model platform to mould and probe 1D phonon-polariton excitations in the THz regime, to achieve selective growth of atoms, aggregates, and molecular adsorbates for organic optoelectronics and catalysis, or to tailor the 3D stacking with other 2D materials, such as graphene.





Hexagonal boron nitride nanostripes can be grown on vicinal rhodium surfaces

How aromatic are molecular nanorings? The case of a six-porphyrin nanoring

Casademont-Reig I, Guerrero-Avilés R, Ramos-Cordoba E, Torrent-Sucarrat M and Matito E *Angewandte Chemie International Edition 60, 24080* (2021)

Aromaticity is a property of cyclic structures with delocalized electrons, which give rise to some intriguing molecular properties: increased stability, certain geometrical features such as planarity, and exhibit a ring current under the presence of an external magnetic field. A molecule's aromatic character is typically verified experimentally using nuclear magnetic resonance (¹H-NMR), as the protons oriented toward the center of the ring are affected by the presence of the ring current in aromatic compounds.

Annulenes are monocyclic hydrocarbons that contain the maximum number of non-cumulated double bonds. They have the general formula C_nH_n (when n is an even number) or C_nH_{n+1} (when n is an odd number). Benzene is the smallest neutral annulene that presents π -conjugated aromaticity because it satisfies the Hückel rule, which states that molecules $4n+2\pi$ electrons are aromatic. This rule helps to predict the aromaticity of relatively small annulenes, but it breaks for large annulenes. It is well established that large annulenes suffer out-of-plane distortions and exhibit a poor overlap between π orbitals, thus favoring non-symmetric conformations that are much less aromatic. The larger the annulene, the less aromatic the molecule is expected. For this reason, it is difficult to find large aromatic macrocycles. Geometrical constraints are actually imposed in some large macrocyclic structures with the hope of preserving conjugation, aromaticity, and quantum coherence.

Anderson and co-workers have recently synthesized and analyzed the aromaticity of a six-porphyrin nanoring (c-P6·T6) in four different oxidation states (c-P6·T6, c-P6T6⁴⁺, c-P6·T6⁶⁺, and c-P6·T6¹²⁺), concluding from ¹H-NMR and computational analyses that c-P6·T6 and the c-P6·T6¹²⁺ are nonaromatic, whereas c-P6·T6⁴⁺ and c-P6·T6⁶⁺ are, respectively, antiaromatic and aromatic. c-P6·T6⁶⁺ is thus one of the largest aromatic rings ever synthesized.

A team of researchers from DIPC demonstrates that the aromaticity of these large macrocycles is questionable. They provide compelling evidence that the conclusions are highly sensitive to the simulation employed, which should avoid the so-called delocalization errors. Using density functional approximations that minimize the delocalization error, they find that the main reason behind the absence of an aromatic ring current in these nanorings is the low delocalization in the transition from the porphyrins to the bridging butadiyne linkers, which disrupts the overall conjugated circuit. They also demonstrate that ¹H-NMR are not infallible probes of aromaticity and, therefore, the ¹H-NMR experimental evidence should not be blindly trusted.



Figure 1. Methods with a low percentage of Hartree-Fock exchange suffer from delocalization errors and wrongly reflect the aromaticity of the nanoring structure.



None of the large nanorings can be considered aromatic, and the quest for large aromatic nanorings should be continued. These results highlight the importance of choosing a suitable computational method to study large conjugated molecules and the appropriate aromaticity descriptors to identify the part responsible for the loss of aromaticity.



Density functional approximations can suffer from delocalization errors that artificially increase the aromaticity of the molecule

Figure 2. Methods with a low percentage of Hartree-Fock exchange give a spuriously enhanced chemical shielding that suggests the presence of a ring current.

Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection

Buchs G, Marganska M, González JW, Eimre K, Pignedoli CA, Passerone D, Ayuela A, Gröning O and Bercioux D Applied Physics Reviews 8, 021406 (2021)

Terahertz (THz) radiation is all around us. For example, this page emits blackbody radiation mainly in the THz region (broadly from 0.3 THz to 30 THz). Because terahertz radiation begins at a wavelength of around one millimeter and proceeds into shorter wavelengths, it is sometimes known as the submillimeter band, and its radiation as submillimeter waves, especially in astronomy.

This band of electromagnetic radiation can be regarded either as microwave radio waves or far-infrared. The technology for its generation and manipulation is in its infancy; that is why engineers talk about the THz gap (in this case, from 0.1 to 10 THz). One of the reasons is that THz radiation from traditional microwave sources is usually too weak to have any measurable impact on the properties of materials.

The situation drastically changed at the beginning of the 2000s, when the technique of optical rectification with phase matching in crystals lacking inversion symmetry such as lithium niobate was developed. This technological breakthrough enabled the development of table-top sources of singlecycle THz pulses with field strengths comparable to the intrinsic field strength in a wide range of strongly correlated materials. Consequently, it became possible to modify their intrinsic fields to engineer new dynamic states of materials.

In condensed matter physics and in general, THz radiation is an efficient tool to investigate a multitude of low-energy excitations existing in the THz region. Important examples are resonances of phonons and plasmons (collective lattice and electron vibrations, respectively), spins, intersubband transitions (subbands are electronic energy bands formed in quantum wells, in which the electrons are confined in two directions), excitons (bound electron-hole pairs), macro-molecular vibrations and molecular rotations.

THz radiation can penetrate most dielectric materials non-invasively, opening the way for numerous possible applications in the fields of medicine, security, chemical spectroscopy, and data transmission, notably in the framework of the future 6, G cellular network. This is why photodetection and emission in the THz regime have recently attracted much attention from fundamental and applied research communities.



or a broadband terahertz detector

The proposed device is largely unaffected by temperatures up to 100 K, making carbon nanotube guantum dots with broken symmetries a promising platform to design tunable THz detectors that could operate at liquid nitrogen temperatures

A team of researchers, including the theorists from DIPC - Dario Bercioux & Andrés Ayuela - have proposed a theoretical scheme for a fully tunable THz detector based on carbon nanotubes. Specifically, using numerical simulations and scanning tunnelling spectroscopy, Buch et al. show that breaking simultaneously various symmetries in metallic nanotube guantum dots of arbitrary chirality strongly relaxes the selection rules in the electric dipole approximation removes energy degeneracies. This leads to a richer set of allowed optical transitions spanning frequencies from 1THz to several tens of THz for a ~10nm guantum dot. The researcher team proposed a terahertz detector device based on a metallic singlewalled carbon nanotube quantum dot defined by artificial defects based on these findings. The operating regimes range from a high-resolution gate-tunable THz sensor to a broadband THz detector, depending on its length and contacts transparency. Their calculations indicate that the device is mainly unaffected by temperatures up to 100K, making carbon nanotube quantum dots with broken symmetries a promising platform to design tunable terahertz detectors that could operate at liquid nitrogen temperatures.



Proposed device to be used as either a high-resolution gate-tunable terahertz sensor

A dissolution model of alite coupling surface topography and ions transport under different hydrodynamics conditions at microscale

Chen J, Martin P, Xu Z, Manzano H, Dolado JS and Ye G Cement and Concrete Research 142, 106377 (2021)

A cement is any of various substances used for bonding or setting to a hard material. A popular one, Portland cement, is a mixture of calcium silicates and aluminates made by heating limestone (CaCO₃) with clay (that contains aluminosilicates) in a kiln. The product is then ground to a fine powder. When Portland cement is mixed with water, it sets in a few hours and then hardens over a longer period of time due to the formation of hydrated aluminates and silicates.

Portland cement contains four main components: Alite, Belite, calcium aluminate and calcium aluminoferrite. Alite (tricalcium silicate) is the major and characteristic mineral phase. The thermodynamics and kinetics of Alite hydration has being studied for more than 100 years, still, it is not completely understood.

In the past decades, many hydration models were proposed for the hydration process of Portland cement. These models favored either particle reaction kinetics or integrated reaction kinetics, and focused on the dissolution of cement grains, but individual chemical components were not considered explicitly.

Some models have been proposed in order to predict the dissolution of alite. Some take the vector approach, with arbitrarily chosen hydration kinetics to calculate the hydration rate and convert the amount of hydration product into a volumetric term; however, thermodynamics and ions transport are not taken into account. Others proposed an analytical model to simulate the dissolution of alite. This model described the etch pit formation on the surface of Alite, and calculated the corresponding dissolution rate, but diffusion and chemistry were not considered.

