Swimming Gold Nanoparticles

Chinese scientists have redesigned collective chemotaxis by creating artificial model nanoswimmers from chemically and biochemically modified gold nanoparticles. [43]

"We discovered a new structure in gold that exists at extreme states—two thirds of the pressure found at the center of Earth," said lead author Richard Briggs, a postdoctoral researcher at LLNL. [42]

The properties of gold in nanoscale are significantly different to those of bulk gold. Of special interest are gold nanoclusters, that are composed of between tens to some hundreds of gold atoms. [41]

A team at Osaka University has created single-molecule nanowires, complete with an insulation layer, up to 10 nanometers in length. [40]

Using optical and electrical measurements, a two-dimensional anisotropic crystal of rhenium disulfide was found to show opposite piezoresistant effects along two principle axes, i.e. positive along one axis and negative along another. [39]

A team of researchers from the University of Konstanz has demonstrated a new aqueous polymerization procedure for generating polymer nanoparticles with a single chain and uniform shape, which, by contrast to previous methods, involves high particle concentrations. [38]

A team of researchers from China, the U.S. and Japan has developed a way to strengthen graphene-based membranes intended for use in desalination projects—by fortifying them with nanotubes. [37]

The team arrived at their results by imaging gold nanoparticles, with diameters ranging from 2 to 5 nanometres, via aberration corrected scanning transmission electron microscope. [36]

Nanoparticles of less than 100 nanometres in size are used to engineer new materials and nanotechnologies across a variety of sectors. [35]

For years, researchers have been trying to find ways to grow an optimal nanowire, using crystals with perfectly aligned layers all along the wire. [34]

Ferroelectric <u>materials</u> have a spontaneous dipole moment which can point up or down. [33] Researchers have successfully demonstrated that hypothetical particles that were proposed by Franz Preisach in 1935 actually exist. [32]

Scientists from the Department of Energy's SLAC National Accelerator Laboratory and the Massachusetts Institute of Technology have demonstrated a surprisingly simple way of flipping a material from one state into another, and then back again, with single flashes of laser light. [31]

Materials scientists at Duke University computationally predicted the electrical and optical properties of semiconductors made from extended organic molecules sandwiched by inorganic structures. [30]

KU Leuven researchers from the Roeffaers Lab and the Hofkens Group have now put forward a very promising direct X-ray detector design, based on a rapidly emerging halide <u>perovskite</u> semiconductor, with chemical formula Cs₂AgBiBr₆. [29]

Physicists at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) have proven that incoming light causes the electrons in warm perovskites to rotate, thus influencing the direction of the flow of electrical current. [28]

Self-assembly and crystallisation of nanoparticles (NPs) is generally a complex process, based on the evaporation or precipitation of NP-building blocks. [27]

New nanoparticle-based films that are more than 80 times thinner than a human hair may help to fill this need by providing materials that can holographically archive more than 1000 times more data than a DVD in a 10-by-10-centimeter piece of film. [26]

Researches of scientists from South Ural State University are implemented within this area. [25]

Following three years of extensive research, Hebrew University of Jerusalem (HU) physicist Dr. Uriel Levy and his team have created technology that will enable computers and all optic communication devices to run 100 times faster through terahertz microchips. [24]

When the energy efficiency of electronics poses a challenge, magnetic materials may have a solution. [23]

An exotic state of matter that is dazzling scientists with its electrical properties, can also exhibit unusual optical properties, as shown in a theoretical study by researchers at A*STAR. [22]

The breakthrough was made in the lab of Andrea Alù, director of the ASRC's Photonics Initiative. Alù and his colleagues from The City College of New York, University of Texas at Austin and Tel Aviv University were inspired by the seminal work of three British researchers who won the 2016 Noble Prize in Physics for their work, which teased out that particular properties of matter (such as electrical conductivity) can be preserved in certain materials despite continuous changes in the matter's form or shape. [21] Researchers at the University of Illinois at Urbana-Champaign have developed a new technology for switching heat flows 'on' or 'off'. [20] Thermoelectric materials can use thermal differences to generate electricity. Now there is an inexpensive and environmentally friendly way of producing them with the simplest tools: a pencil, photocopy paper, and conductive paint. [19] A team of researchers with the University of California and SRI International has

developed a new type of cooling device that is both portable and efficient. [18]

Thermal conductivity is one of the most crucial physical properties of matter when it comes to understanding heat transport, hydrodynamic evolution and energy balance in systems ranging from astrophysical objects to fusion plasmas. [17]

Researchers from the Theory Department of the MPSD have realized the control of thermal and electrical currents in nanoscale devices by means of quantum local observations. [16]

Physicists have proposed a new type of Maxwell's demon—the hypothetical agent that extracts work from a system by decreasing the system's entropy—in which the demon can extract work just by making a measurement, by taking advantage of quantum fluctuations and quantum superposition. [15]

Pioneering research offers a fascinating view into the inner workings of the mind of 'Maxwell's Demon', a famous thought experiment in physics. [14]

For more than a century and a half of physics, the Second Law of Thermodynamics, which states that entropy always increases, has been as close to inviolable as any law we know. In this universe, chaos reigns supreme. [13]

Physicists have shown that the three main types of engines (four-stroke, twostroke, and continuous) are thermodynamically equivalent in a certain quantum regime, but not at the classical level. [12]

For the first time, physicists have performed an experiment confirming that thermodynamic processes are irreversible in a quantum system—meaning that, even on the quantum level, you can't put a broken egg back into its shell. The results have implications for understanding thermodynamics in quantum systems and, in turn, designing quantum computers and other quantum information technologies. [11] Disorder, or entropy, in a microscopic quantum system has been measured by an international group of physicists. The team hopes that the feat will shed light on the "arrow of time": the observation that time always marches towards the future. The experiment involved continually flipping the spin of carbon atoms with an oscillating magnetic field and links the emergence of the arrow of time to quantum fluctuations between one atomic spin state and another. [10]

Mark M. Wilde, Assistant Professor at Louisiana State University, has improved this theorem in a way that allows for understanding how quantum measurements can be approximately reversed under certain circumstances. The new results allow for understanding how quantum information that has been lost during a measurement can be nearly recovered, which has potential implications for a variety of quantum technologies. [9]

Today, we are capable of measuring the position of an object with unprecedented accuracy, but quantum physics and the Heisenberg uncertainty principle place fundamental limits on our ability to measure. Noise that arises as a result of the quantum nature of the fields used to make those measurements imposes what is called the "standard quantum limit." This same limit influences both the ultrasensitive measurements in nanoscale devices and the kilometer-scale gravitational wave detector at LIGO. Because of this troublesome background noise, we can never know an object's exact location, but a recent study provides a solution for rerouting some of that noise away from the measurement. [8]

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the Wave-Particle Duality and the electron's spin also, building the Bridge between the Classical and Quantum Theories.

The Planck Distribution Law of the electromagnetic oscillators explains the electron/proton mass rate and the Weak and Strong Interactions by the diffraction patterns. The Weak Interaction changes the diffraction patterns by moving the electric charge from one side to the other side of the diffraction pattern, which violates the CP and Time reversal symmetry.

The diffraction patterns and the locality of the self-maintaining electromagnetic potential explains also the Quantum Entanglement, giving it as a natural part of the relativistic quantum theory.

Contents

Preface	7
Actively swimming gold nanoparticles	7
Study reveals new structure of gold at extremes	8
Solvent pH controls interactions of gold nanoclusters, offers potential applications in dru and imaging	•

The acidity controls gold nanoclusters' binding to virus	10
Plot twist: Straightening single-molecule conductors improves their performance	11
Opposite piezoresistant effects of rhenium disulfide in two principle directions	12
Researchers create uniform-shape polymer nanocrystals	14
Using carbon nanotubes to strengthen graphene-based membranes used desalination	
Research reveals liquid gold on the nanoscale	16
Scientists explore the unknown behaviour of gold nanoparticles with neutrons	17
Research team discovers perfectly imperfect twist on nanowire growth	18
Nanosized ferroelectrics become a reality	20
Skepticism	21
Polar phase	21
Wake up cycle	21
Researchers validate 80-year-old ferroelectric theory	22
Researchers switch material from one state to another with a single flash of light	24
Frozen waves of electrons	25
Surprising material switch	25
Supercomputer predicts optical and thermal properties of complex hybrid materials	27
Perovskite semiconductors seeing right through next generation X-ray detectors	29
Researchers decipher the dynamics of electrons in perovskite crystals	30
Orderly atomic structure	30
Nanoparticles form supercrystals under pressure	31
Researchers develop nanoparticle films for high-density data storage	32
Storing more data in less space	33
Changing the electron flow	34
Researchers developing materials for quantum computing	34
Terahertz computer chip now within reach	36
Revolutionizing computer memory—with magnets	37
The quantum states on the surface of conducting materials can strongly interact with lig	ht39
Breakthrough in circuit design makes electronics more resistant to damage and defects	40
Researchers develop heat switch for electronics	41
Converting heat into electricity with pencil and paper	42
Tiny effect	42
A new efficient and portable electrocaloric cooling device	43
Fast heat flows in warm, dense aluminum	43

Controlling heat and particle currents in nanodevices by quantum observation	44
Maxwell's demon extracts work from quantum measurement	46
Physicists read Maxwell's Demon's mind	47
Researchers posit way to locally circumvent Second Law of Thermodynamics	48
What is quantum in quantum thermodynamics?	49
Physicists confirm thermodynamic irreversibility in a quantum system	50
Physicists put the arrow of time under a quantum microscope	51
Egging on	52
Murky territory	52
Many questions remain	53
Small entropy changes allow quantum measurements to be nearly reversed	53
Quantum relative entropy never increases	53
Wide implications	54
Tricking the uncertainty principle	56
Particle Measurement Sidesteps the Uncertainty Principle	57
A new experiment shows that measuring a quantum system does not necessarily intro uncertainty	
Delicate measurement	59
Quantum entanglement	59
The Bridge	60
Accelerating charges	60
Relativistic effect	60
Heisenberg Uncertainty Relation	60
Wave – Particle Duality	61
Atomic model	61
The Relativistic Bridge	61
The weak interaction	61
The General Weak Interaction	63
Fermions and Bosons	63
Van Der Waals force	63
Electromagnetic inertia and mass	63
Electromagnetic Induction	63
Relativistic change of mass	63
The frequency dependence of mass	64
Electron – Proton mass rate	64

Gravity from the point of view of quantum physics	.64
The Gravitational force	.64
The Higgs boson	.65
Higgs mechanism and Quantum Gravity	.65
What is the Spin?	.66
The Graviton	.66
Conclusions	.66
References	.67

Author: George Rajna

Preface

Physicists are continually looking for ways to unify the theory of relativity, which describes largescale phenomena, with quantum theory, which describes small-scale phenomena. In a new proposed experiment in this area, two toaster-sized "nanosatellites" carrying entangled condensates orbit around the Earth, until one of them moves to a different orbit with different gravitational field strength. As a result of the change in gravity, the entanglement between the condensates is predicted to degrade by up to 20%. Experimentally testing the proposal may be possible in the near future. [5]

Quantum entanglement is a physical phenomenon that occurs when pairs or groups of particles are generated or interact in ways such that the quantum state of each particle cannot be described independently – instead, a quantum state may be given for the system as a whole. [4]

I think that we have a simple bridge between the classical and quantum mechanics by understanding the Heisenberg Uncertainty Relations. It makes clear that the particles are not point like but have a dx and dp uncertainty.

Actively swimming gold nanoparticles

Bacteria can actively move towards a nutrient source—a phenomenon known as chemotaxis—and they can move collectively in a process known as swarming. Chinese scientists have redesigned collective chemotaxis by creating artificial model nanoswimmers from chemically and biochemically modified gold nanoparticles. The model could help understand the dynamics of chemotactic motility in a bacterial swarm, concludes the study published in the journal *Angewandte Chemie*.

What causes swarming, and whether such collective behavior can be translated into artificial intelligent systems, is currently a topic of intensive scientific research. It is known that bacteria swimming in a dense pack feel the surrounding fluid differently from a sole <u>Swimmer</u>. But to

what degree swimmers are sped up in a swarm, and what other factors play a role, is still unclear. Colloidal chemist Qiang He at the Harbin Institute of Technology, China, and his colleagues, have now constructed a simple artificial model of bacteria-like nanoswimmers. They observed active chemotactic behavior and formation of the swimmers into a distinctly moving swarm.

He and his colleagues constructed their artificial swimmers from tiny spheres of <u>**GOld</u>**. With a size 40 times smaller than a usual bacterium, the <u>**GOld nanoparticles**</u> were below the detection limit of the microscope. However, thanks to a light-scattering phenomenon called the Tyndall effect, the scientists could observe larger changes in the solution containing swimmers, even with the naked eye. Using other analytical techniques, they also resolved the speed, orientation, and concentration of the particles in finer detail.</u>

Scientists enjoy working with gold <u>nanoparticles</u> because the tiny spheres form a stable, disperse solution, are readily observed with an electron microscope, and molecules can be attached to them relatively easily. He and his team first loaded the surface of large silica spheres with gold particles. Then they attached <u>polymer brushes</u> on the exposed side of the gold spheres. These brushes were made of <u>polymer chains</u>, and with a length of up to 80 nanometers, they rendered the gold particles highly asymmetric.

The researchers dissolved the silica carrier and tethered an enzyme on the exposed side of the gold spheres so that the resulting nanoparticles were covered with long and thick polymer brushes on one side and with the enzyme on the other. In the presence of oxygen, the glucose oxidase enzyme decomposes glucose into a compound called gluconic acid.

To determine if the nanoswimmers would actively swim in a given direction, the authors placed them at one end of a small channel and placed a permanent glucose source at the other end. Similarly to living bacteria, the model swimmers actively traveled along the glucose gradient towards the <u>glucose</u> source. This fact alone was not surprising as enzymatically driven, self-propelling swimmers are known from experiment and theory. But the authors could also detect swarming behavior. The asymmetric nanoparticles condensed into a separate phase that moved collectively along the nutrient gradient.

The authors imagine that the nanoswimmers could be further developed as valuable and easily accessible physical models to study the chemotactic and swarming behavior of living or non-living things on the nanoscale. [43]

Study reveals new structure of gold at extremes

Gold is an extremely important material for high-pressure experiments and is considered the "gold standard" for calculating pressure in static diamond anvil cell experiments. When compressed slowly at room temperature (on the order of seconds to minutes), gold prefers to be the face-centered cubic (fcc) structure at pressures up to three times the center of the Earth.

However, researchers from Lawrence Livermore National Laboratory (LLNL) and the Carnegie Institution of Washington have found that when gold is compressed rapidly over nanoseconds (1 billionth of a second), the increase in pressure and temperature changes the <u>CryStalline</u> <u>Structure</u> to a new phase of gold. This well-known body-centered cubic (bcc) <u>Structure</u> morphs to a more open crystal structure than the fcc structure. These results were published recently in *Physical Review Letters*.

"We discovered a new structure in gold that exists at extreme states—two thirds of the pressure found at the center of Earth," said lead author Richard Briggs, a postdoctoral researcher at LLNL. "The new structure actually has less efficient packing at higher pressures than the starting structure, which was surprising considering the vast amount of theoretical predictions that pointed to more tightly packed structures that should exist."

The experiments were carried out at the Dynamic Compression Sector (DCS) at the Advanced Photon Source, Argonne National Laboratory. DCS is the first synchrotron X-ray facility dedicated to dynamic compression science. These user experiments were some of the first conducted on hutch-C, the dedicated high energy laser station of DCS. Gold was the ideal subject to study due to its high-Z (providing a strong X-ray scattering signal) and relatively unexplored phase diagram at high temperatures.

The team found that that the structure of gold began to change at a pressure of 220 GPa (2.2 million times Earth's atmospheric pressure) and started to melt when compressed beyond 250 GPa.

"The observation of liquid gold at 330 GPa is astonishing," Briggs said. "This is the pressure at the center of the Earth and is more than 300 GPa higher than previous measurements of liquid gold at high pressure."

The transition from fcc to bcc structure is perhaps one of the most studied phase

<u>transitions</u> due to its importance in the manufacturing of steel, where high temperatures or stress causes a change in structure between the two fcc/bcc structures. However, it is not known what phase transition mechanism is responsible. The research team's results show that gold undergoes the same phase transition before it melts, as a consequence of both pressure and temperature, and future experiments focusing on the mechanism of the transition can help clarify key details of this important transition for manufacturing strong steels.