In 2109, Pablo Martin, Hegoi Manzano and Jorge S. Dolado [Pablo Martin, Hegoi Manzano and Jorge S. Dolado (2019); Advanced Theory and Simulations doi: 10.1002/adts.201900114] proposed a Kinetic Monte Carlo model (KMC) at the nanoscale, which could simulate the dissolution of crystals not only in dilute solutions but also at close-to-saturated conditions. It simulated all dissolution mechanisms at nano/ micro scales. Now, an integrated model is proposed to simulate the dissolution of Alite under different hydrodynamic conditions at microscale, combining KMC with the Lattice Boltzmann method (LBM) and the concept of diffusion boundary layer (DBL)



Influence of the flow rate on the dissolution rate of Alite for solutions having different initial calcium hydroxide concentrations. Comparison between the model and available experiments.

All aspects of the dissolution process are incorporated in the new model. The dissolution of Alite itself is modelled with KMC; two multiple-relaxation-time LBM models are used, one to simulate the flow and the other for the transport of ions. The solid-liquid interface is considered using an adapted DBL to calculate the concentration gradient and the dissolution flux. The model is validated with experimental data from literature.

The simulation results show good agreements with published results. At higher initial concentration, the simulation shows a greater dissolution rate than the experimental data. The plateau value is reached at saturated condition, which indicates that the simulation model can be used to predict the dissolution rate of Alite under extreme hydrodynamic conditions, i.e., high flow rates.

For a complete study on the dissolution of cement particle, it is necessary to involve all of its components individually and simultaneously. This new model for Alite provides a good start point for the simulation of the other cement components.



A integrated dissolution model is proposed to deal with different hydrodynamics conditions, coupling surface topography and ions transport

Synthetic conjugates of ursodeoxycholic acid inhibit cystogenesis in experimental models of polycystic liver disease

Caballero-Camino FJ, Rivilla I, Herraez E, Briz O, Santos-Laso A, Izquierdo-Sanchez L, Lee-Law PY, Rodrigues PM, Munoz-Garrido P, Jin S, Peixoto E, Richard E, Gradilone SA Perugorria MJ, Esteller M, Bujanda L, Marin JJG, Banales JM and Cossío FP *Hepatology 73*, 186 (2021)

Polycystic liver diseases (PLDs) are genetic disorders characterized by progressive development of symptomatic biliary cysts. Current surgical and pharmacological approaches are ineffective, and liver transplantation represents the only curative option. Ursodeoxycholic acid (UDCA) and histone deacetylase 6 inhibitors (HDAC6is) have arisen as promising therapeutic strategies, but with partial benefits. Here, we tested an approach based on the design, synthesis, and validation of a family of UDCA synthetic conjugates with selective HDAC6i capacity (UDCA-HDAC6i). According to our results, these UDCA-HDAC6i conjugates open a therapeutic avenue for PLDs.

Epigenetic enzymes have emerged as very promising therapeutic targets in medicinal and biological sciences. PLDs do not have any pharmacologically efficient treatment and constitute a heterogeneous group of genetic disorders characterized by progressive development of multiple fluid-filled biliary cysts (>10), which are the main cause of morbidity. Within this context, based on previous biological results, we decided to combine the structural and electronic features of UDCA with a spacer and a Zn-binding chelating group to generate by chemical synthesis a new family of conjugates able to inhibit histone deacetylases, especially cytoplasmic HDAC6.

Our chemical synthesis of the UDCA-HDAC6i molecules started with the coupling reaction of UDCA with amines to yield amide esters. Cleavage of the ester groups and in situ reaction with hydroxylamine or ortho-phenylendiamine permitted the isolation and characterization of UDCA-hydroxamates and ortho-aminophenylenamides shown in Figure 1 (a).

The potential HDAC6 inhibitory capacity of this family of UDCA synthetic conjugates was first evaluated in silico with a docking model (Figure 1 (b)). Significant binding affinities to HDAC6 were predicted for some of these compounds. Interestingly, three compounds oriented the hydrocarbon skeleton of UDCA toward the same region of the protein surface. We decomposed the total binding energy of each synthetic derivative into the contribution of different descriptors (i.e., hydrogen bonds, van der Waals and Coulombic interactions) to the overall score. Importantly, the contribution of UDCA to the final binding energy of UDCA-HDAC6i #1, #2, and #9 was approximately one-third of the total value, and was mainly integrated by van der Waals interactions and hydrogen bonds established by the two hydroxyl groups of the steroid skeleton of the BA.



This novel family of histone deacetylase inhibitors opens a therapeutic avenue for polycystic diseases and other pathologies in which these enzymes play a significant role

This family of novel HDAC6is was tested in different biological assays and it was concluded that UDCA-HDAC6i #1 inhibited hepatorenal cystogenesis in vivo, improved ciliogenesis in cystic cholangiocytes, and inhibited their hyperproliferation. These therapeutic effects are superior to the simple sum of the individual or combined effects of its constituting pharmacologically active elements. These UDCA synthetic conjugates have preferential targeting to the liver through specific bile acid and organic cation transport properties and are highly concentrated into the enterohepatic circulation. These particular features make UDCA-HDAC6i molecules especially promising for the treatment of hepatic and gastrointestinal disorders where HDAC6 inhibition is considered a therapeutic target, such as acute liver failure, hepatocellular carcinoma, cholangiocarcinoma, pancreatic cancer, or colon cancer, among others, highlighting the high degree of translational potential of this family of chemical entities.



Figure 1. (a) Chemical structures of the UDCA-HDACi conjugates designed and synthetized for testing in animal models of polycystic liver diseases. (b) Optimized poses in docking experiments on human HDAC enzymes.



Cover of Hepatology highlighting the therapeutic potential of our UDCA-HDACis.

Sensitivity of a tonne-scale NEXT detector for neutrinoless doublebeta decay searches

The NEXT collaboration, Adams C et al Journal of High Energy Physics 8, 164 (2021)

NEXT-HD will optimize the ability to separate signal from backgrounds in terms of a topological signature. Thus its name, HD which refers to the high definition of the topological signature. In addition, NEXT-HD will deploy an excellent energy resolution (around 0.5 % FWHM at the relevant of the decay) and a very low radioactive budget. The combination of all these features, together with its large mass will increase the sensitivity to bb0nu processes by at least one order of magnitude with respect to NEXT-100, resulting in a large discovery potential.

The NEXT international collaboration formed and led by Ikerbasque Professor Gomez-Cadenas JJ, is developing the technology of High-Pressure Xenon gas Time Projection Chambers (HPXe) to search for neutrinoless double beta decay processes (bb0nu) in xenon. The detection of such events, in which an atom of the isotope Xe-137 decays into Ba-137, emitting two electrons and no neutrinos, would signal that the neutrino is its own antiparticle, a major discovery, which could explain, in particular, the cosmic asymmetry between matter and antimatter.

The NEXT collaboration is developing the HPXe technology in incremental steps. The initial prototype, NEXT-DEMO, with 1 kg of xenon, was followed by the successful NEXT-White demonstrator (10 kg of xenon), which has demonstrated the powerful topological signature (discussed below) low radioactive budget and excellent energy resolution of the technology. The NEXT-100 detector, deploying 100 kg of xenon is currently being commissioned at the Canfranc Underground Laboratory. NEXT-100 will reach a sensitivity to bbonu processes competitive with the best experiments currently in operation. In particular the experiment can make a discovery if the lifetime of the process is up to 1026 years.

Current data from oscillation experiments, however, suggest that the lifetime of bb0nu processes may be one order of magnitude larger (1027 years). If NEXT-100 does not find a signal, the next step is to build a detector with ten times more mass, while keeping the backgrounds from radioactive and cosmological events to essentially negligible levels.



The NEXT detectors are able to reconstruct the trajectory of the electrons moving in the chamber, measuring the energy of the end-points of the track. The signal (left) is characterized by high energy deposition in both end of the track (corresponding to two electrons), while the background only deposit energy in one of the ends. As shown in the figure, this allows a very effective separation between both types of events.

NEXT-HD will deploy an excellent energy resolution (around 0.5 % FWHM at the relevant of the decay) and a very low radioactive budget

The selected paper describes the main features and expected performance of such a detector, call NEXT-HD, which is currently being planned, and could start operations in about 5 years. Central to the large discovery potential of the NEXT detectors is their ability to discriminate the signal produced by bb0nu events (two electrons) from the spurious events produced by backgrounds, which result in single electrons, as illustrated in the figure.



Chemical tuning of exciton versus charge-transfer excited states in conformationally restricted arylene cages

Lewis TN, Tonnelé C, Shuler WG, Kasun ZA, Sato H, Berges AJ, Rodriguez JR, Krische MJ, Casanova D and Bardeen CJ Journal of the American Chemical Society 143, 18548 (2021)

Materials design for organic electronics requires to go beyond the molecular properties and address the solid-state properties instead, i.e., the collective behavior of multiple units in active layer thin films that depends on the supramolecular arrangement and nature of the intermolecular interactions. One major challenge thus lies in understanding and controlling these interactions, which can give rise to new emergent properties of the assembly.

Bulk solid-state samples, where disorder and the large number of interacting molecules make difficult a first-principles description, are not the best place to start. This complexity motivated the synthesis and study of discrete multiunit assemblies of conjugated molecules with controlled chemical and geometrical structures and restricted conformational freedom that can be purified and studied in isolation, for example, in dilute solution. Examples of such conjugated assemblies include donor-bridge-acceptor molecules, bichromophores and dendrimers. In these supermolecules, covalent linker groups define both the number and connectivity of the interacting conjugated subunits.

Yet, even in these smaller systems, the conformational flexibility of covalent assemblies can lead to multiple configurations that have different subunit interactions and, consequently, different electronic states and dynamics. In many cases, the conformational freedom of these covalent assemblies complicates their interpretation as structurally well-defined model systems. Additionally, although we would like to assume that the linker is inert, the truth is that a large body of work says otherwise, showing that it can play an important role in facilitating charge and energy transfer. Any new architecture that would limit conformational freedom and help establish the actual role of the linker would be, thus, most welcome.

In a combined theoretical/experimental study, a team of researchers used a novel cage architecture to demonstrate how chemical tuning can allow to precisely control the nature of the excited states. In particular, they reported the synthesis and photophysics of two triple-stranded thiophene based cages differing in the nature of the aromatic cap, namely benzene and triazine, that links the individual branches of the cage at both top and bottom. This strategy enables improved control of both molecular spacing and orientation as it provides two points of attachment for each conjugated subunit, bringing the assembly closer to crystalline order. Furthermore, the capping group acts as a constant structural element while providing chemical tunability that can be used to actively modify the electronic structure of the assembly.



Schematic of capped bithiophene cage. Dependent on the capping unit used to lock the bithiophenes into the cage conformation, it can undergo charge transfer or exciton delocalization.

Chemical tuning of novel multichromophoric cage architecture enables engineering of excited states nature

Combining steady-state and time-resolved spectroscopies and (time-dependent) density functional theory calculations, they showed that an inert benzene cap supports through-space interchromophore Coulomb interaction generating a neutral Frenkel H-type exciton state that can undergo rapid intersystem crossing (ISC), in turn associated with a strongly decreased fluorescence. On the contrary, using a triazine cap allows the formation of low-lying charge transfer states that can avoid ISC and enhance the fluorescence quantum yield.

The ability to create different nanoscale heterostructures while retaining the overall morphology provides an unprecedented opportunity to tune the properties of these discrete assemblies. These results provide a new route toward structurally well-defined multichromophoric assemblies whose excited states can be rationally designed using the tools of organic synthesis and computational chemistry. As this architecture is in principle scalable, it may provide a path to systematically bridge the gap between molecular properties and solid-state material performance.



The BACCO simulation project: exploiting the full power of largescale structure for cosmology

Angulo RE, Zennaro M, Contreras S, Aricò G, Pellejero-Ibañez M and Stücker J Monthly Notices of the Astronomical Society, 507, 5869 (2021)

This paper presents a new suite of supercomputer simulations of the nonlinear gravitational interactions of matter in the Universe. These calculations were then used to train artificial intelligence algorithms to generate millions of new synthetic universes. These predictions will be used to interpret observations made by the forthcoming ESA's satellite mission "Euclid".

Over the last 20 years, our understanding of the Universe has grown tremendously. There is a relatively simple model, referred to as LCDM, which can explain the main observed properties of the Universe - from its infancy state to the present-day structure. There are, however, major unanswered guestions in this model. For instance: the nature of dark energy that causes an accelerated cosmic expansion, the origin of the seeds from which structure emerged, and the properties of "dark matter" - the most abundant form of mass in the Universe.

In the upcoming years, a new generation of telescopes - located in different places around the world and in outer space - will map the distribution of dark matter, gas, and millions of galaxies. This will offer the possibility of profound discovery. We will be able to carry out tests where perhaps Einstein's General Relativity will break down, a new fundamental particle will appear, or where we would find a clue to explain the accelerated cosmic expansion.

The goal of this paper is to increase the chances for such discoveries by developing a new generation of supercomputer simulations mimicking large regions of the Universe. These simulations - designed to match the new telescopes' observations - have generated hundreds of virtual universes which can be compared to the real one. In each of these computer-generated universes, various cosmic ingredients are varied: the strength of gravity; the processes that govern the formation of galaxies; and the amount of massive neutrinos, dark matter, spatial curvature.

Cosmological simulations typically need tens of thousands of computer cores and millions of hours in computing time, thus it is only possible to carry them out for a small number of parameter sets. To avoid this limitation, we have used existing simulations to train neural networks which are able to create new predictions in unseen parameter sets in under one second of computer time. This enables a thorough exploration of the cosmological parameter space, finding the combination that best describes the observed Universe.



The projected mass density field at the present day, as predicted by one of the eight simulations in the BACCO suite. Each image corresponds to a 100 million light-years deep projection employing a phase-space interpolation method. Top, middle, and bottom panels progressively zoom onto regions 6, 1, and 0.4 billion light-years across.

These tools are currently being incorporated in the data analysis pipeline of the "Euclid" mission. "Euclid" is a satellite telescope developed by the European Space Agency with an expected launch in February 2023. Euclid will detect around 10 billion astronomical sources with which it will map the distribution and evolution of dark matter in over a third of the sky. This will be the most detailed map of the cosmos ever made.

By combining Euclid's data with supercomputer simulations and machine learning, it will be possible to find signatures that distinguish between competing theories for, e.g., dark matter or for the origin of the Universe. We will also be able to investigate whether we can explain the distribution of galaxies and matter within our current galaxy and structure formation theories and whether it will be necessary to include new ingredients, or even change the laws of physics!



Supercomputer simulations are needed to understand the nonlinear processes that give rise to complexity in the universe

Van der Waals driven anharmonic melting of the 3D charge density wave in VSe₂

Diego J, Said AH, Mahatha SK, Bianco R, Monacelli L, Calandra M, Mauri F, Rossnagel K, Errea I and Blanco-Canosa S Nature Communications 12, 598 (2021)

A charge density wave (CDW) is a many-body state of matter characterized by the static modulation of conduction electron density together with the corresponding crystal lattice distortion. Phase transitions to this electronic charge ordering state have been reported in many low dimensional materials at low temperatures, in which there is a big debate on the interplay with the superconducting phase. Indeed, the origin and stabilization of this phenomenon is still an underdebate topic, especially in high dimension systems, as it is the case of quasi-2D layered transition metal dichalcogenides (TMDs). TMDs are particularly interesting because they are the first crystalline structures where 3D CDWs were discovered. Their high dimensionality may imply that the one-dimensional Fermi surface nesting scenario may not be entirely suitable, acquiring electron-phonon interaction particular importance.

The CDW transition of some TMD compounds like 2H-NbSe2 and 1T-TiSe2 has been found to be characterized by the softening of a low energy acoustic phonon branch at the critical wave vector, which goes to zero frequency at the transition temperature. In this work we study this behaviour both experimental and theoretically in the 1T phase of VSe₂ which develops a complex 3D incommensurate pattern in its CDW phase with a $q_{CDW} = (0.250 - 0.3)$ r.l.u CDW wave vector. Motivated by the good results obtained, we finally analyze the origin of the CDW in VSe₂.