"Many of the theoretical models of <u>**GOld</u>** that are used to understand the high-pressure/hightemperature behavior did not predict the formation of a body-centered structure—only two out of more than 10 published works," Briggs said. "Our results can help theorists improve their models of elements under extreme compression and look toward using those new models to examine the effects of chemical bonding to aid the development of new materials that can be formed at extreme states." [42]</u>

Solvent pH controls interactions of gold nanoclusters, offers potential applications in drugs and imaging

The properties of gold in nanoscale are significantly different to those of bulk gold. Of special interest are gold nanoclusters, that are composed of between tens to some hundreds of gold atoms. Numerous of such cluster structures are known and synthesizable to atomic precision. The aim of this thesis was to apply molecular dynamics simulations on investigating properties of gold nanoclusters in different environments. The simulations reveal that gold nanocluster can bind to viruses by different interactions, and that the strength of the interactions are dependent on pH conditions.

The applicability of gold nanoclusters in medicine is widely studied. At the University of Jyväskylä, their usage has been demonstrated for example in virus imaging. Gold nanoclusters are generally composed of a gold core covered by a protective layer of different molecules. The protecting layer thus essentially determines how the gold nanocluster interacts with its environment. Moreover, the properties of the gold nanoclusters may be altered by tailoring the type of the molecules in the protective layer.

The aim of M.Sc Emmi Pohjolainen's dissertation at University of Jyväskylä, Finland, was to study different gold nanoclusters in various environments by means of <u>molecular dynamics</u> <u>Simulations</u>. Molecular dynamics simulations are an established tool in studies of systems whose properties and dynamics need to be investigated in atomic precision, while keeping the computation time reasonable.

While molecular dynamics simulations have been widely used in studies of biomolecules, their use in metal nanocluster research has been relatively sparse. The very first aim of this thesis was to develop and validate parameters to enable simulating such systems. These parameters have since been used by other groups outside the University of Jyväskylä as well.

The acidity controls gold nanoclusters' binding to virus

All the <u>simulation results</u> essentially need to be connected to the <u>experimental data</u>. On one hand the <u>experimental results</u> may be complemented by <u>simulation</u> results, on the other hand available experimental information need to be used in validating the goodness of the simulation. The simulations performed for this thesis included for example simulating gold nanoclusters in interactions with virus, by constructing a system with a full virus capsid covered with 60 gold nanoclusters. This system contained some 3.5 million atoms, and is as such a notably large system to simulate at atomistic scale.

The results revealed that gold nanoclusters may interact with the virus by different means, and the strength of these interactions is dependent on the pH conditions. This information may be in future utilized in design of imaging and drug molecules that need to bound to specific locations on the virus surface. Also binding of different types of drug molecules to the <u>Virus</u> were simulated, and binding strengths were compared to those of <u>QOId</u> nanoclusters.

In this thesis also self-assembly of <u>gold nanoclusters</u> into flakes or spherical structures, previously observed experimentally, were simulated. The simulations revealed that the stability of such superstructures is dependent on both solvent conditions and the distribution of charges on the cluster surface. Thus, self-assembling or disassembling could be controlled by changing the solvent and pH conditions. This property could be usable for example in drug-carrier molecules. [41]

Plot twist: Straightening single-molecule conductors improves their performance

A team at Osaka University has created single-molecule nanowires, complete with an insulation layer, up to 10 nanometers in length. When they measured the electrical properties of these nanowires, the researchers found that forcing the ribbon-like chains to be flat significantly improved their conductivity compared with a twisted conformation. The findings may allow for a new generation of inexpensive high-tech devices, including smartphone screens and photovoltaics.

Carbon-based polymers, which are long molecular chains made of repeating units, can be found everywhere, from the rubber in the soles of your shoes to the proteins that make up your body. We used to think that these molecules could not conduct electricity, but that all changed with the discovery of conducting polymers. These are a small subset of carbon-based molecules that can act like tiny wires owing to their alternating single and double chemical bonds, also called conjugated bonds. Since carbon-based conductors are much easier and cheaper to make and customize than conventional electronics, they have seen rapid adoption in OLED TVs, iPhone screens, and solar panels, while drastically reducing their cost.

Now, researchers at Osaka University have synthesized chains of oligothiophene of various lengths, with up to 24 repeat units. This means that single nanowires could be up to 10 nanometers in length. Insulation of the wires was needed to avoid interwire currents, so that the intrinsic conductivity of a single molecule could be measured accurately. On the basis of the rules of quantum mechanics, electrons in <u>MOIECUIES</u> behave more like spread-out waves than localized particles. The overlapping bonds in oligothiophene allow electrons to be entirely spread out over the polymer backbone, so they can easily transverse the molecule to create an <u>electrical</u> current.

This charge transport can occur is two very different ways. "Over short distances, electrons rely on their wave-like nature to 'tunnel' directly through barriers, but over long distances, they hop from site to site to reach their destination," first author Dr. Yutaka le explained. The team at Osaka University found that changing the oligothiophene chain from twisted to flat led to much greater overlap of the conjugated backbone of oligothiophene, which in turn meant a larger overall conductivity. As a result, the crossover from tunneling to hopping conduction took place with flat chains at shorter Chain lengths, compared with those with the twisted conformation.

The researchers believe that this work can open a whole new world of devices. "This study demonstrates that our insulated nanowires have the potential to be used in novel "single-molecule' electronics," lead author Dr. Yoshio Aso said. The work is published in the *Journal of Physical*

Chemistry Letters as "Highly Planar and Completely Insulated Oligothiophenes: Effects of π -Conjugation on Hopping Charge Transport." [40]

Opposite piezoresistant effects of rhenium disulfide in two principle directions

Using optical and electrical measurements, a two-dimensional anisotropic crystal of rhenium disulfide was found to show opposite piezoresistant effects along two principle axes, i.e. positive along one axis and negative along another. Piezoresistance was also reversible; it appeared upon application of a strain, but the relative resistance returned to its original value on strain removal. This novel finding is expected to lead to wide application of rhenium disulfide.

Upon application of mechanical stress such as pressure on crystals and some kinds of ceramics, a surface charge proportional to the applied strain is induced; this phenomenon is called the piezoelectric effect. The piezoelectric effect has been known since the mid-18th century and has found use, for example, in the ignition device of cigarette lighters. Today it is widely applied in sensors, actuators, etc. On the other hand, when mechanical strain is applied to semiconducting materials, some of them show a change in <u>electrical resistance</u>, called the piezoresistive effect. Materials showing the piezoresistive effect are used in pressure sensors, strain sensors etc.

Rhenium disulfide (ReS₂) is a two-dimensional (2-D) material crystallizing into a flake-like structure, as a black platelet (plate-like crystal), showing thickness-independent direct bandgap*1) and anisotropic physical properties. It is classified into the transition metal dichalcogenides*2) subgroup. According to theoretical calculations, it has two anisotropic directions along different principle axes. Two anisotropic directions are predicted to respond differently to a uniaxial strain. Upon validation of this property, ReS₂ should be useful in the accurate detection and recognition of multidimensional strain/stress and gestures, which will have wide applications in the fields of electronic skin*3), human–machine interfaces, strain sensors etc.

This international research team from China and Japan, in which Dr. Liu from Tianjin University and Dr. Yang from WPI-NanoLSI, Kanazawa University, played important roles, not only confirmed the anisotropic piezoresistive effect of rhenium disulfide but also discovered a novel phenomenon that, depending on the direction of strain applied along two crystalline axes, a 2-D device of ReS₂ showed opposite, i.e. positive and negative piezoresistance.

A 2-D device of ReS₂ was fabricated as schematically depicted in Figure 1. After examining its configuration using <u>atomic force microscopy</u> (AFM), anisotropic properties were investigated by both optical and electrical methods.

First, optical measurements were performed using reflectance difference microscopy*4) (RDM) developed by the present research team. A device of ReS₂ with an 8 nm thickness was irradiated with polarized light from various directions to determine the two axial (principle) directions of the 2-D crystal (Figure 2).

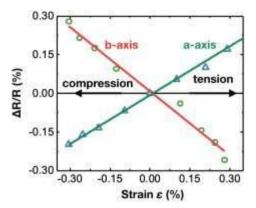


Figure 2. Relative resistance changes of the device

along two axes as a function of strain. It shows the relative resistance change of this ReS₂ device along the a- and b-axes, respectively, as a function of the strain. As expected, the a/b-axis showed positive/negative piezoresistance and almost linear change with the strain. Credit: Kanazawa University

Next, electric anisotropy was measured with the same sample for Optical

<u>measurements</u> along 12 directions with a spacing of 30 degrees. These measurements also determined the two principle directions which showed a 110 degree difference. The same measurements were carried out with another device of ReS₂, but with a different thickness (70 nm). The latter also yielded very similar anisotropic behavior, indicating the thickness-independent nature of the phenomenon. These results are consistent with previous work.

The 2-D crystal ReS₂ device whose principle axes were determined as above was clamped at one end along a principle axis and the other end was moved towards the fixed end at a specified speed, i.e. a compressive strain was applied. The device generated piezoresistance due to the strain. With one end fixed, piezoresistance recovered completely when the compressive strain of the other end was returned to its original state.

On the other hand, when the same experiment was performed along the other principle axis, the piezoresistance due to the strain was smaller when a larger strain was applied and increased when the applied strain was smaller. The same experiment was repeated with different ReS₂ devices, but the results were always consistent. Thus, ReS₂ 2-D crystalline devices showed opposite, i.e. positive or negative piezoresistance depending on the principle axes.

In addition, when the same experiment using a single device was repeated 28 times, almost the same results were obtained. This indicates that after applying a strain to the ReS₂ device, releasing the strain allowed the piezoresistant effect to return to its original state.

While the piezoresistant effect is a result of the bandgap adjustment induced by a strain, the piezoelectric effect is a result of a strain-dependent distortion of the crystal lattice. Various electrical measurements were performed, which also demonstrated that the phenomenon observed was piezoresistance and not the piezoelectric effect.

The present study demonstrated that the ReS₂ 2-D devices showed opposite, i.e. positive and negative piezoresistance depending on the principle axes along which a strain was applied. Such

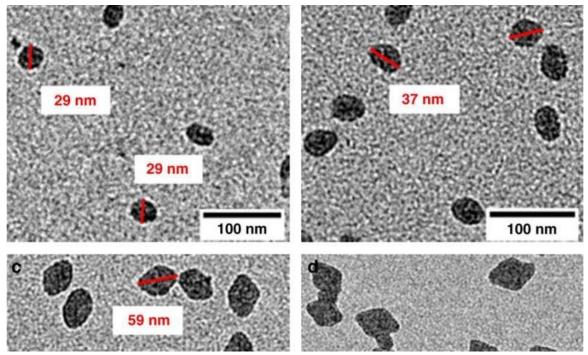
positive and negative piezoresistant effects depending on the principle axes were not observed in previous studies. Thus, the present study is the first to identify such an effect. It is expected that this study will lead to wide applications of ReS₂ to electronics, such as electronic skin, human-machine interfaces, strain sensors and so on. [39]

Researchers create uniform-shape polymer nanocrystals

A team of researchers from the University of Konstanz has demonstrated a new aqueous polymerization procedure for generating polymer nanoparticles with a single chain and uniform shape, which, by contrast to previous methods, involves high particle concentrations. A corresponding paper titled "Uniform shape monodisperse single chain nanocrystals by living aqueous catalytic polymerization" is set for publication in *Nature Communications*.

To build nanomaterials, <u>nanoparticles</u> with uniform shapes and sizes are required. While inorganic metal or metal oxide nanoparticles suitable for assembly can be generated in a variety of shapes, it has been very difficult until now to manufacture <u>polymer nanoparticles</u> in shapes other than spheres. Stefan Mecking, professor of chemical materials science at the University of Konstanz says, "In previous approaches, single-chain particles were prepared by post-<u>polymerization</u> collapse or assembled from solutions of separately synthesized chains. What we have managed to do is to demonstrate direct polymerization to single-chain uniform-shape monodisperse nanocrystals for polyethylene, which is the largest and most important synthetic <u>polymer</u> material."

One major challenge associated with this approach is to achieve living chain and particle growth that can be sustained for several hours and up to very high molecular weights, ideally yielding single-chain nanocrystals of ultra-high molecular weight polyethylene. To achieve this, the researchers developed advanced catalysts. "We then conducted a series of pressure reactor tests to identify ideal conditions for maintaining <u>Catalytic activity</u> over longer periods of time and to gain insights into the chain and particle growth process," explains Mecking. "In addition to the novel catalysts, control of the colloidal state of the reaction mixture is another key element in obtaining the desired aqueous particle dispersions."



TEM images of UHMWPE nanocrystals. a–d Nanocrystals obtained from aqueous polymerization after different reaction times showing the evolution of size and shape (entries 1 (a), 3 (b), 5 (c), and 7 (d), Table 2); e, f layered structures with short-range order formed by drying of uniform particle dispersions with different sizes (entries 2 (e) and 7 (f), Table 2), particle boundaries marked in red.

In contrast to many post-polymerization procedures, the aqueous polymerization procedure elaborated by Stefan Mecking and his team yields high particle number densities, which are comparable to commercial polymer dispersions used for coatings, paints and other applications. Using <u>transmission electron microscopy</u> (TEM), the researchers were able to confirm that the <u>particles</u> thus generated are composed of a single chain, display a uniform shape and size distribution and do not aggregate.

"While our assemblies may not fully match the extensively optimized assemblies of inorganic nanoparticles, they seem to be very promising," concludes Mecking. "In time, our insights into the creation of anisotropic polymer nanocrystals using aqueous catalytic polymerization may enable us to create polymer materials based on nanoparticle assembly." [38]

Using carbon nanotubes to strengthen graphene-based membranes used for desalination

A team of researchers from China, the U.S. and Japan has developed a way to strengthen graphenebased membranes intended for use in desalination projects—by fortifying them with nanotubes. In their paper published in the journal *Science*, the group describes how they created their fortified membranes and how well the membranes worked when tested. Baoxia Mi, with the University of California, has published a <u>Perspective piece</u> on the work by the team in the same journal issue.

As time passes and the human population grows, access to <u>Water</u> becomes more of a serious problem for many people around the world. To address the problem, scientists have been putting a lot of effort into creating better <u>Water filtration</u>systems to remove salt from water. Part of this effort has focused on finding better filters. One idea is to use a <u>graphene membrane</u>; prior research has shown that it would be faster and more efficient than current materials. But graphene sheets are also prone to defects and damage if struck by objects in the water, and they deteriorate quickly under the constant flow of water. In this new effort, the researchers have found a way to improve the strength of graphene-based membranes by using carbon nanotubes.

Prior research had shown that graphene-based membranes are more likely to have defects and are more prone to damage as their surface area increases. To get around that problem, the researchers created small cells of graphene nanomesh connected and held together by single-walled carbon nanotubes. The result was a centimeter-sized mesh with a honeycomb appearance—one that was large enough to test as a <u>membrane</u> in a filtration system. The researchers report that testing showed their membrane to be highly efficient, and just as important, less prone to damage migration—if damage occurred to the mesh in one of the cells, it was constrained to that cell alone.

The researchers claim that their technique could be used to produce membranes large enough for commercial applications. Mi points out, however, that despite the good work done by the team in creating the membrane, more work is required before <u>**Graphene</u>** can be used in any kind of real-world application. [37]</u>

Research reveals liquid gold on the nanoscale

The research published in *Nature Communications* set out to answer a simple question—how do nanoparticles melt? Although this question has been a focus of researchers for the past century, it still is an open problem—initial theoretical models describing melting date from around 100 years, and even the most relevant models being some 50 years old.

Professor Richard Palmer, who led the team based at the University's College of Engineering said of the research: "Although melting behaviour was known to change on the nanoscale, the way in which <u>nanoparticles</u> melt was an open question. Given that the theoretical models are now rather old, there was a clear case for us to carry out our new imaging experiments to see if we could test and improve these <u>theoretical models</u>."

The research team used gold in their experiments as it acts as a model system for noble and other metals. The team arrived at their results by imaging gold nanoparticles, with diameters ranging from 2 to 5 nanometres, via aberration corrected scanning transmission electron microscope. Their observations were later supported by large-scale quantum mechanical simulations.

Professor Palmer said: "We were able to prove the dependence of the melting point of the nanoparticles on their size and for the first time see directly the formation of a liquid shell around a solid core in the nanoparticles over a wide region of elevated temperatures, in fact for hundreds of degrees.