This work is the result of a cooperative work between experimentalists and theoreticians. Our highresolution inelastic x-ray scattering experiments have shown for the first time that the CDW transition in this compound is characterized by the collapse at 110K of a low energy acoustic mode. This behavior has been ratified by our ab initio anharmonic phonon calculations with the stochastic self-consistent harmonic approximation (SSCHA), a variational method that fully accounts for non-perturbative anharmonic effects. These theoretical calculations have pointed to anharmonicity as the responsible for stabilizing the 1T phase of VSe₂ at high temperatures. Indeed, remarkably our theoretical phonons are only comparable to experimental results if interlayer weak van der Waals corrections are considered. Definitely, both anharmonic effects and van der Waals interactions between neighbouring VSe₂ layers are vital to melt the CDW.

The dominant role of van der Waals forces here may be attributed to the out-of-plane nature of the CDW, which modulates the interlayer distance. This is not the case in 2H-NbSe₂, where the bulk and monolayer transition temperatures seem to be similar as reported experimentally by Ugeda et al. and theoretically by Bianco et al. This line of thinking is consistent with the enhancement of the CDW in monolayer VSe₂ since the out-of-plane van der Waals interactions are absent in this case.



Figure 1. Momentum dependence of the frequency represents the acoustic mode that is silent in IXS. CDW region.

Definitely, both anharmonic effects and van der Waals interactions between neighbouring VSe₂ layers are vital to melt the CDW



Finally, our work sheds light on the crucial role of the EPI and nesting mechanism in the formation of the charge modulated state. We conclude that the electron-phonon interaction is the main driving force of the CDW transition in 1T-VSe₂ despite the presence of nesting at the critical wave vector. This conclusion is supported by the wide softening in momentum space observed in the experiments, in addition to the calculated strongly momentum dependent electron-phonon linewidth peaking at the critical wave vector, and the weaker dependence on the wave vector of the susceptibility.





Figure 2. Temperature dependence of the energy of the ω_1 and ω_2 branches at 150 K. The anharmonic of the ω_1 CDW driving branch and the anharmonic phonon dispersions of the acoustic modes obtained theoretical frequencies obtained with and without van at 150 K are plotted as solid lines. The gray line der Waals corrections. The shaded area defines the

Figure 3. Electron-phonon interaction vs Fermi surface nesting. (a) Calculated harmonic phonon spectra of 1T-VSe₂ along (h 0 -1/3) r.l.u. Only acoustic modes are shown. The gray line denotes the mode silent in IXS, which is labeled as ω 3 here. (b) Phonon linewidth (full width at half maximum) given by the electron-phonon interaction for the same modes. (c) Real part of the non-interacting susceptibility, χ_0 , as well as the nesting function, ζ , at the same wave vectors. (d) Ratio between the full width at half maximum given by the electron-phonon interaction and the nesting function.

Complex plasmon-exciton dynamics revealed through quantum dot light emission in a nanocavity

Gupta SN, Bitton O, Neuman T, Esteban R, Chuntonov L, Aizpurua J and Haran G Nature Communications 12, 1310 (2021)

Light emitted by quantum dots coupled to plasmonic nanocavities and the underlaying dynamics of the excited states in the system can be strongly affected by dark excitonic states in the quantum dots, as recently revealed by a combined theory-experiment study of the system scattering spectrum, photoluminescence and two photon correlations.

The manipulation of optical transitions in semiconductor materials enables new possibilities to engineer the absorption and emission of light, with applications such as the design of more energetically efficient light sources. For example, discrete atom-like excitonic states at optical energies are obtained by fabricating structures of nanometric size in all three dimensions, so-called quantum dots.

The properties of guantum dot excitonic states are not intrinsic, but can be modified by the surrounding environment. A particularly large modification of the optical properties of quantum dots can be produced when interacting with metallic nanocavities (sketch in top panel of the figure). These nanocavities present plasmonic resonances produced by collective oscillations of the free electrons in the metal, and are able to localize electromagnetic energy into very small volumes, leading to very efficient coupling with excitons. A typical effect of plasmons is to induce an increase of the exciton radiative rate, of interest in the design of fast and efficient light sources. For very intense exciton-plasmon interaction, the regime of strong coupling is achieved, characterized by the emergence of new polaritonic modes that combine the properties of the excitons and those of the plasmonic resonances.

The study of emission dynamics in quantum dots usually focuses on bright excitonic states that radiate photons efficiently and can be easily excited by a laser, while difficult-to-excite dark excitons are often ignored. In this work, DIPC researchers use a cavity electrodynamics framework to show that a dark excitonic state in a quantum dot can play a key role in the dynamics of a coupled plasmonic cavityquantum dot system, which allows for explaining several unexpected experimental findings by colleagues at the Weizmann Institute of Science in Israel (bottom panels in the figure). The dark exciton does not significantly affect the light scattered or absorbed at the energy of the illumination laser, but it does strongly modify the photoluminescence spectrum as well as the behaviour of the two-photon correlations, a key property to identify the emission of non-classical light. These results thus emphasize the importance of considering both bright and dark excitons to fully understand the optical response of complex nanoscale systems formed by plasmonic nanostructures coupled to one or a few quantum dots.



the presence of a dark exciton in the quantum dot.



Light emission of quantum dots in plasmonic antennas reveals a complex excitonic dynamics

Coupling of a guantum dot and a plasmonic nanocavity. Top: sketch of the system considered, where a guantum dot interacts with a plasmonic nanocavity. In the experimental realization a bowtie configuration is used with two triangular nanoparticles separated by a very narrow nanogap. The system is close to the strong coupling regime. Bottom left: calculated scattering spectra (light emitted elastically at the frequency of the illumination) and photoluminescence, PL, spectra (light emitted inelastically at lower energy than the illumination). Bottom right: measured scattering and PL spectra. In both theory and experiments the spectral shape of the scattering is very different to that of the PL, showing spectral peaks of different width and at different positions, attributed to

Topological phase transition in chiral graphene nanoribbons: from edge bands to end states

Li J, Sanz S, Merino-Díez N, Vilas-Varela M, Garcia-Lekue A, Corso M, G de Oteyza D, Frederiksen T, Peña D and Pascual JI Nature Communications 12, 5538 (2021)

In the last decades, a mathematical description of symmetries in nature called topology has been applied to describe and predict new electronic and magnetic properties of materials. A very simple aspect of topology connects a symmetry in the atomic structure of a crystal with a class of materials. Many materials that we know or use in current technology (silicon, diamond, gallium arsenide, etc.) belong to a topological class called trivial, meaning standard, and behave as normal semiconductors or insulators.

Novel materials with "anomalous" topology (technically called non-trivial) can be fabricated with advanced techniques of material science, which achieve control of their structure with atomic precision. For such materials, mathematical models predict "exotic" properties that can be utilized in future technology, such as that they are insulating inside and metallic at their surfaces.

In this study, published in Nature Communications a multidisciplinary group of Spanish research teams reported that certain stripes of graphene called graphene nanoribbons (GNRs) acquire the anomalous topological state of matter when narrowed down to just a few nanometres in width.

GNRs are atomically thin, planar carbon nanostructures that can be obtained from a sheet of graphene (carbon atoms arranged in a hexagonal lattice) by cutting in different directions. Conceptually, they can be thought of as stripes of graphene aligned along different directions, i.e., as nanoscale wires that may be used to transport an electronic current.

The scientists fabricated with atomic precision narrow GNRs of different width and orientation, like in the figure below, and demonstrated that all types convert from a metallic into an insulating state when the width is reduced below a few nanometers. Unexpectedly, they found that this new state corresponds to a non-trivial topological class.

Because of their anomalous topology, electronic states were found localized at the ends of the ribbons (as shown in the figure). These states represent a novel source of non-conventional magnetism with promising applications in quantum technologies.



at the end of the ribbon.