"This helps us to describe accurately how nanoparticles melt and to predict their behaviour at elevated temperatures. This is a science breakthrough in a field we can all relate to—melting—and will also help those producing nanotech devices for a range of practical and everyday uses, including medicine, catalysis and electronics." [36]

Scientists explore the unknown behaviour of gold nanoparticles with neutrons

Nanoparticles of less than 100 nanometres in size are used to engineer new materials and nanotechnologies across a variety of sectors. Their small size means these particles have a very high surface area to volume ratio and their properties depend strongly on their size, shape and bound molecules. This offers engineers greater flexibility when designing materials that can be used in our everyday lives. Nanoparticles are found in sunblock creams and cosmetics as well as inside our bodies, as drug delivery vehicles and as contrast agents for pharmaceuticals. Gold nanoparticles are proving to be a next-generation tool in nanoengineering as an effective catalyst at such small dimensions. However, nanomaterials also pose a potential risk, as their interactions with living matter and the environment are not fully understood—meaning that they might not perform as expected, for instance in the human body.

While scientists have been able to fine-tune and engineer the properties of nanoparticles by changing their size, shape, surface chemistry and even physical state, such a variety of possibilities means that dictating precisely how the particles behave at that small scale also becomes extremely difficult. This is of particular concern as we rely on the potential use of nanoparticles within the human body. Gold nanoparticles are good carriers of large and small molecules, making them ideal for transporting drugs to human cells. However, predicting how far they are then absorbed by the cells and their toxicity, is difficult, as is understanding any associated risks to health using these nanomaterials.

A European collaboration of researchers, including scientists from the Institut Laue-Langevin (ILL), Tampere University, University of Helsinki, Norwegian University of Science and Technology, and Université Grenoble Alpes, investigated the physical and chemical influences when gold nanoparticles interact with a model <u>biological membrane</u> in order to identify the behavioural mechanisms taking place. Better understanding the factors that determine whether nanoparticles are attracted or repelled by the cell membrane, whether they are adsorbed or internalised, or whether they cause membrane destabilisation, will help us to ensure that nanoparticles interact with our cells in a controlled way. This is particularly important when using gold nanoparticles for drug delivery, for example. As outlined in the journal *Small*, the researchers used a combination of neutron scattering techniques and <u>COMPUTATIONAL methods</u> to study the interaction between positively charged cationic gold nanoparticles and model lipid membranes. The study showed how the temperature and the lipid charge modulate the presence of energy barriers that affect the interaction of the nanoparticle with the membrane. Furthermore, different molecular mechanisms for nanoparticle-membrane interactions are revealed which explain how nanoparticles become internalised in the lipid membranes, and how they cooperatively act to destabilise a negatively charged lipid membrane.

Using Molecular Dynamics (MD), a computational simulation method for studying the movement of atoms, the researchers demonstrated how <u>gold nanoparticles</u> interacted within the system at the atomic level. This gives a complementary tool to interpret and explain the data obtained on real systems by <u>neutron reflectometry</u>. This study shows convincingly that the combination of neutron scattering and computational methods provides a better understanding than just one of the methods alone.

Giovanna Fragneto, Head of Soft Matter Science and Support at ILL said: "Nanoparticles are proving to be an invaluable tool to help us address a number of social challenges. For instance, as well as mechanisms for drug delivery, gold particles can prove useful for cancer imaging. With so much promise for the future, it is important that we develop the tools to better investigate nanomaterials, so we can harness them effectively and safely. This is made possible through developments in neutron science techniques and advances in sample environment and sample preparation, performed at facilities such as ILL."

Marco Maccarini, research scientist at the Université Grenoble Alpes, said: "There are thousands of different nanoparticles of different sizes and compositions, which all impact cells differently. The complementarity of computational and neutron techniques highlighted in this study has helped to provide a clearer indication of what influences the behaviour of nanoparticles. This will help us predict how cells will interact with <u>nanoparticles</u> in future." [35]

Research team discovers perfectly imperfect twist on nanowire growth

For years, researchers have been trying to find ways to grow an optimal nanowire, using crystals with perfectly aligned layers all along the wire.

A team of Nebraska Engineering researchers—Peter Sutter, Eli Sutter and Shawn Wimer—sees an advantage to natural imperfection.

Through their research, highlighted in a letter published in the April 22 edition of the journal *Nature*, the group found that a defect—a screw dislocation—that occurs in the growth process causes the layers of crystals to rotate along an axis as they form. This defect creates twists that give these nanowires advantages, particularly in electronics and light emission.

"In layered nanowires, we basically have a new architecture that implements a crystal twist between two-dimensional materials," said Peter Sutter, professor of electrical and computer engineering. "We take the approach that you can (either) make such twist moiré structures or have them make themselves, and when we let the wires do the job on their own, nature introduces this defect, a twist."

Typically, materials with twisted interfaces are artificially created from two atomically thin 2-D crystals. When these crystals are painstakingly placed on top of each other, a small rotation among them—an interlayer twist—causes a moiré, or a beat pattern that changes with the twist angle and is much larger than the spacing of the atoms in the material. The motion of electrons in this beat pattern cause new phenomena, such as superconductivity or systematic changes in the color of emitted light.

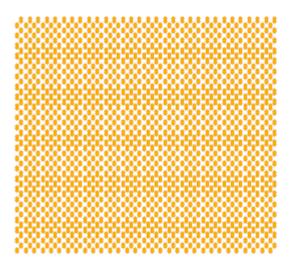
The Sutters' team took a different approach to realizing these twists by growing nanowires that consist of 2-D layers. They took small particles of gold, heated them up and inundated them with a vapor of germanium sulfide. At <u>high temperatures</u>, the gold particles melted and alloyed with the germanium sulfide.

"At some point, it gets saturated and can't take any more of it in. Then it has a choice: don't take in any more and let a film grow over it on the surface, or continue to try to absorb more," said Eli Sutter, professor of electrical and computer engineering. "It turns out these particles are greedy for germanium sulfide."

The gold particles kept absorbing the vapor but became too saturated to hold it all and began growing layered crystals of germanium sulfide, one per gold particle. When the germanium sulfide was expelled, the <u>Crystals</u> lengthened and turned into nanowires that are about 1,000 times thinner than a human hair.

The team discovered that each of these wires had a screw dislocation, which produced a helical structure and the twist between their crystal layers.

To explore the properties of their helical twisted nanowires, the team used a focused beam of electrons to stimulate the emission of light from minute portions of their nanowires. When the excited electrons relax, they emit light of a characteristic color or frequency, which the researchers recorded.



An animation showing the twist moiré

pattern that emerges when stacking crystals on each other and introducing a small rotation. Credit: University of Nebraska-Lincoln

By allowing for an imperfect stack of twisted layers, the germanium sulfide nanowires emit different colors of light at different points along the wire. This makes it possible to tune the band gap and control the energy of absorbed or emitted light.

"We were able to show there are new, accessible <u>light-emission</u> properties that change along the wire because the moiré registry changes," Eli Sutter said.

Twisted nanowires of <u>**Germanium**</u> <u>**Sulfide**</u>, a semiconductor, could have applications that include energy harvesting, tunable light sources, or next-generation computing.

The researchers, however, said their next step is understanding why the color of emitted light changes along the wire and possibly achieving similar results with other materials.

"We have to better understand the consequences of the helical twist structure. We expect that twisted <u>nanowires</u> still have many other surprises in store for us," Peter Sutter said.

This material is based upon work supported by the National Science Foundation under Grant No. DMR-1607795. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation. [34]

Nanosized ferroelectrics become a reality

Using ferroelectricity instead of magnetism in computer memory saves energy. If ferroelectric bits were nanosized, this would also save space. But conventional wisdom dictates that ferroelectric

properties disappear when the bits are made smaller. Reports that hafnium oxide can be used to make a nanoscale ferroelectric have not yet convinced the field, however University of Groningen (UG) physicists have now gathered evidence that could persuade the skeptics, published in *Nature Materials* on 22 October.

Ferroelectric <u>materials</u> have a spontaneous dipole moment which can point up or down. This means that they can be used to store information, just like magnetic bits on a hard disk. The advantage of ferroelectric bits is that they can be written at a low voltage and power. Magnetic bits require large currents to create a magnetic field for switching, and thus more power. The disadvantage of ferroelectrics is that the aligned dipoles are only stable in fairly large groups, so if you make the crystals smaller, the dipole moment eventually disappears.

Skepticism

"Reducing the size of <u>ferroelectric materials</u> has been a research topic for more than 20 years," says UG Functional Nanomaterials Professor Beatriz Noheda. Some eight years ago, a breakthrough was announced by the Nanoelectronic Materials Laboratory in Dresden, Germany. They claimed that <u>hafnium oxide</u> thin films were ferroelectric when thinner than ten nanometres and that thicker films actually lost their <u>ferroelectric properties</u>. Noheda says, "This went against everything we knew, so most scientists were skeptical, including me." Some of the skepticism was because the ferroelectric <u>hafnium</u> samples used in these studies were polycrystalline and showed multiple phases, obscuring any clear fundamental understanding of such an unconventional phenomenon.

Noheda and her group decided to investigate. They wanted to study these crystals by growing clean (single-phase) films on a substrate. Using X-ray scattering and high-resolution electron microscopy techniques, they observed that very thin films (under ten nanometres) grow in an entirely unexpected and previously unknown polar structure, which is necessary for ferroelectricity. Combining these observations with meticulous transport measurements, they confirmed that the material was indeed ferroelectric. "In the substrate that we used, the atoms were a little bit closer than those in hafnium <u>oxide</u>, so the hafnium crystals would be a little strained," Noheda explains.

Polar phase

To their surprise, they noticed that the crystal structure changed when the layers exceeded ten nanometres, thus reproducing the results of the Dresden lab. Noheda: "We used a totally different method, but we reached similar conclusions. This confirmed that ferroelectricity in nanosized hafnium oxide crystals is indeed real and unconventional. And that begged the question: why does this happen?"

The common denominator in both studies was size. Small crystals became ferroelectric, whereas larger crystals lost this property. This led the scientists to study the phase diagrams of hafnium oxide. At a very small size, particles have a very large surface energy, creating pressures of up to 5 gigapascals in the crystal. The phase diagrams show a different crystal arrangement at such a pressure. "This pressure, along with the substrate-imposed strain, induces a polar phase, which is in line with the observation that these crystals are ferroelectric," concludes Noheda.

Wake up cycle

One more important finding is that, in contrast to the thin films in Dresden, the new crystals do not need a 'wake-up' cycle to become ferroelectric. Noheda: "The previously studied thin films only

became ferroelectric after going through a number of switching cycles. This increased the suspicion that ferroelectricity was some sort of artefact. We now believe that the wake-up cycles were necessary to align the dipoles in "unclean" samples grown via other techniques. In our material, the alignment is already present in the crystals."

In Noheda's opinion, the results are conclusive: hafnium oxide is ferroelectric at the nanoscale. This means that very small bits can be constructed from this material, with the added advantage that they switch at low voltage. Furthermore, the particular substrate used in this study is magnetic, and this combination of magnetic and ferroelectric bits brings an extra degree of freedom, allowing each bit to store double the information. Now that the mechanism of nanosized ferroelectricity is clear, it seems likely that other simple oxides could have similar properties. Noheda expects that together, this will spark a lot of new research. [33]

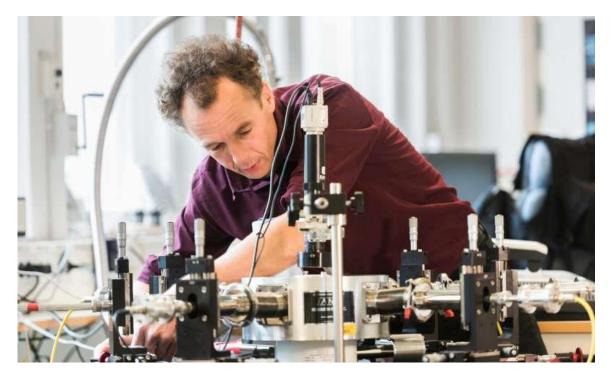
Researchers validate 80-year-old ferroelectric theory

Researchers have successfully demonstrated that hypothetical particles that were proposed by Franz Preisach in 1935 actually exist. In an article published in *Nature Communications*, scientists from the universities in Linköping and Eindhoven show why ferroelectric materials act as they do.

Ferroelectricity is the lesser-known twin of ferromagnetism. Iron, cobalt and nickel are examples of common ferromagnetic materials. The electrons in such materials function as small magnets, dipoles, with a north pole and a south pole. In a ferroelectric, the dipoles are electric rather than magnetic, and have a positive and negative pole.

In absence of an applied magnetic (for a ferromagnet) or electric (for a ferroelectric) <u>field</u>, the orientation of the dipoles is random. When a sufficiently strong field is applied, the dipoles align with it. This field is known as the critical (or coercive) field. Surprisingly, in a ferroic material, the alignment remains when the field is removed, and the material is permanently polarized. To change the direction of the polarization, a field at least as strong as the critical field must be applied in the opposite direction. This effect is known as hysteresis—the behaviour of the material depends on what has previously happened to it. Hysteresis makes these materials highly suitable as rewritable memory, for example, in hard disks.

In an ideal ferroelectric material, the whole piece switches its polarization when the critical field is reached and it does so with a well-defined speed. In real ferroelectric materials, different parts of the material switch polarization at different critical fields, and at different speeds. Understanding this non-ideality is key to application in computer memory.

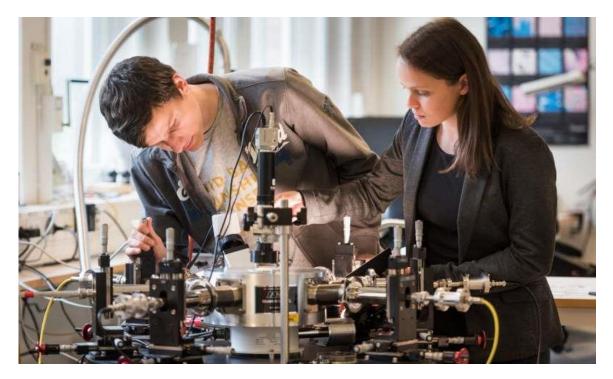


Professor Martijn Kemerink. Credit: Thor Balkhed

A model for ferroelectricity and ferromagnetism was developed by the German researcher Franz Preisach as early as 1935. The purely mathematical Preisach model describes ferroic materials as a large collection of small, independent modules called hysterons. Each hysteron shows ideal ferroic behaviour, but has its own critical field that can differ from hysteron to hysteron. It has been generally agreed that the model gives an accurate description of real materials, but scientists have not understood the physics on which the model is built. What are the hysterons? Why do their critical fields differ as they do? In other words, why do ferroelectric materials act as they do?

Professor Martijn Kemerink's research group (Complex Materials and Devices at LiU), in collaboration with researchers at the University of Eindhoven, has now studied two organic ferroelectric model systems and found the explanation. The molecules in the studied organic ferroelectric materials like to lie on top of each other, forming cylindrical stacks of around a nanometre wide and several nanometres long.

"We could prove that these stacks actually are the sought-after hysterons. The trick is that they have different sizes and strongly interact with each other since they are so closely packed. Apart from its own unique size, each stack therefore feels a different environment of other stacks, which explains the Preisach distribution," says Martijn Kemerink.



Tim Cornelissen and Indre Urbanaviciute, Linköping University. Credit: Thor Balkhed

The researchers have shown that the non-ideal switching of a ferroelectric material depends on its nanostructure—in particular, how many stacks interact with each other, and the details of the way in which they do this.

"We had to develop new methods to measure the switching of individual hysterons to test our ideas. Now that we have shown how the molecules interact with each other on the nanometre scale, we can predict the shape of the hysteresis curve. This also explains why the phenomenon acts as it does. We have shown how the hysteron distribution arises in two specific organic <u>ferroelectric materials</u>, but it's quite likely that this is a general phenomenon. I am extremely proud of my doctoral students, Indre Urbanaviciute and Tim Cornelissen, who have managed to achieve this," says Martijn Kemerink.

The results can guide the design of <u>materials</u> for new, so-called multi-bit memories, and are a further step along the pathway to the small and flexible memories of the future. [32]

Researchers switch material from one state to another with a single flash of light

Scientists from the Department of Energy's SLAC National Accelerator Laboratory and the Massachusetts Institute of Technology have demonstrated a surprisingly simple way of flipping a material from one state into another, and then back again, with single flashes of laser light.

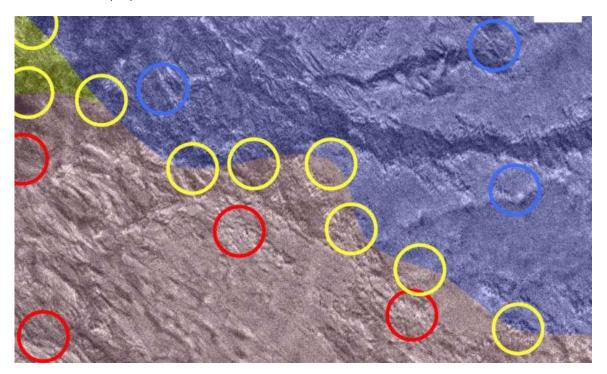
This switching behavior is similar to what happens in magnetic data storage <u>materials</u>, and making the switch with <u>laser light</u> could offer a new way to read and write information in next-generation

data storage devices, among other unprecedented applications, says Nuh Gedik, the study's principal investigator at MIT. The team reported their results today in *Science Advances*.

Frozen waves of electrons

In today's devices, information is stored and retrieved by flipping the spin of electrons with a magnetic field. "But here we flipped a different material property known as <u>charge density</u> <u>waves</u>," says Alfred Zong, a graduate student in Gedik's group and one of the study's lead authors.

Charge density waves are periodic peaks and valleys in the way electrons are distributed in a material. They are motionless, like icy waves on a frozen lake. Scientists want to learn more about these waves because they often coexist with other interesting material properties, such as the ability to conduct electricity without loss at relatively high temperatures, and could potentially be related to those properties.



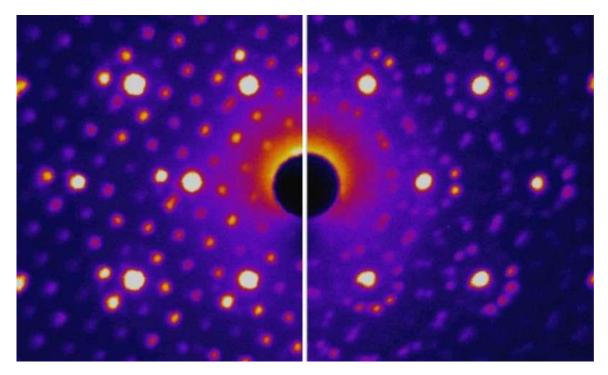
This transmission electron microscopy image shows a domain wall (marked with yellow circles) between two different states, alpha (red area) and beta (blue area), in a tantalum disulfide crystal. The beta state and domain wall formed after ...<u>more</u>

The new study focused on tantalum disulfide, a material with charge density waves that are all oriented in the same direction in what's called the alpha state. When the researchers zapped a thin crystal of the material with a very brief laser pulse, some of the waves flipped into a beta state with a different electron orientation, and the alpha and beta regions were separated by domain walls. A second flash of light dissolved the domain walls and returned the material to its pure alpha state.

Surprising material switch

These changes in the material, which had never been seen before, were detected with SLAC's instrument for ultrafast electron diffraction (UED), a high-speed "electron camera" that probes the motions of a material's atomic structure with a powerful beam of very energetic electrons.

"We were looking for other effects in our experiment, so we were taken by complete surprise when we saw that we can write and erase domain walls with single light pulses," says Xijie Wang, head of SLAC's UED group.



Intensity patterns recorded with SLAC's "electron camera" showed researchers how the atomic structure of a tantalum disulfide crystal responded to laser flashes, switching from an alpha state (left) to an alpha/beta state (right) and back. ...<u>more</u>

Anshul Kogar, a postdoctoral researcher in Gedik's group, says, "The <u>domain walls</u> are a particularly interesting feature because they have properties that differ from the rest of the material." For example, they might play a role in the drastic change seen in tantalum disulfide's electrical resistance when it's exposed to ultrashort light pulses, which was previously observed by another group.

SLAC staff scientist Xiaozhe Shen, one of the study's lead authors on Wang's team, says, "UED allowed us to analyze in detail how the domains formed over time, how large they were and how they were distributed in the material."

The researchers also found that they can fine-tune the process by adjusting the temperature of the crystal and the energy of the light pulse, giving them control over the material switch. In a next step, the team wants to gain even more control, for example by shaping the light pulse in a way that it allows generating particular domain patterns in the material.

"The fact that we can tune a material in a very simple manner seems very fundamental," Wang says. "So fundamental, in fact, that it could turn out to be an important step toward using <u>light</u> in creating the exact material properties we want." [31]

Supercomputer predicts optical and thermal properties of complex hybrid materials

Materials scientists at Duke University computationally predicted the electrical and optical properties of semiconductors made from extended organic molecules sandwiched by inorganic structures.

These types of so-called layered "hybrid organic-inorganic perovskites"—or HOIPs—are popular targets for light-based devices such as solar cells and light-emitting diodes (LEDs). The ability to build accurate models of these materials atom-by-atom will allow researchers to explore new material designs for next-generation devices.

The results appeared online on October 4 in Physical Review Letters.

"Ideally we would like to be able to manipulate the organic and <u>inorganic components</u> of these types of materials independently and create semiconductors with new, predictable properties," said David Mitzi, the Simon Family Professor of Mechanical Engineering and Materials Science at Duke. "This study shows that we are able to match and explain the experimental properties of these materials through complex supercomputer simulations, which is quite exciting."

HOIPs are a promising class of materials because of the combined strengths of their constituent organic and inorganic pieces. Organic materials have more desirable optical properties and may be bendable, but can be ineffective at transporting electrical charge. Inorganic structures, on the other hand, are typically good at conducting electricity and offer more robust mechanical strength.

Combining the two can affect their individual properties while creating hybrid materials with the best of both worlds. Understanding the electronic and atomic-scale consequences of their interaction, however, is challenging at best, since the resulting crystals or films can be structurally complex. But because these particular HOIPs have their organic and inorganic components in well-ordered layers, their structures are somewhat easier to model, and researchers are now beginning to have success at computationally predicting their behaviors on an atomic level.

"The computational approach we used has rarely been applied to structures of this size," said Volker Blum, associate professor of mechanical engineering and <u>materials science</u> and of chemistry at Duke. "We couldn't have done it even just 10 years ago. Even today, this work would not have been possible without access to one of the fastest supercomputers in the world."

That supercomputer—dubbed Theta—is currently the 21st fastest in the world and resides at Argonne National Laboratory. The group was able to gain time on the behemoth through Blum securing one of only a dozen Theta Early Science Projects, aimed at paving the way for other applications to run on the system first launched in late 2017. They are now co-investigators on one of Department of Energy's prestigious "Innovative and Novel Computational Impact on Theory and Experiment" (INCITE) awards, enabling them to continue their work.

In the new study, Chi Liu, a graduate student in Blum's laboratory; Yosuke Kanai, a fellow theorist at the University of North Carolina – Chapel Hill; and Alvaro Vazquez-Mayagoitia, a scientist at Argonne National Laboratory, used Theta's computational power to model the electronic states

within a layered HOIP first synthesized by Mitzi more than a decade ago. While the electrical and <u>optical properties</u> of the material are well-known, the physics behind how they emerge have been much debated.

The team has now settled the debate.

In a series of computational models, the team calculates the electronic states and localizes the valence band and conduction band of the HOIP's constituent materials, the organic bis(aminoethyl)-quaterthiophene (AE4T) and the inorganic lead bromide (PbBr4). These properties dictate how electrons travel through and between the two materials, which determines the wavelengths and energies of light it absorbs and emits, among other important properties such as electrical conduction.

The results showed that the team's computations and experimental observations match, proving that the computations can accurately model the behaviors of the material.

Liu then went further by tweaking the materials—varying the length of the organic molecular chain and substituting chlorine or iodine for the bromine in the inorganic structure—and running additional computations. On the experimental side, Mitzi and collaborator Wei You, professor of chemistry and applied physical sciences at the University of North Carolina – Chapel Hill, are working on the difficult task of synthesizing these variations to further verify their colleagues' theoretical models.

The work is part of a larger initiative called the HybriD3 project aimed at discovering and fine-tuning new functional semiconductor materials. The collaborative effort features a total of six teams of researchers. Joining those researchers located at Duke University and the University of North Carolina at Chapel Hill, professors Kenan Gundogdu and Franky So at North Carolina State University are working to further characterize the materials made in the project, as well as exploring prototype light-emitting devices.

"By using the same type of computation, we can now try to predict the properties of similar materials that do not yet exist," said Mitzi. "We can fill in the components and, assuming that the structure doesn't change radically, provide promising targets for materials scientists to pursue."

This ability will allow scientists to more easily search for better materials for a wide range of applications. For this particular class of materials, that includes lighting and water purification.

Inorganic light sources are typically surrounded by diffusers to scatter and soften their intense, concentrated light, which leads to inefficiencies. This class of layered HOIPs could make films that achieve this more naturally while wasting less of the light. For water purification, the material could be tailored for efficient high-energy emissions in the ultraviolet range, which can be used to kill bacteria.

"The broader aim of the project is to figure out the material space in this class of <u>materials</u> in general, well beyond the organic thiophene seen in this study," said Blum. "The key point is that we've demonstrated we can do these calculations through this proof of concept. Now we have to work on expanding it." [30]

Perovskite semiconductors seeing right through next generation X-ray detectors

From observing celestial objects to medical imaging, the sensitive detection of X-rays plays a central role in countless applications. However, the methods used to detect them have undergone an interesting evolution of their own.

X-ray detector designs vary in shape, function and ultimately performance. For example, indirect scintillators detect X-rays by converting the high energy of X-ray photons into light which is visible to the naked eye. This down-shifting makes it possible to use well-established optical detectors to generate a detectable electronic signal. Besides the need for large, complicated multi-component devices, such designs inherent significant limitations when applied for imaging. Direct conversion semiconductor detectors directly absorb and convert X-ray photons into electrical charge, which can then be collected to generate a digital signal. Direct conversion configurations are not only much simpler, but also allow for the imaging smaller details.

KU Leuven researchers from the Roeffaers Lab and the Hofkens Group have now put forward a very promising direct X-ray detector design, based on a rapidly emerging halide <u>perovskite</u> semiconductor, with chemical formula Cs₂AgBiBr₆. Perovskite is the general name for a particular type of periodic crystal structure, which, when composed of heavy elements like silver (Ag) and bismuth (Bi), are ideal for direct X-ray conversion because of their ability to combine both heavy atomic nuclei – for efficient X-ray absorption – with their excellent charge formation and transport properties.

The researchers singled out the all-inorganic double metal halide perovskite $Cs_2AgBiBr_6$ as one of the strongest candidates because of its high X-ray sensitivity and excellent structural stability. By optimising the materials and lowering the operating temperature, they were even able to improve the X-ray sensitivity of the device tenfold, ultimately peaking near 500 times more sensitive than commercial direct conversion X-ray detectors on the market – commonly based on pure selenium (Se).

Importantly, the researchers studied their simple single crystal $Cs_2AgBiBr_6 \underline{detector}$ at both room and low temperatures to track physical features that are beneficial for the efficient conversion of Xrays into a collectible signal. This is an extremely novel approach, and one that offers a generic method for screening other potentially good X-ray detecting mediums. Using this method, the researchers developed an extensive photo-physical model to account for the large jump in X-ray sensitivity when operating at reduced temperatures.

This research is a big step forward in the development of new, cheap and easy to make, and highly sensitive X-ray detectors based on perovskite semiconductors. The breadth of possible applications is vast, stretching from more refined fundamental research, all the way to improved medical diagnostics.

The researchers recently published their discovery in the high-impact material science journal *Advanced Materials*. [29]

Researchers decipher the dynamics of electrons in perovskite crystals

Physicists at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) have proven that incoming light causes the electrons in warm perovskites to rotate, thus influencing the direction of the flow of electrical current. They have thus found the key to an important characteristic of these crystals, which could play an important role in the development of new solar cells. The results have now been published in *Proceedings of the National Academy of Sciences*.

The sun is an important source of renewable energy. Its radiation energy provides heat, and sunlight can be converted into electricity thanks to photovoltaics. Perovskites, crystalline compounds that can be simply manufactured using chemical processes, are considered a promising material for photovoltaics. Under laboratory conditions, prototypes have achieved surprising levels of efficiency.

There is little knowledge about precisely why perovskites are so powerful. "Two factors are decisive for generating electrical energy cost-efficiently from sunlight," says Dr. Daniel Niesner from the Chair of Solid State Physics at FAU. "On the one hand, the light must excite as many <u>electrons</u> as possible in a layer that's as thin as possible. On the other, the electrons must be able to flow as freely as possible to the electrodes that pick up the current."

Researchers suspect that perovskites make particularly good use of the rotation of electrons for efficient current flow. "Each electron has spin, similar to the intrinsic rotation of a billiard ball," explains Niesner. "As is the case with billiard balls, where left-hand or right-hand spin when they are hit with the cue leads to a curved path on the table, scientists have suspected that rotation and forward movement in electrons in perovskites could also be linked."

Orderly atomic structure

Physicists at FAU in Erlangen have now confirmed this suspicion for the first time. In their experiments, they used a laser whose light also has spin or a direction of rotation. The result: If a crystal is exposed to light with a left-hand spin, the electrons move to the left. If the direction of the light is reversed, the direction of the flow of electrons also reverses. "The experiments clearly demonstrate that the direction of rotation of the electrons and the direction of flow of current are linked."

Until now, scientists presumed that the atomic structure of perovskites was too 'orderly' for such behaviour. In actual fact, experiments with cooled <u>perovskite</u> crystals show only a very weak link between the direction of rotation of the electrons and the direction of current flow. "This changes, however, when the crystals are heated to room temperature because the movement of the atoms leads to fluctuating deviations of the highly-ordered structure," says Nieser. "The heat enables the crystals of perovskite to link the <u>direction</u> of rotation and flow of the electrons. A 'normal' crystal couldn't do that."

The discovery of the connection between heat and spin in electrons means that the FAU researchers have uncovered a vital aspect of the unusual flow of current in perovskites. Their work could contribute to improving the understanding of the high energy efficiency of these crystals and to developing new materials for photovoltaics in the future. [28]

Nanoparticles form supercrystals under pressure

Self-assembly and crystallisation of nanoparticles (NPs) is generally a complex process, based on the evaporation or precipitation of NP-building blocks. Obtaining high-quality supercrystals is slow, dependent on forming and maintaining homogenous crystallisation conditions. Recent studies have used applied pressure as a homogenous method to induce various structural transformations and phase transitions in pre-ordered nanoparticle assemblies. Now, in work recently published in the *Journal of Physical Chemistry Letters*, a team of German researchers studying solutions of gold nanoparticles coated with poly(ethylene glycol)- (PEG-) based ligands has discovered that supercrystals can be induced to form rapidly within the whole suspension.

Over the last few decades, there has been considerable interest in the formation of nanoparticle (NP) supercrystals, which can exhibit tunable and collective properties that are different from that of their component parts, and which have potential applications in areas such as optics, electronics, and sensor platforms. Whilst the formation of high-quality supercrystals is normally a slow and complex process, recent research has shown that applying <u>pressure</u> can induce gold nanoparticles to form supercrystals. Building on this and the established effect of salts on the solubility of gold nanoparticles (AuNP) coated with PEG-based ligands, Dr. Martin Schroer and his team carried out a series of experiments investigating the effect of varying pressure on <u>gold nanoparticles</u> in aqueous solutions. They made an unexpected observation – when a salt is added to the solution, the <u>nanoparticles</u> crystallise at a certain pressure. The phase diagram is very sensitive, and the crystallisation can be tuned by varying the type of salt added, and its concentration.

The team used small angle x-ray scattering (SAXS) on beamline I22 to study the crystallisation in situ with different chloride salts (NaCl, KCl, RbCl, CsCl). As Dr. Schroer explains,

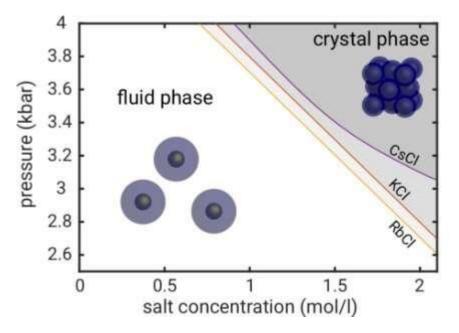


Fig. 2: Pressure – salt concentration phase diagram of AuNP@PEG. For low pressures, the particles are in the liquid state, beyond a critical pressure, face-centred cubic (fcc) superlattices are formed within solution. The crystallisation ...<u>more</u>

122 is one of the few beamlines to offer a high-pressure environment, and it is unusual because the experimental setup is easily managed by the users themselves. The beamline staff are excellent, and we are particularly grateful for their expertise in data processing, which was invaluable."