This study was achieved through a multidisciplinary collaboration combining tools and methods of chemistry and physics. First, organic chemists at the CIQUS institute in the University of Santiago de Compostela synthesized molecular precursors for GNRs using solution chemistry. Physicists at CIC nanoGUNE and at the Centro de Física de Materiales (CFM), in San Sebastian, did the assembling reaction on metal surfaces to produce the desired GNRs with atomic precision and investigated their anomalous electronic properties with scanning tunneling microscopy. The physicists at the Donostia International Physics Center (DIPC) did theoretical simulations that demonstrated the anomalous topology of the narrow GNRs. This result widens the scope for the use of graphene nanostructures in emerging quantum technologies



Scanning tunneling microscopy image resolving the hexagonal structure (schematically indicated by black lines) of one of the studied GNRs. The bright, localized feature at the right side reveals the emergent "exotic" state

> Novel electronic states were found at the end of specific chiral graphene nanoribbons

Cubic 3D Chern photonic insulators with orientable large Chern vectors

Devescovi C, García-Díez M, Robredo I, Blanco de Paz M, Lasa-Alonso J, Bradlyn B, Mañes JL, Vergniory MG and García-Etxarri A Nature Communications 12, 7330 (2021)

Some materials have special universal properties protected against perturbations. Such properties are theoretically described by topology, a branch of mathematics concerned with the properties of geometrical objects that are unchanged by continuous deformations. So-called topological insulators are electronic materials that have a bulk band gap like an ordinary insulator but have conducting states on their boundaries, i.e., edges or surfaces. The conducting surface is not what makes topological insulators unique, but the fact that it is protected due to the combination of spin-orbit interactions and time-reversal symmetry.

A topological invariant is a geometrical quantity that remains unchanged by continuous deformations. Topological invariants have found widespread applications in physics, chemistry, and materials science. One of the best known topological invariants in condensed matter physics is the Chern number.

The definition of the Chern number is not exactly simple. But it could be enough to understand the Chern number as an integer that characterizes the topology of filled bands in two-dimensional lattice systems. A band with a non-zero Chern number is topologically non-trivial. When the highest occupied band is nontrivial and completely filled, the state is called a topological insulator. A material whose topological phases can be characterized by the Chern number is called a Chern insulator, a class of topological insulators.

But when we make Chern insulators interact with light, something interesting happens. Electrons are spin-1/2 particles, whereas photons are spin-1 particles. The distinct spin difference between these two kinds of particles means that their corresponding symmetry is fundamentally different. An electronic topological insulator is protected by the electron's spin-1/2 (fermionic) time-reversal symmetry; however, due to photon's spin-1 (bosonic) time-reversal symmetry, the same protection does not exist under normal circumstances for a photonic topological insulator. In other words, we could have a Chern photonic insulator with broken time-reversal symmetry. Time reversal symmetry broken topological phases provide gapless surface states protected by topology, regardless of additional internal symmetries, spin or valley degrees of freedom. Thus, the topology of the propagation of light in photonic crystals has been the subject of much recent attention.



Unit cell of on of the designed 3D Photonic Chern insulators.

Despite the numerous demonstrations of 2D topological phases, few examples of 3D topological systems with time reversal symmetry breaking exist. In contrast to 2D, a 3D Chern insulator is a topological phase that can be characterized by three first Chern invariants-or a Chern vector C = (Cx, Cy, Cz) – defined on lower dimensional surfaces: such a state of matter can support chiral surface states propagating on the planes with Miller indices indicated by the Chern vector.

Now, our team of researchers proposes a method to design cubic 3D topological photonic crystals where Chern vectors of any magnitude, sign or direction can be implemented at will. The new method is based on the merging and annihilation of Weyl points through multifold supercell modulations in three dimensions. The designs achieved this way display topologically protected chiral and unidirectional surface states with disjoint equifrequency loops.

The resulting crystals present the following characteristics: First, by increasing the Chern number, multiple surface states channels can be supported. Second, the Chern vector can be oriented along any direction simply changing the magnetization axis, opening up larger cube/cube interfacing possibilities as compared to 2D. Third, by lowering the time reversal symmetry breaking requirements, the system is ideal for realistic photonic applications where the magnetic response is weak.





Our team of researchers proposes a method to design cubic 3D topological photonic crystals where Chern vectors of any magnitude, sign or direction can be implemented at will

Avoiding a replication crisis in deep-learning-based bioimage analysis

Laine RF, Arganda-Carreras I, Henriques R and Jacquemet G Nature Methods 18, 1136 (2021)

Microscopy is a leading technology in biological research. Today, a typical microscopy session may generate hundreds to thousands of images, generally requiring computational analysis to extract meaningful results. But a simple analysis is not enough any more. Over the last few years, deep learning (DL) has increasingly become one of the gold standards for high-performance microscopy image analysis. DL algorithms have become powerful tools for analyzing, restoring and transforming bioimaging data. One promise of DL is parameter-free one-click image analysis with expert-level performance in a fraction of the time previously required. Is it a realistic promise? As with most emerging technologies, the potential for inappropriate use is raising concerns among the research community, what should we do to make sure the results provided are reliable and reproducible?

For image analysis, DL usually uses algorithms called artificial neural networks (ANNs). Unlike classical algorithms, before an ANN is used, it first needs to be trained. During training, the ANN is presented with a range of data, from which it attempts to learn how to perform a specific task. More specifically, the ANN builds a model of the mathematical transformation that needs to be applied to data to obtain the desired output. ANNs can therefore be considered as non-linear transformation machines, performing sequential mathematical operations on the input data. As we inspect deeper into these sequences of operations, it becomes difficult to understand what features of the original images are used. For that reason, they are often thought of as 'black boxes' as, for most users, only the input images and output predictions are readily available.

Learning how to perform an analysis from example data is both the principal strength and the main weakness of DL. By learning directly from the data, the ANN tries to identify the most suitable way to perform the analysis, leading to models with excellent performances for that particular dataset. However, trained DL models are only as good as the data, and the parameters used to train them. Thus, one powerful approach is to produce general models with high reusability potential using a large and diverse training dataset.

As DL models are becoming accessible through public repositories (so-called model zoos, such as bioimage.io) or web interfaces, it becomes straightforward to use the models directly to analyze new data. This has the advantages of speeding up DL uptake but, unless the researchers can confirm that their own data were well-represented within the training dataset used initially (which can be very difficult to do), the performance of such portable models on the new data often remains unclear.

This is the reason why despite its incredible potential, the application of DL in microscopy analysis has raised concerns due to a lack of transparency and understanding of its limitations, especially for generalizability. In addition to this, DL is developing at an incredible rate, which places a significant burden on users to determine the most appropriate tools for their needs. It remains challenging to assess the validity and performance of a range of approaches that are often difficult to compare, especially when widely accepted benchmark datasets are unavailable.



Spiderman's Uncle Ben has never been more right than today: "With great powers comes great responsibility"

Now a team of researchers at Universidad del Pais Vasco, University College London, Instituto Gulbenkian de Ciência and Åbo Akademi University, in order to help define adequate guidelines and ensure the appropriate use of this transformative technology, has reviewed key concepts that they believe are important for researchers to consider when using DL for their microscopy studies. They also describe in this work how results obtained using DL can be validated and propose what should, in their view, be considered when choosing a suitable tool. Finally, they also suggest what aspects of a deep learning analysis should be reported in publications to ensure reproducibility.

The researchers argue the importance of validating any model using a purposefully built evaluation dataset containing ground-truth target images or labels. Similarly, the use of DL models should be reported appropriately to ensure reproducibility and transparency. This is a challenging task for DL as many components, both internal (hyperparameters) and external (training dataset) to the network used, can dramatically influence the results obtained.

With the increasing availability of networks and models, finding ways to identify what might be a 'good tool' becomes critical. The authors believe that a good tool should not be only a performant one, but that its transparency of what it does to the data, usability and reliability are equally important.

The responsibility of proper use of DL in microscopy is now equally shared between users and developers. Spiderman's Uncle Ben has never been more right than today: "With great powers comes great responsibility".





Deep learning (DL) methods can offer excellent performances but only when the model used matches the data to be analysed. a,b, Noisy images of cells stained to visualize their nuclei (a) or F-actin (b) were acquired using a spinning disk confocal microscope and denoised using two different DL (CARE) models or a classic algorithm (PureDenoise). One DL model was trained to denoise these images, while the other was trained to denoise structured illumination microscopy images of F-actin. Note that in both cases, the appropriate DL model outperforms the classic algorithm, while the inappropriate DL model fails to denoise these images correctly. In b, the inappropriate DL model was trained to denoise the nuclei images shown in a. c,d, Examples to highlight how segmentation models can offer variable performance even on similar images. Images of cells migrating on cell-derived matrices were acquired using a brightfield microscope and segmented with DL models (cellpose). Note how the DL cyto model performs well in c but poorly in d. Also, note how the DL cyto2 model, a model trained with additional data, performs better than the cyto model in d.

Time for NanoNeuro

Garcia-Etxarri A and Yuste R Nature Methods 18, 1287 (2021)

Because of their unique physical properties, nanomaterials have intrinsic advantages as biosensors and actuators, and they may be applicable to humans without the need for genetic modifications. It follows, then, that nanoscience could make major methodological contributions to the future of biomedical sciences, especially neuroscience. Meet NanoNeuro, a new field defined as the intersection of nanoscience and neuroscience, that aims to develop nanoscale methods to record and stimulate neuronal activity.

Traditional neuroscience tools, such a metal or glass-based electrodes, have been used for over a century to record the activity of individual neurons, but are inadequate for characterizing the function of vast numbers of them in their form in the brain. More recently, optical imaging using fluorescent calcium or voltage probes and magnetic resonance imaging, which detects haemoglobin oxygenation, have enabled a more comprehensive recording of neural circuits. Still, in terms of spatial and temporal resolution, current methods are far from recording 'every spike from every neuron'.

Methods for manipulating brain activity have similar shortcomings in spatio-temporal resolution. For example, traditional stimulating electrodes, used in the clinic for deep-brain stimulation, and newer optical and magnetic methods for activating single neurons or groups of them, either with optogenetics, optochemistry, or transmagnetic stimulation, are still far from achieving systematic stimulation of entire neural circuits, with single-cell precision, in three dimensions (3D) in awake, behaving animals. To perform such a systematic recording and manipulation of neural circuits, new technologies are necessary.

In 1959, Richard Feynman, in his talk 'There's Plenty of Room at the Bottom', described the possibility of chemical synthesis by direct manipulation of atoms, thus marking the start of nanoscience. Aside from being a technological breakthrough, nanomaterials have enabled the development of new technological tools and the discovery of new physical laws. Indeed, over the last few decades, nanomaterials with previously unknown properties and functions have been developed, with applications in research fields ranging from electronics and energy harvesting to biomedicine.

In order to learn where NanoNeuro currently stands, Aitzol Garcia-Etxarri and Rafael Yuste discuss in a review article nanoscience-based methods and tools to record and stimulate neuronal activity as a potential technological platform to propel neurotechnology forward. They consider both electrode and particle-based approaches to these methods.



Artistic view of nanoparticles interacting with neurons to record and induce neural activity.

The authors find that the NanoNeuro is still in its infancy as a scientific field. From the variety of approaches they discuss, it is clear that there is not a one-size-fits-all method, as different nanomaterials have different advantages and disadvantages when compared with existing neuroscience methods. They envision a future where the combination of nanomaterials with existing methods facilitates the creation of new and powerful hybrid technologies. But, there are substantial challenges that NanoNeuro methods should still overcome to reach technological maturity and to enable real-world applications.

Probably, one of the major challenges will be the isolationist tendencies of scientific fields. For NanoNeuro to grow, it will be necessary to break barriers betweeWn disciplines, with strong collaborations and interdisciplinary training for the next generations. Because, paraphrasing Feynman, there's plenty of room at the bottom, also for neuroscience.



Nanoscience-based methods and tools to record and stimulate neuronal activity

Real-space observation of vibrational strong coupling between propagating phonon polaritons and organic molecules

Bylinkin A, Schnell M, Autore M, Calavalle F, Li P, Taboada-Gutièrrez J, Liu S, H. Edgar J, Casanova F, Hueso Luis E, Alonso-Gonzalez P, Y Nikitin A and Hillenbrand R Nature Photonics 15, 197 (2021)

Van der Waals materials consist of two-dimensional layers bound by weak van der Waals forces. After the isolation of graphene, the field of two-dimensional van der Waals materials has experienced an explosive growth and new families of two-dimensional systems and block-layered bulk materials have been created.

This growth has been fueled mainly by the possibility of tuning a set of remarkable electronic properties using a variety of methods (thickness control, doping, intercalation, proximity effects, to name a few) and a relative simplicity of fabrication. These two characteristics, that make layered van der Waals materials similar to Lego constructions, are attractive from both practical and fundamental points of view.

In a parallel development, phonon polaritons – the result from the coupling of an infrared photon with an optic phonon – with extraordinary properties have been discovered in polar van der Waals crystals. A remarkable example is a dielectric hexagonal boron nitride (h-BN), where such exotic phenomena as ray propagation or hyper-lensing effects can be observed, offering opportunities for the development of a planar directional control of light-matter interactions at the nanoscale.

Since phonon polaritons in h-BN spectrally coincide with typical mid-infrared molecular vibrational resonances, these polaritons could be a way to achieve a strong vibrational coupling. Theoretically, this interaction could be the key for developing ultrasensitive infrared spectroscopy and a new way to modifying chemical properties of molecules. However, until now this most interesting interaction has not been proven experimentally.

A team of researchers has just demonstrated by nanoimaging that vibrational strong coupling can be achieved between propagating phonon polaritons in thin van der Waals crystals (h-BN) and molecular vibrations in adjacent thin molecular organic layers.

Mid-infrared nanoimaging experiments were used to study the interaction of ultra-confined propagating phonon polaritons in van der Waals materials with molecular vibrations in sub-100 nm thick organic layers. Specifically, phonon-polariton interferometry was performed in thin, continuous hexagonal boron nitride layers interacting with 4,4'-bis(N-carbazolyl)-1,1'-biphenyl molecules. The researchers retrieved—in an excellent agreement-experimentally and theoretically the guasi-normal modes of the coupled system, revealing a strong coupling.

Interestingly, a numerical study predicts that few-layer h-BN layers may enable strong coupling to be reached even in the case of atomically thin molecular layers, thus underlining the potential of phonon polaritons to become a platform for ultrasensitive on-chip spectroscopy devices.

Researchers visualize a mixed light-matter state by near-field optical microscopy



Artistic representation of nanoimaging of the strong coupling between molecular vibrations and phonon polaritons (circular waves) in a thin slab of h-BN. Nanoimaging is performed by a near-field microscope that scans a sharp tip across the sample surface. Nature Photonics cover (Nature.com/nphoton/volumes/15/issues/3)



Probing quantum speed limits with ultracold gases

del Campo A Physical Review Letters 126, 180603 (2021)

In recent years, the understanding of time-energy uncertainty relations as quantum speed limits has provided deep insights in nonequilibrium processes and quantum technologies. Quantum speed limits (QSLs) rule the pace at which quantum systems can change and thus have applications ranging from quantum metrology to quantum control, orthogonality catastrophe, and the limits of computation, among other relevant examples.

Quantum physics dictates the existence of Quantum Speed Limits (QSL), that impose a minimum time for a physical process to unfold. Not surprisingly, QSL have broad applications in quantum computing, quantum metrology, and other quantum technologies. And yet, their experimental study has remained elusive for decades. The work by Prof. del Campo shows how recent advances in experimental ultracold atom physics can be harnessed to probe QSL in the laboratory, further unveiling their implication in optimal control theory.

The common understanding of the uncertainty relation says that it is impossible to measure both the position and the momentum of a subatomic particle, in the same instant to unlimited accuracy. The more accurate is the measurement of the momentum, the less accurate is the measurement of the position in that instant, and vice versa.

Momentum is certainly related to time through velocity, but introducing time in the quantum realm turns everything a little bit blurry. The time-energy uncertainty relation is a fundamental result in quantum physics relating characteristic times to the inverse of energy fluctuations, Still, as Busch puts it, different types of time energy uncertainty relation can indeed be deduced in specific contexts, but that there is no unique universal relation that could stand on equal footing with the position-momentum uncertainty relation.

The modern formulation of the time-energy uncertainty relation relies on quantum speed limits that bound the minimum time for a physical process to unfold in terms of energy fluctuations. As the state of a system in quantum mechanics is represented by a vector in a linear vector space that can have an infinite number of dimensions, called a Hilbert space, quantum speed limits represent quantum dynamics geometrically, where the quantum state of a system evolves in time by sweeping a distance in Hilbert space. Therefore, quantum speed limits involve the notions of speed and distance in Hilbert space.

Quantifying the distance between the initial and time-evolving quantum states requires estimating state overlaps, which is challenging, if not unfeasible, for many-particle systems with continuous variables.



In spite of the fundamental nature of quantum speed limits, there is currently a lack of experimental studies probing them. Now, Adolfo del Campo theoretically proposes the experimental study of quantum speed limits with many-body systems of trapped ultracold atoms by measuring the mean atomic cloud size as a function of the evolution time.