The resulting pressure-salt concentration phase diagram shows that the crystallisation is a result of the combined effect of salt and pressure on the PEG coatings. Supercrystal formation occurs only at high salt concentrations, and is reversible. Increasing the salt concentration leads to a continuous decrease of the crystallisation pressure, whereas the lattice structure and degree of crystallinity is independent of the <u>salt</u> type and concentration.

When reaching the crystallisation pressure, supercrystals form within the whole suspension; compressing the liquid further results in changes of the lattice constant, but no further crystallisation or structural transitions. This technique should be applicable to a variety of nanomaterials, and future studies may reveal insights into supercrystal formation that will help to understand crystallisation processes and enable the development of new and quicker methods for the synthesis of NP supercrystals.

The NP <u>crystallisation</u> appears to be instantaneous, but in this set of experiments there was a delay of around 30 seconds between applying the pressure and taking the SAXS measurements. Dr. Schroer and his team are returning to Diamond later this year to carry out time-resolved studies to further investigate this phenomenon. [27]

Researchers develop nanoparticle films for high-density data storage

As we generate more and more data, the need for high-density data storage that remains stable over time is becoming critical. New nanoparticle-based films that are more than 80 times thinner than a human hair may help to fill this need by providing materials that can holographically archive more than 1000 times more data than a DVD in a 10-by-10-centimeter piece of film. The new technology could one day enable tiny wearable devices that capture and store 3-D images of objects or people.

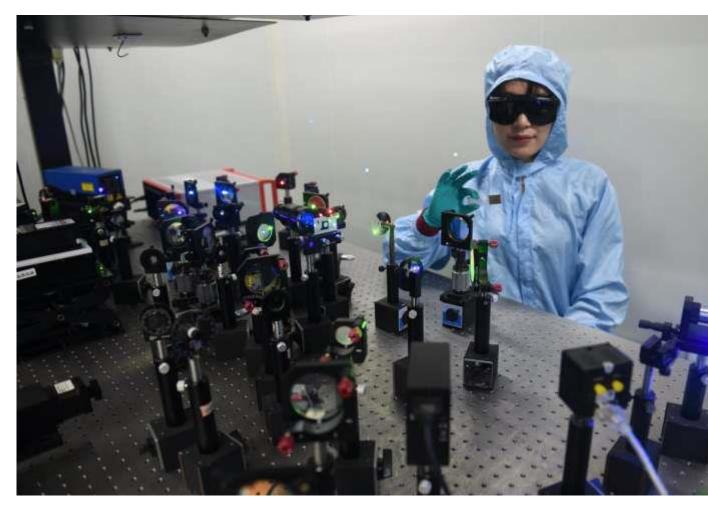
"In the future, these new films could be incorporated into a tiny <u>storage</u> chip that records 3-D color information that could later be viewed as a 3-D hologram with realistic detail," said Shencheng Fu, who led researchers from Northeast Normal University in China who developed the new films. "Because the storage medium is environmentally stable, the device could be used outside or even brought into the harsh radiation conditions of outer space."

In the journal *Optical Materials Express*, the researchers detail their fabrication of the new films and demonstrate the technology's ability to be used for an environmentally-stable holographic storage system. The films not only hold large amounts of data, but that data can also be retrieved at speeds up to 1 GB per second, which is about twenty times the reading speed of today's flash memory.

Storing more data in less space

The new films are designed for holographic data storage, a technique that uses lasers to create and read a 3-D holographic recreation of data in a material. Because it can record and read millions of bits at once, holographic data storage is much faster than optical and magnetic approaches typically used for data storage today, which record and read individual bits one at a time. Holographic approaches are also inherently high-density because they record information throughout the 3-D volume of the material, not just on the surface, and can record multiple images in the same area using light at different angles or consisting of different colors.

Recently, researchers have been experimenting with using metal-semiconductor nanocomposites as a medium for storing nanoscale holograms with high spatial resolution. Porous films made of the semiconductor titania and silver nanoparticles are promising for this application because they change color when exposed to various wavelengths, or colors, of laser light and because a set of 3-D images can be recorded at the focus area of laser beam using a single step. Although the films could be used for multiwavelength holographic data storage, exposure to UV light has been shown to erase the data, making the films unstable for long-term information storage.



Shuangyan Liu is holding the new UV-resistant holographic storage film. The new technology could one day be used to make tiny wearable devices that capture and store 3-D images of objects or people. Credit: Northeast Normal University

Recording a holographic image into titania-silver films involves using a laser to convert the silver particles into silver cations, which have a positive charge due to extra electrons. "We noticed that UV light could erase the data because it caused electrons to transfer from the semiconductor film to the metal nanoparticles, inducing the same photo transformation as the laser," said Fu. "Introducing electron-accepting molecules into the system causes some of the electrons to flow from the semiconductor to these molecules, weakening the ability of UV light to erase the data and creating an environmentally stable high-density data storage medium."

Changing the electron flow

For the new films, the researchers used electron-accepting molecules that measured only 1 to 2 nanometers to disrupt the electron flow from the semiconductor to the metal nanoparticles. They fabricated semiconductor films with a honeycomb nanopore structure that allowed the nanoparticles, electron-accepting molecules and the semiconductor to all interface with each other. The ultrasmall size of the electron-accepting molecules allowed them to attach inside the pores without affecting the pore structure. The final films were just 620 nanometers thick.

The researchers tested their new films and found that holograms can be written into them efficiently and with high stability even in the presence of UV light. The researchers also demonstrated that using the electron-acceptors to change the <u>electron flow</u> formed multiple electron transferring paths, making the material respond faster to the laser light and greatly accelerating the speed of data writing.

"Particles made from noble metals such as silver are typically viewed as a slow-response media for optical storage," said Fu. "We show that using a new electron transport flow improves the optical response speed of the particles while still maintaining the particle's other advantages for information storage."

The researchers plan to test the environmental stability of the new films by performing outdoor tests. They also point out that real-life application of the <u>films</u> would require the development of high efficiency 3-D image reconstruction techniques and methods for color presentation for displaying or reading the stored data. [26]

Researchers developing materials for quantum computing

Creation of innovative materials is one of the most important areas of modern science. Active development of Industry 4.0 requires new properties from composite elements of electronics. Researches of scientists from South Ural State University are implemented within this area. SUSU's Crystal Growth Laboratory performs modification of properties and structure of ferrites, which are oxides of iron with other metals' oxides. This task is performed by introducing other chemical elements into the structure of barium hexaferrite in order to obtain new working characteristics of the material.

One of the latest research articles dedicated to this topic was published at the end of 2017 in *Ceramics International*.

"The specificity of ferrite crystal structure is in the fact that it has five different positions of iron in the crystal lattice. This is exactly what allows modifying the structure and properties of the material in a sufficiently wide range. Structure of the initial material changes its properties after introduction of other elements, which expands the possibilities for its use. Therefore, by changing material's chemical composition, we can modify its working characteristics. We researched distribution of indium on positions of the substitute element," says Denis Vinnik, Head of the Crystal Growth Laboratory.

The scientists have a special interest in determining which of iron's positions in the lattice of barium hexaferrite is the most preferential for the new <u>element</u>: properties of the modified material depend on its structure. At the present time, the crystallographic positions that indium will place have been determined. Research is being carried out in the area of studying super-high frequency characteristics and the nature of other various properties of ferrites.



Viktoria Matveychuk. Credit: A. Trukhanov

"Our interest to barium ferrites is conditioned by their high functional properties," explains Aleksey Valentinovich. "Chemical stability and corrosion resistance makes these <u>materials</u> environmentally safe and usable fro practically unlimited time. Hexaferrites possess excellent magnetic parameters. Low specific electrical conductivity allows applying hexaferrite magnets at the presence of high-

frequency magnet fields, which is prospective for microelectronics. Nowadays this material has a great potential in absorbing electromagnetic interference (EMI) in the microwave range. Therefore, hexaferrites are applicable for microwave technologies and for data transmission and protection from wave exposure at high frequencies."

"We are working with a 'palette' of various <u>chemical elements</u>, including wolframium, aluminum, titanium, manganese and silicon. We would like to find out how such substitutions affect the material's properties," says Svetlana Aleksandrovna. "Now, we are working with lead germanate. Additionally, we are studying physical characteristics of barium hexaferrite with placeable lead and its behavior at high temperatures. At some point of heating till a specific temperature, the sample starts shrinking; this is a quite extraordinary phenomenon. Within this experiment, we calculated the linear expansion coefficient and obtained interesting dependences. There are materials with negative or zero expansion coefficient; they don't change their size during heating. This is important at extreme temperatures, because some electronic details get overheated even under normal conditions."

Barium hexaferrite with placeable lead is one of study fields of the Crystal Growth Laboratory. The scientists have now grown monocrystals with low defect density that can be applied as working elements of electronic devices. Potentially, the material can be used for creation of a quantum computer which would have the highest performance capacity among the existing computational devices.

Development of new magnetic materials in the 21st century will allow creating memory elements with high-speed response, significant volume, and reliability. This class of materials has many applications. [25]

Terahertz computer chip now within reach

Following three years of extensive research, Hebrew University of Jerusalem (HU) physicist Dr. Uriel Levy and his team have created technology that will enable computers and all optic communication devices to run 100 times faster through terahertz microchips.

Until now, two major challenges stood in the way of creating the terahertz <u>microchip</u>: overheating and scalability.

However, in a paper published this week in *Laser & Photonics Reviews*, Dr. Levy, head of HU's Nano-Opto Group and HU emeritus professor Joseph Shappir have shown proof of concept for an optic <u>technology</u> that integrates the speed of optic (light) communications with the reliability—and manufacturing scalability—of electronics.

Optic communications encompass all technologies that use light and transmit through <u>fiber optic</u> <u>cables</u>, such as the internet, email, text messages, phone calls, the cloud and data centers, among others. Optic communications are super fast but in microchips they become unreliable and difficult to replicate in large quanitites.

Now, by using a Metal-Oxide-Nitride-Oxide-Silicon (MONOS) structure, Levy and his team have come up with a new integrated circuit that uses flash memory technology—the kind used in flash drives and discs-on-key—in microchips. If successful, this technology will enable standard 8-16 gigahertz computers to run 100 times faster and will bring all optic devices closer to the holy grail of communications: the terahertz chip.

As Dr. Uriel Levy shared, "this discovery could help fill the "THz gap' and create new and more powerful wireless devices that could transmit data at significantly higher speeds than currently possible. In the world of hi-tech advances, this is game-changing technology,"

Meir Grajower, the leading HU Ph.D. student on the project, added, "It will now be possible to manufacture any optical <u>device</u> with the precision and cost-effectiveness of flash technology." [24]

Revolutionizing computer memory—with magnets

When the energy efficiency of electronics poses a challenge, magnetic materials may have a solution.

Energy efficiency will make or break the future. As the demand for energy from electronics continues growing, the Semiconductor Research Corporation warns that within two decades, the global computational demand for energy will be greater than the total amount produced. Vincent Sokalski, an assistant professor of <u>materials</u> science and engineering at Carnegie Mellon University, is working on a solution to this problem—using <u>magnetic materials</u> for energy-efficient memory and computing.

Sokalski recently received a \$1.8 million grant from the Defense Advanced Research Projects Agency (DARPA) for his project, "Domain wall skyrmions: Topological excitations confined to 1-D channels." Along with CMU Professors Marc De Graef (MSE) and Di Xiao (Physics), Sokalski will explore new ways to efficiently process and store information with magnetic materials.

Although magnetic materials are already used in today's hard disk drives for long-term storage, semiconductors are currently used for short-term memory and processing, which is where most of the energy is consumed. However, as semiconductors shrink to meet consumer expectations for speed and density, there comes a limit to how small they can be made without risking the loss of information. DARPA recognizes this challenge, and <u>research projects</u> funded by DARPA's "Topological Excitations in Electronics" program center on finding ways to use "topological protection" to improve magnetic materials that can be used for computer memory storage or processors.

Imagine a bowl with a small ball rolling inside. As you shake it, the ball moves up and down the walls of the bowl, staying inside. However, if you did this with a smaller bowl, the ball might eventually fall out. Similarly, when a semiconductor is exposed to heat, it is at risk of losing information. The smaller you manufacture semiconductors, the more risk there is of data loss.

Credit: Carnegie Mellon University College of Engineering

"The fundamental physics behind that isn't something we can readily change," explains Sokalski, "but we can look at entirely different material systems and mechanisms where we're moving around magnetic features, and using those magnetic features to change the resistance of a computing device. But in order to do that, we really need to explore and discover new materials that can serve that purpose."

Enter magnetic materials. By improving magnetic materials, Sokalski hopes to one day find <u>new</u> <u>materials</u> that could augment, or even replace, semiconductors in computing.

Sokalski's project begins with magnetic skyrmions, or 2-D magnetic bubbles. If used in computer memory, each bubble would store a single bit of data.

"Skyrmions are a rebirth of the idea of bubble memory" that was widely studied in the 1970s and 80s, says Sokalski. "Except now the bubbles are much smaller, more stable, and have topological protection, so we can move them around with greater <u>energy efficiency</u> than we ever could have moved them around 40 or 50 years ago."

In magnetic materials, think of each electron as a tiny bar magnet with a north and south pole that are all pointing in the same direction. These are called spins. Sokalski is interested in how to create topological defects in lines of these spins.

To understand the importance of topological protection, you first have to understand topological defects. Imagine stacking a cheese tray with a friend. One of you starts on the right side of the tray, stacking up each piece of cheese on top of the next, and the other starts on the left side. Eventually, you'll meet in the middle, and your slices of cheese will collide, rather than aligning at the same angle. That point where they collide is the essence of a topological defect.

To erase a topological defect, you'd have to flip every "slice of cheese" on one side of the defect. In magnetism, if half of your spins in a chain point inward to the left, and all the others point the opposite direction, you'd get a defect in the middle. In order to make the defect disappear, you'd have to reverse every spin on one side, moving it away to the edge of the chain.

In magnetism, these topological defects are very valuable. If you have a topological defect, that means your data are topologically protected, because if just one spin spontaneously flips to point in the opposite direction, the <u>defect</u> just shifts, rather than goes away.

Why is this topic suddenly emerging in magnetic materials research? All magnetism is based on something called the Heisenberg Exchange, a quantum mechanical effect that causes electron spins to align in a parallel orientation. However, the discovery of a new phenomenon called the Dzyaloshinskii-Moriya Interaction (DMI) leads to a perpendicular alignment of neighboring spins. The combination of Heisenberg Exchange and DMI, which is what Sokalski studies, gives rise to a new kind of magnetism that causes electron spins to have a continuously spiraling configuration.

"It turns out that features in magnetic materials that are stabilized by this new interaction can actually be manipulated with better efficiency than in cases where it's only the Heisenberg Exchange," says Sokalski.

Having greater control over skyrmions and <u>topological defects</u> would mean more reliable data storage and energy efficiency in computing.

"DARPA is looking to circumvent the pending challenge of energy-efficient electronics," says Sokalski, "and that scales from the most fundamental physical concepts of spin to the design of computers that have an entirely different circuit architecture. Our research will lead to energyefficient computing that meets the needs of artificial intelligence and small-scale computers, while mitigating their global energy footprint."

MSE Ph.D. students Maxwell Li and Derek Lau and Physics postdoctoral researcher Ran Cheng are collaborators on this project, in addition to Co-PIs Tim Mewes and Claudia Mewes at the University of Alabama. [23]

The quantum states on the surface of conducting materials can strongly interact with light

An exotic state of matter that is dazzling scientists with its electrical properties, can also exhibit unusual optical properties, as shown in a theoretical study by researchers at A*STAR.

Atomically thin materials, such as graphene, derive some of their properties from the fact that electrons are confined to traveling in just two-dimensions. Similar phenomena are also seen in some three-dimensional materials, in which electrons confined to the <u>surface</u> behave very differently from those within the bulk—for example, <u>topological insulators</u>, whose surface electrons conduct electricity even though their bulk electrons do not. Recently, another exciting class of materials has been identified: the topological semimetal.

The difference in insulator and conductor <u>electrical properties</u> is down to the bandgap: a gap between the ranges, or bands, of energy that an electron traveling through the material can assume. In an insulator, the lower band is full of electrons and the bandgap is too large to enable a current to flow. In a semimetal, the lower band is also full but the lower and upper bands touch at some points, enabling the flow of a small current.

This lack of a full bandgap means that topological semimetals should theoretically exhibit very different properties from those of the more conventional topological insulators.

To prove this, Li-kun Shi and Justin Song from the A*STAR Institute of High Performance Computing used an 'effective Hamiltonian' approximation to show that the two-dimensional surface states in semimetals, known as Fermi arcs, possess a light–matter interaction much stronger than that found in other gapless two-dimensional systems, such as graphene.

"Typically, the bulk dominates material absorption," explains Song. "But we show that Dirac semimetals are unusual in that they possess a very optically active surface due to these peculiar Fermi arc states."

Shi and Song analyzed a proto-typical semimetal with a symmetric band structure where the electronic bands touch at two places, known as Dirac points, and predicted the strength with which incident radiation induces electron transitions from the lower band to the upper one. They found that surface absorption depends heavily on the polarization of light, being 100 to 1,000 times

stronger when light is polarized perpendicular—rather than parallel—to the crystal's rotational axis. This strong anisotropy offers a way of optically investigating and probing the topological surfaces states of Dirac semimetals.

"Our goal is to identify more unconventional optics that arise due to Fermi arcs," says Song. "Topological semimetals could host unusual opto-electronic behavior that goes beyond conventional materials." [22]

Breakthrough in circuit design makes electronics more resistant to damage and defects

People are growing increasingly dependent on their mobile phones, tablets and other portable devices that help them navigate daily life. But these gadgets are prone to failure, often caused by small defects in their complex electronics, which can result from regular use. Now, a paper in today's *Nature Electronics* details an innovation from researchers at the Advanced Science Research Center (ASRC) at The Graduate Center of The City University of New York that provides robust protection against circuitry damage that affects signal transmission.

The breakthrough was made in the lab of Andrea Alù, director of the ASRC's Photonics Initiative. Alù and his colleagues from The City College of New York, University of Texas at Austin and Tel Aviv University were inspired by the seminal work of three British researchers who won the 2016 Noble Prize in Physics for their work, which teased out that particular properties of matter (such as electrical conductivity) can be preserved in certain materials despite continuous changes in the matter's form or shape. This concept is associated with topology—a branch of mathematics that studies the properties of space that are preserved under continuous deformations.

"In the past few years there has been a strong interest in translating this concept of matter topology from material science to light propagation," said Alù. "We achieved two goals with this project: First, we showed that we can use the science of topology to facilitate robust electromagnetic-wave propagation in electronics and circuit components. Second, we showed that the inherent robustness associated with these topological phenomena can be self-induced by the signal traveling in the circuit, and that we can achieve this robustness using suitably tailored nonlinearities in circuit arrays."

To achieve their goals, the team used nonlinear resonators to mold a band-diagram of the circuit array. The array was designed so that a change in signal intensity could induce a change in the band diagram's topology. For low signal intensities, the electronic circuit was designed to support a trivial topology, and therefore provide no protection from defects. In this case, as defects were introduced into the array, the <u>signal transmission</u> and the functionality of the circuit were negatively affected.

As the voltage was increased beyond a specific threshold, however, the band-diagram's topology was automatically modified, and the signal transmission was not impeded by arbitrary defects introduced across the circuit array. This provided direct evidence of a topological transition in the circuitry that translated into a self-induced robustness against defects and disorder.

"As soon as we applied the higher-voltage signal, the system reconfigured itself, inducing a topology that propagated across the entire chain of resonators allowing the signal to transmit without any problem," said A. Khanikaev, professor at The City College of New York and co-author in the study. "Because the system is nonlinear, it's able to undergo an unusual transition that makes signal transmission robust even when there are defects or damage to the circuitry."

"These ideas open up exciting opportunities for inherently robust electronics and show how complex concepts in mathematics, like the one of topology, can have real-life impact on common electronic devices," said Yakir Hadad, lead author and former postdoc in Alù's group, currently a professor at Tel-Aviv University, Israel. "Similar ideas can be applied to nonlinear optical <u>circuits</u> and extended to two and three-dimensional nonlinear metamaterials." [21]

Researchers develop heat switch for electronics

Researchers at the University of Illinois at Urbana-Champaign have developed a new technology for switching heat flows 'on' or 'off'. The findings were published in the article "Millimeter-scale liquid metal droplet thermal switch," which appeared in *Applied Physics Letters*.

Switches are used to control many technical products and engineered systems. Mechanical switches are used to lock or unlock doors, or to select gears in a car's transmission system. Electrical switches are used to turn on and off the lights in a room. At a smaller scale, <u>electrical</u> <u>switches</u> in the form of transistors are used to turn electronic devices on and off, or to route logic signals within a circuit.

Engineers have long desired a switch for heat flows, especially in electronics systems where controlling heat flows can significantly improve system performance and reliability. There are however significant challenges in creating such a heat switch.

"Heat <u>flow</u> occurs whenever you have a region of higher temperature near a region of lower temperature," said William King, the Andersen Chair Professor in the Department of Mechanical Science and Engineering and the project co-leader. "In order to control the <u>heat flow</u>, we engineered a specific heat flow path between the hot region and cold region, and then created a way to break the heat flow path when desired."

"The technology is based on the motion of a liquid metal droplet," said Nenad Miljkovic, Assistant Professor in the Department of Mechanical Science and Engineering and the project co-leader. "The metal droplet can be positioned to connect a heat flow path, or moved away from the heat flow path in order to limit the heat flow."

The researchers demonstrated the technology in a system modeled after modern electronics systems. On one side of the switch there was a heat source representing the power electronics component, and on the other side of the switch, there was liquid cooling for heat removal. When the switch was on, they were able to extract heat at more than 10 W/cm2. When the switch was off, the <u>heat</u>flow dropped by nearly 100X.

Besides King and Miljkovic, other authors of the paper include Paul Braun, Racheff Professor of Materials Science and Engineering and the Director of Materials Research Laboratory; and graduate students Tianyu Yang, Beomjin Kwon and Patricia B. Weisensee (now an assistant professor at Washington University in St. Louis) from mechanical science and engineering and Jin Gu Kang and Xuejiao Li from materials science and engineering.

King says that the next step for the research is to integrate the <u>switch</u> with power electronics on a circuit board. The researchers will have a working prototype later this year. [20]

Converting heat into electricity with pencil and paper

Thermoelectric materials can use thermal differences to generate electricity. Now there is an inexpensive and environmentally friendly way of producing them with the simplest tools: a pencil, photocopy paper, and conductive paint. These are sufficient to convert a temperature difference into electricity via the thermoelectric effect, which has now been demonstrated by a team at the Helmholtz-Zentrum Berlin.

The <u>thermoelectric effect</u> was discovered almost 200 years ago by Thomas J. Seebeck. If two metals of different temperatures are brought together, they can develop an electrical voltage. This effect allows residual heat to be converted partially into electrical energy. Residual heat is a by-product of almost all technological and natural processes, such as in power plants and household appliances, not to mention the human body. It is also one of the most under-utilised energy sources in the world.

Tiny effect

However, as useful an effect as it is, it is extremely small in ordinary metals. This is because metals not only have high electrical conductivity, but <u>high thermal conductivity</u> as well, so that differences in temperature disappear immediately. Thermoelectric <u>materials</u> need to have <u>low</u> <u>thermal conductivity</u> despite their <u>high electrical conductivity</u>. Thermoelectric devices made of inorganic semiconductor materials such as bismuth telluride are already being used today in certain technological applications. However, such material systems are expensive and their use only pays off in certain situations. Researchers are exploring whether flexible, nontoxic organic materials based on carbon nanostructures, for example, might also be used in the human body.

The team led by Prof. Norbert Nickel at the HZB has now shown that the effect can be obtained much more simply—using a normal HB-grade <u>pencil</u>, they covered a small area with pencil on ordinary photocopy paper. As a second material, they applied a transparent, conductive co-polymer paint (PEDOT: PSS) to the surface.

The pencil traces on the paper delivered a voltage comparable to other far more expensive nanocomposites that are currently used for flexible thermoelectric elements. And this voltage could be increased tenfold by adding indium selenide to the graphite from the pencil.

The researchers investigated graphite and co-polymer coating films using a scanning electron microscope and Raman scattering at HZB. "The results were very surprising for us as well," says Nickel. "But we have now found an explanation of why this works so well—the pencil deposit left on the paper forms a surface characterised by unordered graphite flakes, some graphene, and clay.

While this only slightly reduces the electrical conductivity, heat is transported much less effectively."

These simple constituents might be usable in the future to print extremely inexpensive, environmentally friendly, and non-toxic thermoelectric components onto paper. Such tiny and flexible components could also be used directly on the body and could use body heat to operate small devices or sensors. [19]

A new efficient and portable electrocaloric cooling device

A team of researchers with the University of California and SRI International has developed a new type of cooling device that is both portable and efficient. In their paper published in the journal Science, the team describes their new device and possible applications for its use. Q.M. Zhang and Tian Zhang with the Pennsylvania State University offer some background on electrocaloric theory and outline the work done by the team in California in a Perspectives piece in the same journal issue.

As most everyone knows, conventional air conditioners are bulky, heavy, use a lot of electricity and often leak greenhouse gases into the atmosphere. Thus, conditions are ripe for something new. Some new devices have been developed such as thermoelectric coolers, which make use of ceramics, but they are not efficient enough to play a major role in cooling. A more recent development is the use of devices exploiting the electrocaloric effect, which is where heat moves through certain materials when an electric current is applied. In this new effort, the researchers used a polymer as the material.

The new cooling device was made by layering a polymer between a heat sink and a heat source. Applying electric current to the polymer when it was touching the heat sink caused its molecules to line up, which reduced entropy, forcing heat into the sink. The polymer was then moved into contact with the heat source while the current was turned off. The molecules relaxed, which caused the temperature to drop. Repeating this process resulted in cooling.

The researchers report that the device is extremely efficient, portable and configurable. They suggest the same technology could be used to create coolers for a chair or hat, for example, or perhaps to chill smartphone batteries. They proved this last claim by actually building such a device and using it to cool down a battery heated by ordinary use—after only five seconds, the temperature of the battery had lessened by 8° C. Comparatively, air cooling the battery reduced its temperature just 3° C in 50 seconds. [18]

Fast heat flows in warm, dense aluminum

Thermal conductivity is one of the most crucial physical properties of matter when it comes to understanding heat transport, hydrodynamic evolution and energy balance in systems ranging from astrophysical objects to fusion plasmas. In the warm dense matter (WDM) regime, experimental data are very rare, so many theoretical models remain untested.

But LLNL researchers have tested theory by developing a platform called "differential heating" to conduct thermal conductivity measurements. Just as land and water on Earth heat up differently in sunlight, a temperature gradient can be induced between two different materials. The subsequent heat flow from the hotter material to the cooler material is detected by time-resolved diagnostics to determine thermal conductivity.

In an experiment using the Titan laser at the Lab's Jupiter Laser Facility, LLNL researchers and collaborators achieved the first measurements of thermal conductivity of warm dense aluminum— a prototype material commonly used in model development—by heating a dual-layer target of gold and aluminum with laser-generated protons.

"Two simultaneous time-resolved diagnostics provided excellent data for gold, the hotter material, and aluminum, the colder material," said Andrew Mckelvey, a graduate student from the University of Michigan and the first author of a paper appearing in Scientific Reports . "The systematic data sets can constrain both the release equation of state (EOS) and thermal conductivity."

By comparing the data with simulations using five existing thermal conductivity models, the team found that only two agree with the data. The most commonly used model in WDM, called the LeeMore model, did not agree with data. "I am glad to see that Purgatorio, an LLNL-based model, agrees with the data," said Phil Sterne, LLNL co-author and the group leader of EOS development and application group in the Physics Division. "This is the first time these thermal conductivity models of aluminum have been tested in the WDM regime."

"Discrepancy still exists at early time up to 15 picoseconds," said Elijah Kemp, who is responsible for the simulation efforts. "This is likely due to non-equilibrium conditions, another active research area in WDM."

The team is led by Yuan Ping through her early career project funded by the Department of Energy Office of Fusion Energy Science Early Career Program. "This platform can be applied to many pairs of materials and by various heating methods including particle and X-ray heating," Ping said. [17]

Controlling heat and particle currents in nanodevices by quantum observation

Researchers from the Theory Department of the MPSD have realized the control of thermal and electrical currents in nanoscale devices by means of quantum local observations.

Measurement plays a fundamental role in quantum mechanics. The best-known illustration of the principles of superposition and entanglement is Schrödinger's cat. Invisible from the outside, the cat resides in a coherent superposition of two states, alive and dead at the same time.

By means of a measurement, this superposition collapses to a concrete state. The cat is now either dead or alive. In this famous thought experiment, a measurement of the "quantum cat" can be

seen as an interaction with a macroscopic object collapsing the superposition onto a concrete state by destroying its coherence.

In their new article published in npj Quantum Materials, researchers from the Max Planck Institute for the Structure and Dynamics of Matter and collaborators from the University of the Basque Country (UPV/EHU) and the Bremen Center for Computational Materials Science discovered how a microscopic quantum observer is able to control thermal and electrical currents in nanoscale devices. Local quantum observation of a system can induce continuous and dynamic changes in its quantum coherence, which allows better control of particle and energy currents in nanoscale systems.

Classical non-equilibrium thermodynamics was developed to understand the flow of particles and energy between multiple heat and particle reservoirs. The best-known example is Clausius' formulation of the second law of thermodynamics, stating that when two objects with different temperatures are brought in contact, heat will exclusively flow from the hotter to the colder one.

In macroscopic objects, the observation of this process does not influence the flow of energy and particles between them. However, in quantum devices, thermodynamical concepts need to be revisited. When a classical observer measures a quantum system, this interaction destroys most of the coherence inside the system and alters its dynamical response.

Instead, if a quantum observer acts only locally, the system quantum coherence changes continuously and dynamically, thus providing another level of control of its properties. Depending on how strong and where these local quantum observations are performed, novel and surprising quantum transport phenomena arise.

The group of Prof.Dr. Angel Rubio at the Theory Department of the MPSD, along with their colleagues, have demonstrated how the concept of quantum measurements can offer novel possibilities for a thermodynamical control of quantum transport (heat and particle). This concept offers possibilities far beyond those obtained using standard classical thermal reservoirs.

The scientists studied this idea in a theoretical quantum ratchet. Within this system, the left and right side are connected to hot and cold thermal baths, respectively. This configuration forces the energy to flow from hot to cold and the particles to flow clockwise inside the ratchet. The introduction of a quantum observer, however, inverts the particle ring-current against the natural direction of the ratchet—a phenomenon caused by the localized electronic state and the disruption of the system's symmetry.

Furthermore, the quantum observation is also able to invert the direction of the heat flow, contradicting the second law of thermodynamics. "Such heat and particle current control might open the door for different strategies to design quantum transport devices with directionality control of the injection of currents. There could be applications in thermoelectricity, spintronics, photonics, and sensing, among others. These results have been an important contribution to my PhD thesis," says Robert Biele, first author of the paper.

From a more fundamental point of view, this work highlights the role of a quantum observer. In contrast to Schrödinger's cat, where the coherent state is destroyed via the interaction with a macroscopic "observer," here, by introducing a local quantum observer, the coherence is changed

locally and dynamically, allowing researchers to tune between the coherent states of the system. "This shows how thermodynamics is very different in the quantum regime. Schrödinger's cat paradox leads to new thermodynamic forces never seen before," says César A. Rodríguez Rosario.

In the near future, the researchers will apply this concept to control spins for applications in spin injection and novel magnetic memories. Angel Rubio suggests that "The quantum observer— besides controlling the particle and energy transfer at the nanoscale—could also observe spins, select individual components, and give rise to spin-polarized currents without spin-orbit coupling. Observation could be used to write a magnetic memory." [16]

Maxwell's demon extracts work from quantum measurement

Physicists have proposed a new type of Maxwell's demon—the hypothetical agent that extracts work from a system by decreasing the system's entropy—in which the demon can extract work just by making a measurement, by taking advantage of quantum fluctuations and quantum superposition.

The team of Alexia Auffèves at CNRS and Université Grenoble Alpes have published a paper on the new Maxwell's demon in a recent issue of Physical Review Letters.