The proposal relies on measuring the size of the atomic cloud in a given process, such an expansion or compression driven by a modulation of the trap frequency. The scaling factor can be determined by imaging the cloud size via different methods. From it, the distance traveled by the quantum state of the system in Hilbert space (Bures angle) during the evolution can be determined.

This approach circumvents the need for reconstructing a quantum state using measurements of the many-body quantum states of a continuous variable system. These results pave the way to the experimental study of the time-energy uncertainty relation and quantum speed limits in many-body quantum systems and their relation to the orthogonality catastrophe.



The flow of time is marked by the happening of events allowed by quantum speed limits

Artistic representation of the minimum time required for a quantum state to evolve into a distinguishable state, which is encoded in the quantum speed limit (QSL). The existence of a QSL is a fundamental principle in physics and information theory. It sets the ultimate bound on the computational power of physical devices and the complexity of the universe. Thanks to advances in quantum control of ultracold quantum matter, the study of QSL is now at reach in complex many-body systems.

Reaching the ideal glass in polymer spheres: thermodynamics and vibrational density of states

Monnier X, Colmenero J, Wolf M and Cangialosi D Physical Review Letters 126, 118004 (2021)

Glasses, though in the solid state, differ from crystals as they exhibit no long-range order in the atomic distribution. In general, a liquid of any kind can be cooled down below its melting temperature, provided that large cooling rates are used to avoid crystallization. Further cooling leads to the formation of a glass – at a temperature addressed as glass transition temperature, T_{g} – whose thermodynamic state profoundly depends on its thermal history. Once in the glassy state, spontaneous evolution towards low energy states, known as physical aging, takes place.

A deep unresolved question in glass science regards the equality of the glass entropy with that of the crystal at a finite temperature, addressed as the Kauzmann temperature, $T_{\rm K}$, implying an entropy catastrophe with the paradoxical scenario of a liquid having smaller entropy than that of the crystal at $T < T_{\rm K}$. To avoid this unpalatable scenario, it has been largely debated whether a true second order thermodynamic transition, the "ideal" glass transition, at $T_{\rm k}$ takes place. An important aspect related is that, apart from the thermodynamic view, the achievement of low energy glasses may deeply affect the glass vibrational density of state (VDOS). An excess in the VDOS, addressed as the boson peak, is observed in glasses whose magnitude decreases with the energy.

Accessing low energies in bulk glasses is unfeasible due to the astronomical time scales required. Indeed the transformation of the supercooled liquid into a glass takes place at large energies and subsequent glass equilibration below $T_{\rm q}$ is extremely slow. Hence, we exploited the ability of glasses with large free interface to access low energy states. Specifically, aggregates of spheres of a polymeric glass former were aged well below their T_{g} and characterized by calorimetry and inelastic neutron scattering to monitor the thermodynamic state and the VDOS, respectively.

The results show that, when aged at appropriate temperatures, glassy spheres attain a thermodynamic state corresponding to an ideal glass in about one day; indicating that increasing glasses' free interface induces a tremendous reduction of the timescale to recover equilibrium. Via a relaxation process with finite timescale deep in the glassy state, this acceleration allows attaining glass energies relevant to detect a kink in the enthalpy, identified with the transformation from the standard into the ideal glass (see Figure upper right panel). In the ideal glassy state, the boson peak disappears (see Figure lower right panel), thus rendering the VDOS alike that of crystals.



(Left panel) Schematic representation of the potential energy landscape for bulk and spheres glasses, showing how deep in the in the landscape the latter system can fall. (Right upper panel) Thermodynamic plot showing the glass enthalpy of bulk and polymer spheres, the equilibrium (supercooled) line and the kink in the enthalpy at the ideal glass transformation. (Right lower panel) Reduced VDOS for bulk and polymer spheres before aging (rejuvenated) and in the ideal glass state. The inset shows the relation between the glass thermodynamic state and the VDOS.



The existence of the ideal glass is proved by aging glasses with large amount of free interface. The boson peak in the ideal glass is suppressed

Enhancement of spin-charge conversion in dilute magnetic alloys by kondo screening

Huang C, Tokatly Ilya V. and Cazalilla MA Physical Review Letters 127, 176801 (2021)

The importance of impurities in determining the properties of materials cannot be sufficiently understated. After all, our current information technologies are based on devices made from doped semiconductors. Indeed, semiconductors like Silicon would be boring insulators was it not because by randomly introducing impurities they can be turned into metals. Thus, exquisite control of the electric conductivity is possible in devices with metallic gates imprinted on the surface.

However, besides the electrical charge which behaves classically (except for being quantized), electrons also possess an intrinsically quantum mechanical degree of freedom, namely the spin. The field of spintronics was born out of an attempt to control the electron spin and use it for the storage and transport of (quantum) information. In recent years, the generation of spin polarized currents without relying on magnetic materials has become a major research topic. One approach relies on materials whose band structure exhibits a large spin-orbit splitting. Thus, in response to external electric fields, large spin currents can be generated (the so-called intrinsic spin Hall effect, ISHE).

However, synthesizing such materials often requires heavy elements that are scarce or hard to mine from the Earth crust. In addition, it is interesting to use heavy elements in small amounts as contaminants in order to synthesize alloys with interesting spintronic properties. For spin current generation, this relies on the extrinsic spin Hall effect (ESHE). There are two contributions to the ESHE: skew scattering and side jump. The former can be readily incorporated in a kinetic theory describing the transport of electrons in metals. The latter has been extensively discussed by many authors but, unlike skew scattering it has not been possible to account for it within a rigorous kinetic theory until the publication of our work). Instead, various heuristic approaches involving the introduction of an anomalous velocity due to the scattering of electron wave packets with heavy atom impurities have been used so far.

Along with large spin-orbit splittings, electrons in the orbitals of heavy atom impurities also experience strong correlation effects. This has been known to lead to phenomena like the Kondo effect in magnetic alloys. The latter often manifests itself as a minimum in the electrical resistivity of metals contaminated with transition metal impurities like Fe, Co, Mn, or rare earth impurities like Ce, Yb, etc. At low temperatures, this effect eventually results in the disappearance of the impurity's magnetic moment after being screened by the conduction electrons of the metal. What is left behind is often an impurity that resonantly scatters electrons at the Fermi energy.



Simplified model of a Cerium impurity in a rare earth Ce_xLa_{1-x}Cu₆ to which we applied our kinetic theory. The impurity is made rotationally invariant but captures the low-lying multiplet structure of Cerium impurities in the alloy. Two multiplets with (effective) j = 3/2 and j = 1/2 for the f-electron, with the j = 1/2 giving rise to the Kondo effect. An addition scattering channel with $j = \frac{1}{2}$ resulting from other orbitals is also included. The j =1/2 double is Kondo screened at low temperatures.

Our theory uses the density impurities as a small parameter but accounts for arbitrarily strong impurity scattering

The equations obtained in our work provide the first rigorous derivation of side jump contribution within kinetic theory. When deriving the Boltzmann equation and properly accounting for the gradient corrections, we found that gradient corrections to the collision integral readily account for the side jump mechanism. Our theory uses the density impurities as a small parameter but accounts for arbitrarily strong impurity scattering. We solved our kinetic equations and made concrete predictions for the spin Hall conductivity of rare earth alloys like $Ce_xLa_{1-x}Cu_6$, which exhibits the Kondo effect phenomenology for small x. Thus we found 1) a sizeable contribution to the ESHE entirely due to the side jump which does not depend on the interference with other scattering channels 2) A difference in the diffusion coefficients for the longitudinal and transverse components of the spin density.



Global natural orbital functional: towards the complete description of the electron correlation

Piris M Physical Review Letters 127, 233001 (2021)

Our current understanding of how electrons are found in atoms and molecules is based on clouds of probability. According to quantum mechanics, the probabilities of finding an electron in different regions of space can be obtained by solving the Schrödinger equation. Its solution is called the wavefunction, ψ , and the square of the absolute value of the wavefunction, $|\psi|^2$, defines the probability density function.

The solution of the Schrödinger equation for multielectron systems is one of the central problems in physics and is far from trivial. For the most interesting quantum mechanical systems, we don't know how to solve the Schrödinger equation. There are exceptional systems of "exact resolution" such as the free particle, the square well or the harmonic oscillator; however, for other systems, such as a many-electron atom or a molecule, we rely on various approximation methods.