"In the classical world, thermodynamics teaches us how to extract energy from thermal fluctuations induced on a large system (such as a gas or water) by coupling it to a hot source," Auffèves told Phys.org. "In the quantum world, the systems are small, and they can fluctuate— even if they are not hot, but simply because they are measured. In our paper, we show that it is possible to extract energy from these genuinely quantum fluctuations, induced by quantum measurement."

In the years since James Clerk Maxwell proposed the first demon around 1870, many other versions have been theoretically and experimentally investigated. Most recently, physicists have begun investigating Maxwell's demons that operate in the quantum regime, which could one day have implications for quantum information technologies.

Most quantum versions of the demon have a couple things in common: They are thermally driven by a heat bath, and the demon makes measurements to extract information only. The measurements do not actually extract any work, but rather the information gained by the measurements allows the demon to act on the system so that energy is always extracted from the cycle.

The new Maxwell's demon differs from previous versions in that there is no heat bath—the demon is not thermally driven, but measurement-driven. Also, the measurements have multiple purposes: They not only extract information about the state of the system, but they are also the "fuel" for extracting work from the system. This is because, when the demon performs a measurement on a qubit in the proposed system, the measurement projects the qubit from one state into a superposition of states, which provides energy to the qubit simply due to the measurement process. In their paper, the physicists proposed an experiment in which projective quantum nondemolition measurements can be performed with light pulses repeated every 70 nanoseconds or so. Since recent experiments have already demonstrated the possibility of performing measurements at such high frequencies, the physicists expect that the new Maxwell's demon could be readily implemented using existing technology. In the future, they also plan to investigate potential applications for quantum computing.

"This engine is a perfect proof of concept evidencing that quantum measurement has some energetic footprint," Auffèves said. "Now I would like to reverse the game and use this effect to estimate the energetic cost of quantum tasks, if they are performed in the presence of some measuring entity. This is the case in a quantum computer, which is continuously 'measured' by its surroundings. This effect is called decoherence and is the biggest enemy of quantum computation. Our work provides tools to estimate the energy needed to counteract it." [15]

Physicists read Maxwell's Demon's mind

Pioneering research offers a fascinating view into the inner workings of the mind of 'Maxwell's Demon', a famous thought experiment in physics.

An international research team, including Dr Janet Anders from the University of Exeter, have used superconducting circuits to bring the 'demon' to life.

The demon, first proposed by James Clerk Maxwell in 1867, is a hypothetical being that can gain more useful energy from a thermodynamic system than one of the most fundamental laws of physics—the second law of thermodynamics—should allow.

Crucially, the team not only directly observed the gained energy for the first time, they also tracked how information gets stored in the demon's memory.

The research is published in the leading scientific journal Proceedings of the National Academy of Sciences (PNAS).

The original thought experiment was first proposed by mathematical physicist James Clerk Maxwell—one of the most influential scientists in history—150 years ago.

He hypothesised that gas particles in two adjacent boxes could be filtered by a 'demon' operating a tiny door, that allowed only fast energy particles to pass in one direction and low energy particles the opposite way.

As a result, one box gains a higher average energy than the other, which creates a pressure difference. This non-equilibrium situation can be used to gain energy, not unlike the energy obtained when water stored behind a dam is released.

So although the gas was initially in equilibrium, the demon can create a non-equilibrium situation and extract energy, bypassing the second law of thermodynamics.

Dr Anders, a leading theoretical physicist from the University of Exeter's physics department adds: "In the 1980s it was discovered that this is not the full story. The information about the particles' properties remains stored in the memory of the demon. This information leads to an energetic cost which then reduces the demon's energy gain to null, resolving the paradox." In this research, the team created a quantum Maxwell demon, manifested as a microwave cavity, that draws energy from a superconducting qubit. The team was able to fully map out the memory of the demon after its intervention, unveiling the stored information about the qubit state.

Dr Anders adds: "The fact that the system behaves quantum mechanically means that the particle can have a high and low energy at the same time, not only either of these choices as considered by Maxwell."

This ground-breaking experiment gives a fascinating peek into the interplay between quantum information and thermodynamics, and is an important step in the current development of a theory for nanoscale thermodynamic processes.

'Observing a Quantum Maxwell demon at Work' is published in PNAS. [14]

Researchers posit way to locally circumvent Second Law of Thermodynamics

For more than a century and a half of physics, the Second Law of Thermodynamics, which states that entropy always increases, has been as close to inviolable as any law we know. In this universe, chaos reigns supreme.

But researchers with the U.S. Department of Energy's (DOE's) Argonne National Laboratory announced recently that they may have discovered a little loophole in this famous maxim.

Their research, published in Scientific Reports, lays out a possible avenue to a situation where the Second Law is violated on the microscopic level.

The Second Law is underpinned by what is called the H-theorem, which says that if you open a door between two rooms, one hot and one cold, they will eventually settle into lukewarm equilibrium; the hot room will never end up hotter.

But even in the twentieth century, as our knowledge of quantum mechanics advanced, we didn't fully understand the fundamental physical origins of the H-theorem.

Recent advancements in a field called quantum information theory offered a mathematical construction in which entropy increases.

"What we did was formulate how these beautiful abstract mathematical theories could be connected to our crude reality," said Valerii Vinokur, an Argonne Distinguished Fellow and corresponding author on the study.

The scientists took quantum information theory, which is based on abstract mathematical systems, and applied it to condensed matter physics, a well-explored field with many known laws and experiments.

"This allowed us to formulate the quantum H-theorem as it related to things that could be physically observed," said Ivan Sadovskyy, a joint appointee with Argonne's Materials Science Division and the Computation Institute and another author on the paper. "It establishes a connection between welldocumented quantum physics processes and the theoretical quantum channels that make up quantum information theory."

The work predicts certain conditions under which the H-theorem might be violated and entropy in the short term—might actually decrease.

As far back as 1867, physicist James Clerk Maxwell described a hypothetical way to violate the Second Law: if a small theoretical being sat at the door between the hot and cold rooms and only let through particles traveling at a certain speed. This theoretical imp is called "Maxwell's demon."

"Although the violation is only on the local scale, the implications are far-reaching," Vinokur said. "This provides us a platform for the practical realization of a quantum Maxwell's demon, which could make possible a local quantum perpetual motion machine."

For example, he said, the principle could be designed into a "refrigerator" which could be cooled remotely—that is, the energy expended to cool it could take place anywhere.

The authors are planning to work closely with a team of experimentalists to design a proofofconcept system, they said.

The study, "H-theorem in quantum physics," was published September 12 in Nature Scientific Reports. [13]

What is quantum in quantum thermodynamics?

A lot of attention has been given to the differences between the quantum and classical worlds. For example, quantum entanglement, superposition, and teleportation are purely quantum phenomena with no classical counterparts. However, when it comes to certain areas of thermodynamics— specifically, thermal engines and refrigerators—quantum and classical systems so far appear to be nearly identical. It seems that the same thermodynamic laws that govern the engines in our vehicles may also accurately describe the tiniest quantum engines consisting of just a single particle.

In a new study, physicists Raam Uzdin, Amikam Levy, and Ronnie Kosloff at the Hebrew University of Jerusalem have investigated whether there is anything distinctly quantum about thermodynamics at the quantum level, or if "quantum" thermodynamics is really the same as classical thermodynamics.

For the first time, they have shown a difference in the thermodynamics of heat machines on the quantum scale: in part of the quantum regime, the three main engine types (two-stroke, fourstroke, and continuous) are thermodynamically equivalent. This means that, despite operating in different ways, all three types of engines exhibit all of the same thermodynamic properties, including generating the same amounts of power and heat, and doing so at the same efficiency. This new "thermodynamical equivalence principle" is purely quantum, as it depends on quantum effects, and does not occur at the classical level.

The scientists also showed that, in this quantum regime where all engines are thermodynamically equivalent, it's possible to extract a quantum-thermodynamic signature that further confirms the

presence of quantum effects. They did this by calculating an upper limit on the work output of a classical engine, so that any engine that surpasses this bound must be using a quantum effect namely, quantum coherence—to generate the additional work. In this study, quantum coherence, which accounts for the wave-like properties of quantum particles, is shown to be critical for power generation at very fast engine cycles.

"To the best of my knowledge, this is the first time [that a difference between quantum and classical thermodynamics has been shown] in heat machines," Uzdin told Phys.org. "What has been surprising [in the past] is that the classical description has still held at the quantum level, as many authors have shown. The reasons are now understood, and in the face of this classicality, people have started to stray to other types of research, as it was believed that nothing quantum can pop up.

Thus, it was very difficult to isolate a generic effect, not just a numerical simulation of a specific case, with a complementing theory that manages to avoid the classicality and demonstrate quantum effects in thermodynamic quantities, such as work and heat."

One important implication of the new results is that quantum effects may significantly increase the performance of engines at the quantum level. While the current work deals with single-particle engines, the researchers expect that quantum effects may also emerge in multi-particle engines, where quantum entanglement between particles may play a role similar to that of coherence. [12]

Physicists confirm thermodynamic irreversibility in a quantum system

The physicists, Tiago Batalhão at the Federal University of ABC, Brazil, and coauthors, have published their paper on the experimental demonstration of quantum thermodynamic irreversibility in a recent issue of Physical Review Letters.

Irreversibility at the quantum level may seem obvious to most people because it matches our observations of the everyday, macroscopic world. However, it is not as straightforward to physicists because the microscopic laws of physics, such as the Schrödinger equation, are "time-symmetric," or reversible. In theory, forward and backward microscopic processes are indistinguishable.

In reality, however, we only observe forward processes, not reversible ones like broken egg shells being put back together. It's clear that, at the macroscopic level, the laws run counter to what we observe. Now the new study shows that the laws don't match what happens at the quantum level, either.

Observing thermodynamic processes in a quantum system is very difficult and has not been done until now. In their experiment, the scientists measured the entropy change that occurs when applying an oscillating magnetic field to carbon-13 atoms in liquid chloroform. They first applied a magnetic field pulse that causes the atoms' nuclear spins to flip, and then applied the pulse in reverse to make the spins undergo the reversed dynamics.

If the procedure were reversible, the spins would have returned to their starting points—but they didn't. Basically, the forward and reverse magnetic pulses were applied so rapidly that the spins' flipping couldn't always keep up, so the spins were driven out of equilibrium. The measurements of

the spins indicated that entropy was increasing in the isolated system, showing that the quantum thermodynamic process was irreversible.

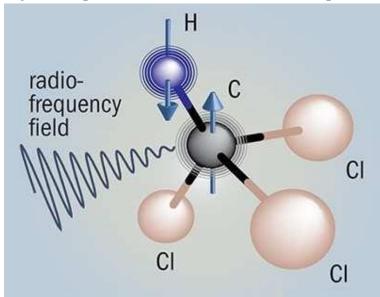
By demonstrating that thermodynamic irreversibility occurs even at the quantum level, the results reveal that thermodynamic irreversibility emerges at a genuine microscopic scale. This finding makes the question of why the microscopic laws of physics don't match our observations even more pressing. If the laws really are reversible, then what are the physical origins of the time-asymmetric entropy production that we observe?

The physicists explain that the answer to this question lies in the choice of the initial conditions. The microscopic laws allow reversible processes only because they begin with "a genuine equilibrium process for which the entropy production vanishes at all times," the scientists write in their paper. Preparing such an ideal initial state in a physical system is extremely complex, and the initial states of all observed processes aren't at "genuine equilibrium," which is why they lead to irreversible processes.

"Our experiment shows the irreversible nature of quantum dynamics, but does not pinpoint, experimentally, what causes it at the microscopic level, what determines the onset of the arrow of time," coauthor Mauro Paternostro at Queen's University in Belfast, UK, told Phys.org. "Addressing it would clarify the ultimate reason for its emergence."

The researchers hope to apply the new understanding of thermodynamics at the quantum level to high-performance quantum technologies in the future.

"Any progress towards the management of finite-time thermodynamic processes at the quantum level is a step forward towards the realization of a fully fledged thermo-machine that can exploit the laws of quantum mechanics to overcome the performance limitations of classical devices," Paternostro said. "This work shows the implications for reversibility (or lack thereof) of nonequilibrium quantum dynamics. Once we characterize it, we can harness it at the technological level." [11]



Physicists put the arrow of time under a quantum microscope

Diagram showing the spin of a carbon atom in a chloroform molecule

Disorder, or entropy, in a microscopic quantum system has been measured by an international group of physicists. The team hopes that the feat will shed light on the "arrow of time": the observation that time always marches towards the future. The experiment involved continually flipping the spin of carbon atoms with an oscillating magnetic field and links the emergence of the arrow of time to quantum fluctuations between one atomic spin state and another.

"That is why we remember yesterday and not tomorrow," explains group member Roberto Serra, a physicist specializing in quantum information at the Federal University of ABC in Santo André, Brazil. At the fundamental level, he says, quantum fluctuations are involved in the asymmetry of time.

Egging on

The arrow of time is often taken for granted in the everyday world. We see an egg breaking, for example, yet we never see the yolk, white and shell fragments come back together again to recreate the egg. It seems obvious that the laws of nature should not be reversible, yet there is nothing in the underlying physics to say so.

The dynamical equations of an egg breaking run just as well forwards as they do backwards.

Entropy, however, provides a window onto the arrow of time. Most eggs look alike, but a broken egg can take on any number of forms: it could be neatly cracked open, scrambled, splattered all over a pavement, and so on. A broken egg is a disordered state – that is, a state of greater entropy – and because there are many more disordered than ordered states, it is more likely for a system to progress towards disorder than order.

This probabilistic reasoning is encapsulated in the second law of thermodynamics, which states that the entropy of a closed system always increases over time.

According to the second law, time cannot suddenly go backwards because this would require entropy to decrease. It is a convincing argument for a complex system made up of a great many interacting particles, like an egg, but what about a system composed of just one particle?

Murky territory

Serra and colleagues have delved into this murky territory with measurements of entropy in an ensemble of carbon-13 atoms contained in a sample of liquid chloroform. Although the sample contained roughly a trillion chloroform molecules, the non-interacting quantum nature of the molecules meant that the experiment was equivalent to performing the same measurement on a single carbon atom, one trillion times.

Serra and colleagues applied an oscillating external magnetic field to the sample, which continually flipped the spin state of a carbon atom between up and down.

They ramped up the intensity of the field oscillations to increase the frequency of the spin-flipping, and then brought the intensity back down again.

Had the system been reversible, the overall distribution of carbon spin states would have been the same at the end as at the start of the process. Using nuclear magnetic resonance and quantum-

state tomography, however, Serra and colleagues measured an increase in disorder among the final spins. Because of the quantum nature of the system, this was equivalent to an increase in entropy in a single carbon atom.

According to the researchers, entropy rises for a single atom because of the speed with which it is forced to flip its spin. Unable to keep up with the field-oscillation intensity, the atom begins to fluctuate randomly, like an inexperienced dancer failing to keep pace with up-tempo music. "It's easier to dance to a slow rhythm than a fast one," says Serra.

Many questions remain

The group has managed to observe the existence of the arrow of time in a quantum system, says experimentalist Mark Raizen of the University of Texas at Austin in the US, who has also studied irreversibility in quantum systems. But Raizen stresses that the group has not observed the "onset" of the arrow of time. "This [study] does not close the book on our understanding of the arrow of time, and many questions remain," he adds.

One of those questions is whether the arrow of time is linked to quantum entanglement – the phenomenon whereby two particles exhibit instantaneous correlations with each other, even when separated by vast distances. This idea is nearly 30 years old and has enjoyed a recent resurgence in popularity. However, this link is less to do with growing entropy and more to do with an unstoppable dispersion of quantum information.

Indeed, Serra believes that by harnessing quantum entanglement, it may even be possible to reverse the arrow of time in a microscopic system. "We're working on it," he says. "In the next generation of

our experiments on quantum thermodynamics we will explore such aspects." [10]

Small entropy changes allow quantum measurements to be nearly reversed

In 1975, Swedish physicist Göran Lindblad developed a theorem that describes the change in entropy that occurs during a quantum measurement. Today, this theorem is a foundational component of quantum information theory, underlying such important concepts as the uncertainty principle, the second law of thermodynamics, and data transmission in quantum communication systems.

Now, 40 years later, physicist Mark M. Wilde, Assistant Professor at Louisiana State University, has improved this theorem in a way that allows for understanding how quantum measurements can be approximately reversed under certain circumstances. The new results allow for understanding how quantum information that has been lost during a measurement can be nearly recovered, which has potential implications for a variety of quantum technologies.