Probably the most popular approaches are based on density functional theory (DFT). In DFT, the electron density completely determines a many-electron system and, in particular, the total energy turns out to be a density functional. This represents a great advantage since it avoids having to know the wave function ψ that contains much more information, significantly lowering the computational costs to solve the many-body problem. Unfortunately, attempts to construct such a functional for the total energy have not been very successful due to its strong non-locality.

Appropriate representations of the electronic structure of atoms, molecules and solids without explicit recourse to the wavefunction can alternatively be obtained by the one-particle reduced density matrix (1RDM) functional theory. The functionals currently in use are constructed in the basis where the 1RDM is diagonal which is the definition of a natural orbital functional (NOF). In NOFT, the electronic structure is described in terms of the natural orbitals and their occupation numbers. The approximate NOFs have proven to be more accurate than those of the density for systems with a significant multiconfigurational character, on one side, and scale better with the number of basis functions than correlated wavefunction methods, on the other side. Several approximate NOFs have been proposed, but they suffer from an important lack of dynamic correlation.



Ionization potentials of transition-metal atoms.

An even more elegant approach for the description of electronic correlation based only on the one-particle reduced density matrix

In 2017, Mario Piris, an Ikerbasque research professor working at DIPC and UPV/EHU, proposed a new method to calculate electron correlations based on the NOF theory. To recover the dynamic correlation, second-order perturbative corrections were considered with significant results. The implementation of the method in an open-source code called DoNOF (Donostia Natural Orbital Functional) was presented three years later. Now, Piris provides the next step towards the complete description of the electron correlation. He has designed an accurate NOF for electronic systems with any spin value independent of the external potential being considered, that is, a global NOF (GNOF).

Piris limits himself to a new two-index reconstruction of the two-particle reduced density matrix for spin multiplets, and introduces the concept of the dynamic part of the occupation numbers. The emergent functional describes the complete intrapair electron correlation, and the correlation between orbitals that make up both the pairs and the individual electrons.

The results for different properties calculated this way agree extremely well with experimental data. Piris now recovers the missing dynamic correlation within the NOF theory framework only.





Potential Energy Curves.

Coulomb interaction, phonons, and superconductivity in twisted bilayer graphene

Cea T and Guinea F PNAS 118, e2107874118 (2021)

Twistology could be the study of unexpected changes or developments in stories or situations, from coups d'état to the fatherhood of Darth Vader. In condensed matter physics there is something similar, although the preferred name is twistronics (from twist and electronics). It is understood as the study of how the angle (the twist) between layers of two-dimensional materials can change their electrical properties. Materials such as twisted bilayer graphene (TBG) have been shown to have vastly different electronic behaviour, ranging from non-conductive to superconductive, that depends sensitively on the angle between the layers.

The development of superconducting devices was greatly stimulated after the acceptance of the basic theory of superconductivity proposed in 1957 by John Bardeen, Leon Cooper, and Robert Schrieffer. The authors of the BCS theory, as it is known, received the Nobel Prize for their work in 1972. The basic idea is that the electron waves in the superconducting state no longer act independently, as in Bloch's model. Instead, they are paired together at the so-called critical temperature so that their wave functions act as one unit as they interact with the crystal lattice. Moreover, all of the electron pairs move together in one collective motion, so that if any single electron is scattered by the lattice it is pulled back into the flow by its partner, and if any pair of electrons is somehow scattered off track, it is pulled back into the collective flow by all the other pairs. Since there is no scattering or inelastic collisions, there is no resistance, and the material becomes a superconductor.

The pairing interaction responsible for superconductivity in TBG has been intensively studied. Among other possible pairing mechanisms, the effect of phonons, the proximity of the chemical potential to a van Hove singularity in the density of states and excitations of insulating phases, and the role of electronic screening have been considered.

Now, Tommaso Cea and Francisco Guinea study 1 how the screened Coulomb interaction induces pairing in TBG. The researchers obtain critical temperatures of magnitude 1 to 10 K and provide estimates and trends in agreement with the experimental measurements.

The long-range Coulomb interaction, projected onto the central bands of TBG, is described by an energy scale in the range of 20 to 100 meV. As a result, this interaction modifies significantly the shape and width of the bands of TBG near the so-called first magic angle. The authors focus on low-energy excitations in TBG, including particle-hole excitations, plasmons, and acoustic phonons, analysing the way in which these excitations lead to superconductivity, by means of well-tested diagrammatic techniques.



Electronic structure and superconductivity in twisted bilayer graphene. The plots show the Fermi surfaces and peaks in the superconducting order parameter for different numbers of electrons.

The article shows that, nevertheless, this interaction induces superconductivity, due to the complex structure of the electronic bands

The scientists find that the screened Coulomb interaction allows for the formation of Cooper pairs and superconductivity in a significant range of twist angles and fillings. The tendency toward superconductivity is enhanced by the coupling between longitudinal phonons and electron-hole pairs. Importantly, scattering processes involving large momentum transfers play a crucial role in the formation of Cooper pairs.

This is another important theoretical contribution to understand superconductivity in general, and particularly in TBG.







The strongest interaction between electrons in twisted bilayer graphene is the long range Coulomb repulsion

Simulation methods for open quantum many-body systems

Weimer H, Kshetrimayum A and Orús R Reviews of Modern Physics 93, 015008 (2021)

It is very difficult to obtain exact solutions to systems involving interactions between more than two bodies, using either classical mechanics or quantum mechanics. To understand the physics of many-body systems, it is necessary to make use of approximation techniques or model systems that capture the essential physics of the problem. The complexity of the problem scales exponentially with the size of the system, requiring the use of sophisticated simulation methods to obtain useful results This is compounded by the fact that no system in nature is perfectly isolated. They are constantly interacting with their environment in the form of heat transfer, decoherence, etc. Actually, all real systems are open systems.

Open quantum many-body systems have witnessed a surge of interest in recent years, chiefly for two reasons. On the one hand, these systems offer the possibility of using controlled dissipation channels to engineer interesting quantum many-body states as the stationary state of their dynamics. On the other hand, open quantum many-body systems are attractive from a fundamental perspective, as their dynamics exhibits a wide range of features not found in equilibrium systems.

Open quantum many-body systems are even harder to simulate on classical computers than closed systems, while at the same time the stationary state of an open quantum system is much easier to experimentally prepare than the ground state of a closed system. These properties make open guantum systems one of the prime candidates to show a guantum advantage of guantum simulators over classical methods within noisy intermediate-scale quantum devices. However, this requires a thorough assessment of the capabilities of classical simulation methods, which a team of researchers now provide in a new review.

The substantial effort to develop novel simulation methods to investigate open quantum many-body systems has produced a variety of numerical methods. Specifically, in this review methods for the Markovian guantum master equation (assuming a weak-coupling limit), including mean-field stochastic methods, tensor networks, variational methods, guantum Monte Carlo methods, a truncated Wigner approximation, BBGKY hierarchy equations, and linked-cluster expansions are considered.



(a) A quantum state described by a Tensor Network includes degrees of freedom for the system (black lines) and the environment (red lines). The projector (b) describes the complete system, and the trace over the environment in (c) produces a quantum state in the form of a Tensor Network capable of describing the physical system directly, by means of a reduced density matrix that can be manipulated computationally for very large systems.

Simulaiting open and noisy systems is now possible by using a variety of computational techniques, allowing for the discovery of new phases of dissipative guantum matter

While no method has yet emerged that is universally optimal for all cases, there have been several promising developments with different methods for different regimes. Even with the major technical advances recently achieved, there are still many open problems that are inaccessible with these stateof-the-art numerical techniques.

The authors come to very interesting conclusions. The first is that mean-field methods are considerably less reliable for open systems than their counterparts for closed systems, although the reason for this discrepancy is still an open question. Secondly, tensor network methods have demonstrated their ability to successfully tackle many hard problems surrounding open many-body systems and resolve longstanding open questions. A particularly interesting and promising case is that of open 2D systems, which are unexplored territory to a large extent. Finally, for the variational methods discussed in this review, there appears to be a trade-off between the formal suitability of the norm and its efficient computability.

Progress in recent years in simulating open quantum systems has brought the field to a level where one has a wide range of tools at hand to systematically make a comparison to experimental results, particularly in the context of quantum simulations. Combined with the experimental ease of preparing the steady state of an open quantum system, these are good reasons to believe that the study of strongly correlated open quantum many-body systems will become a research topic with an impact on other areas of science, such as material design and quantum computation.