Quantum relative entropy never increases

Most people are familiar with entropy as a measure of disorder and the law that "entropy never decreases"—it either increases or stays the same during a thermodynamic process, according to the second law of thermodynamics. However, here the focus is on "quantum relative entropy," which in some sense is the negative of entropy, so the reverse is true: quantum relative entropy never increases, but instead only decreases or stays the same.

In fact, this was the entropy inequality theorem that Lindblad proved in 1975: that the quantum relative entropy cannot increase after a measurement. In this context, quantum relative entropy is interpreted as a measure of how well one can distinguish between two quantum states, so it's this distinguishability that can never increase. (Wilde describes a proof of Lindblad's result in greater detail in his textbook Quantum Information Theory, published by Cambridge University Press.)

One thing that Lindblad's proof doesn't address, however, is whether it makes any difference if the quantum relative entropy decreases by a little or by a lot after a measurement.

In the new paper, Wilde has shown that, if the quantum relative entropy decreases by only a little, then the quantum measurement (or any other type of so-called "quantum physical evolution") can be approximately reversed.

"When looking at Lindblad's entropy inequality, a natural question is to wonder what we could say if the quantum relative entropy goes down only by a little when the quantum physical evolution is applied," Wilde told Phys.org. "It is quite reasonable to suspect that we might be able to approximately reverse the evolution. This was arguably open since the work of Lindblad in 1975, addressed in an important way by Denes Petz in the late 1980s (for the case in which the quantum relative entropy stays the same under the action of the evolution), and finally formulated as a conjecture around 2008 by Andreas Winter. What my work did was to prove this result as a theorem: if the quantum relative entropy goes down only by a little under a quantum physical evolution, then we can approximately reverse its action."

Wide implications

Wilde's improvements to Lindblad's theorem have a variety of implications, but the main one that Wilde discusses in his paper is how the new results allow for recovering quantum information.

"If the decrease in quantum relative entropy between two quantum states after a quantum physical evolution is relatively small," he said, "then it is possible to perform a recovery operation, such that one can perfectly recover one state while approximately recovering the other. This can be interpreted as quantifying how well one can reverse a quantum physical evolution." So the smaller the relative entropy decrease, the better the reversal process.

The ability to recover quantum information could prove useful for quantum error correction, which aims to protect quantum information from damaging external effects. Wilde plans to address this application more in the future with his colleagues.

As Wilde explained, Lindblad's original theorem can also be used to prove the uncertainty principle of quantum mechanics in terms of entropies, as well as the second law of thermodynamics for quantum systems, so the new results have implications in these areas, as well.

"Lindblad's entropy inequality underlies many limiting statements, in some cases said to be physical laws or principles," Wilde said. "Examples are the uncertainty principle and the second law of thermodynamics. Another example is that this entropy inequality is the core step in determining limitations on how much data we can communicate over quantum communication channels. We could go as far as to say that the above entropy inequality constitutes a fundamental law of quantum information theory, which is a direct mathematical consequence of the postulates of quantum mechanics."

Regarding the uncertainty principle, Wilde and two coauthors, Mario Berta and Stephanie Wehner, discuss this angle in a forthcoming paper. They explain that the uncertainty principle involves quantum measurements, which are a type of quantum physical evolution and therefore subject to Lindblad's theorem. In one formulation of the uncertainty principle, two experiments are performed on different copies of the same quantum state, with both experimental outcomes having some uncertainty.

"The uncertainty principle is the statement that you cannot generally make the uncertainties of both experiments arbitrarily small, i.e., there is generally a limitation," Wilde said. "It is now known that a statement of the uncertainty principle in terms of entropies can be proved by using the 'decrease of quantum relative entropy inequality.' So what the new theorem allows for doing is relating the uncertainties of the measurement outcomes to how well we could try to reverse the action of one of the measurements. That is, there is now a single mathematical inequality which captures all of these notions."

In terms of the second law of thermodynamics, Wilde explains how the new results have implications for reversing thermodynamic processes in both classical and quantum systems.

"The new theorem allows for quantifying how well we can approximately reverse a thermodynamic transition from one state to another without using any energy at all," he said.

He explained that this is possible due to the connection between entropy, energy, and work. According to the second law of thermodynamics, a thermodynamic transition from one quantum state to another is allowed only if the free energy decreases from the original state to the final state. During this process, one can gain work and store energy. This law can be rewritten as a statement involving relative entropies and can be proved as a consequence of the decrease of quantum relative entropy.

"What my new work with Stephanie Wehner and Mischa Woods allows for is a refinement of this statement," Wilde said. "We can say that if the free energy does not go down by very much under a thermodynamic transition (i.e., if there is not too much work gained in the process), then it is possible to go back approximately to the original state from the final state, without investing any work at all. The key word here is that you can go back only approximately, so we are not in violation of the second law, only providing a refinement of it."

In addition to these implications, the new theorem can also be applied to other research topics in quantum information theory, including the Holevo bound, quantum discord, and multipartite information measures.

Wilde's work was funded in part by The DARPA Quiness program (ending now), which focused on quantum key distribution, or using quantum mechanics to ensure secret communication between two parties. He describes more about this application, in particular how Alice and Bob might use a quantum state to share secrets that can be kept private from an eavesdropper Eve (and help them survive being attacked by a bear), in a recent blog post. [9]

Tricking the uncertainty principle

"If you want to know where something is, you have to scatter something off of it," explains Professor of Applied Physics Keith Schwab, who led the study. "For example, if you shine light at an object, the photons that scatter off provide information about the object. But the photons don't all hit and scatter at the same time, and the random pattern of scattering creates quantum fluctuations"—that is, noise. "If you shine more light, you have increased sensitivity, but you also have more noise. Here we were looking for a way to beat the uncertainty principle—to increase sensitivity but not noise."

Schwab and his colleagues began by developing a way to actually detect the noise produced during the scattering of microwaves—electromagnetic radiation that has a wavelength longer than that of visible light. To do this, they delivered microwaves of a specific frequency to a superconducting electronic circuit, or resonator, that vibrates at 5 gigahertz—or 5 billion times per second. The electronic circuit was then coupled to a mechanical device formed of two metal plates that vibrate at around 4 megahertz—or 4 million times per second. The researchers observed that the quantum noise of the microwave field, due to the impact of individual photons, made the mechanical device shake randomly with an amplitude of 10-15 meters, about the diameter of a proton.

"Our mechanical device is a tiny square of aluminum—only 40 microns long, or about the diameter of a hair. We think of quantum mechanics as a good description for the behaviors of atoms and electrons and protons and all of that, but normally you don't think of these sorts of quantum effects manifesting themselves on somewhat macroscopic objects," Schwab says. "This is a physical manifestation of the uncertainty principle, seen in single photons impacting a somewhat macroscopic thing."

Once the researchers had a reliable mechanism for detecting the forces generated by the quantum fluctuations of microwaves on a macroscopic object, they could modify their electronic resonator, mechanical device, and mathematical approach to exclude the noise of the position and motion of the vibrating metal plates from their measurement.

The experiment shows that a) the noise is present and can be picked up by a detector, and b) it can be pushed to someplace that won't affect the measurement. "It's a way of tricking the uncertainty principle so that you can dial up the sensitivity of a detector without increasing the noise," Schwab says.

Although this experiment is mostly a fundamental exploration of the quantum nature of microwaves in mechanical devices, Schwab says that this line of research could one day lead to the observation of quantum mechanical effects in much larger mechanical structures. And that, he notes, could allow the demonstration of strange quantum mechanical properties like superposition and entanglement in large objects—for example, allowing a macroscopic object to exist in two places at once.

"Subatomic particles act in quantum ways—they have a wave-like nature—and so can atoms, and so can whole molecules since they're collections of atoms,"

Schwab says. "So the question then is: Can you make bigger and bigger objects behave in these weird wave-like ways? Why not? Right now we're just trying to figure out where the boundary of quantum physics is, but you never know." [8]

Particle Measurement Sidesteps the Uncertainty Principle

Quantum mechanics imposes a limit on what we can know about subatomic particles. If physicists measure a particle's position, they cannot also measure its momentum, so the theory goes. But a new experiment has managed to circumvent this rule—the so-called uncertainty principle—by ascertaining just a little bit about a particle's position, thus retaining the ability to measure its momentum, too.

The uncertainty principle, formulated by Werner Heisenberg in 1927, is a consequence of the fuzziness of the universe at microscopic scales. Quantum mechanics revealed that particles are not just tiny marbles that act like ordinary objects we can see and touch. Instead of being in a particular place at a particular time, particles actually exist in a haze of probability. Their chances of being in any given state are described by an equation called the quantum wavefunction. Any measurement of a particle "collapses" its wavefunction, in effect forcing it to choose a value for the measured characteristic and eliminating the possibility of knowing anything about its related properties.

Recently, physicists decided to see if they could overcome this limitation by using a new engineering technique called compressive sensing. This tool for making efficient measurements has already been applied successfully in digital photographs, MRI scans and many other technologies. Normally, measuring devices would take a detailed reading and afterward compress it for ease of use. For example, cameras take large raw files and then convert them to compressed jpegs. In compressive sensing, however, engineers aim to compress a signal while measuring it, allowing them to take many fewer measurements—the equivalent of capturing images as jpegs rather than raw files.

This same technique of acquiring the minimum amount of information needed for a measurement seemed to offer a way around the uncertainty principle. To test compressive sensing in the quantum world, physicist John C. Howell and his team at the University of Rochester set out to measure the position and momentum of a photon—a particle of light. They shone a laser through a box equipped with an array of mirrors that could either point toward or away from a detector at its

end. These mirrors formed a filter, allowing photons through in some places and blocking them in others. If a photon made it to the detector, the physicists knew it had been in one of the locations where the mirrors offered a throughway. The filter provided a way of measuring a particle's position without knowing exactly where it was—without collapsing its wavefunction. "All we know is either the photon can get through that pattern, or it can't," says Gregory A. Howland, first author of a paper reporting the research published June 26 in Physical Review Letters. "It turns out that because of that we're still able to figure out the momentum—where it's going. The penalty that we pay is that our measurement of where it's going gets a little bit of noise on it." A less precise momentum measurement, however, is better than no momentum measurement at all.

The physicists stress that they have not broken any laws of physics. "We do not violate the uncertainty principle," Howland says. "We just use it in a clever way." The technique could prove powerful for developing technologies such as quantum cryptography and quantum computers, which aim to harness the fuzzy quantum properties of particles for technological applications. The more information quantum measurements can acquire, the better such technologies could work. Howland's experiment offers a more efficient quantum measurement than has traditionally been possible, says Aephraim M. Steinberg, a physicist at the University of Toronto who was not involved in the research. "This is one of a number of novel techniques which seem poised to prove indispensible for economically characterizing large systems." In other words, the physicists seem to have found a way to get more data with less measurement—or more bangs for their buck. [7]

A new experiment shows that measuring a quantum system does not necessarily introduce uncertainty

Contrary to what many students are taught, quantum uncertainty may not always be in the eye of the beholder. A new experiment shows that measuring a quantum system does not necessarily introduce uncertainty. The study overthrows a common classroom explanation of why the quantum world appears so fuzzy, but the fundamental limit to what is knowable at the smallest scales remains unchanged.

At the foundation of quantum mechanics is the Heisenberg uncertainty principle. Simply put, the principle states that there is a fundamental limit to what one can know about a quantum system. For example, the more precisely one knows a particle's position, the less one can know about its momentum, and vice versa. The limit is expressed as a simple equation that is straightforward to prove mathematically.

Heisenberg sometimes explained the uncertainty principle as a problem of making measurements. His most well-known thought experiment involved photographing an electron. To take the picture, a scientist might bounce a light particle off the electron's surface. That would reveal its position, but it would also impart energy to the electron, causing it to move. Learning about the electron's position would create uncertainty in its velocity; and the act of measurement would produce the uncertainty needed to satisfy the principle.

Physics students are still taught this measurement-disturbance version of the uncertainty principle in introductory classes, but it turns out that it's not always true. Aephraim Steinberg of the

University of Toronto in Canada and his team have performed measurements on photons (particles of light) and showed that the act of measuring can introduce less uncertainty than is required by Heisenberg's principle. The total uncertainty of what can be known about the photon's properties, however, remains above Heisenberg's limit.

Delicate measurement

Steinberg's group does not measure position and momentum, but rather two different interrelated properties of a photon: its polarization states. In this case, the polarization along one plane is intrinsically tied to the polarization along the other, and by Heisenberg's principle, there is a limit to the certainty with which both states can be known.

The researchers made a 'weak' measurement of the photon's polarization in one plane — not enough to disturb it, but enough to produce a rough sense of its orientation. Next, they measured the polarization in the second plane. Then they made an exact, or 'strong', measurement of the first polarization to see whether it had been disturbed by the second measurement.

When the researchers did the experiment multiple times, they found that measurement of one polarization did not always disturb the other state as much as the uncertainty principle predicted. In the strongest case, the induced fuzziness was as little as half of what would be predicted by the uncertainty principle.

Don't get too excited: the uncertainty principle still stands, says Steinberg: "In the end, there's no way you can know [both quantum states] accurately at the same time." But the experiment shows that the act of measurement isn't always what causes the uncertainty. "If there's already a lot of uncertainty in the system, then there doesn't need to be any noise from the measurement at all," he says.

The latest experiment is the second to make a measurement below the uncertainty noise limit. Earlier this year, Yuji Hasegawa, a physicist at the Vienna University of Technology in Austria, measured groups of neutron spins and derived results well below what would be predicted if measurements were inserting all the uncertainty into the system.

But the latest results are the clearest example yet of why Heisenberg's explanation was incorrect. "This is the most direct experimental test of the Heisenberg measurement-disturbance uncertainty principle," says Howard Wiseman, a theoretical physicist at Griffith University in Brisbane, Australia "Hopefully it will be useful for educating textbook writers so they know that the naive measurement-disturbance relation is wrong."

Shaking the old measurement-uncertainty explanation may be difficult, however. Even after doing the experiment, Steinberg still included a question about how measurements create uncertainty on a recent homework assignment for his students. "Only as I was grading it did I realize that my homework assignment was wrong," he says. "Now I have to be more careful." [6]

Quantum entanglement

Measurements of physical properties such as position, momentum, spin, polarization, etc.

performed on entangled particles are found to be appropriately correlated. For example, if a pair of particles is generated in such a way that their total spin is known to be zero, and one particle is found to have clockwise spin on a certain axis, then the spin of the other particle, measured on the same axis, will be found to be counterclockwise. Because of the nature of quantum measurement, however, this behavior gives rise to effects that can appear paradoxical: any measurement of a property of a particle can be seen as acting on that particle (e.g. by collapsing a number of superimposed states); and in the case of entangled particles, such action must be on the entangled system as a whole. It thus appears that one particle of an entangled pair "knows" what measurement has been performed on the other, and with what outcome, even though there is no known means for such information to be communicated between the particles, which at the time of measurement may be separated by arbitrarily large distances. [4]

The Bridge

The accelerating electrons explain not only the Maxwell Equations and the Special Relativity, but the Heisenberg Uncertainty Relation, the wave particle duality and the electron's spin also, building the bridge between the Classical and Quantum Theories. [1]

Accelerating charges

The moving charges are self maintain the electromagnetic field locally, causing their movement and this is the result of their acceleration under the force of this field. In the classical physics the charges will distributed along the electric current so that the electric potential lowering along the current, by linearly increasing the way they take every next time period because this accelerated motion. The same thing happens on the atomic scale giving a dp impulse difference and a dx way difference between the different part of the not point like particles.

Relativistic effect

Another bridge between the classical and quantum mechanics in the realm of relativity is that the charge distribution is lowering in the reference frame of the accelerating charges linearly: ds/dt = at (time coordinate), but in the reference frame of the current it is parabolic: $s = a/2 t^2$ (geometric coordinate).

Heisenberg Uncertainty Relation

In the atomic scale the Heisenberg uncertainty relation gives the same result, since the moving electron in the atom accelerating in the electric field of the proton, causing a charge distribution on delta x position difference and with a delta p momentum difference such a way that they product is about the half Planck reduced constant. For the proton this delta x much less in the nucleon, than in the orbit of the electron in the atom, the delta p is much higher because of the greater proton mass.

This means that the electron and proton are not point like particles, but has a real charge distribution.

Wave - Particle Duality

The accelerating electrons explains the wave – particle duality of the electrons and photons, since the elementary charges are distributed on delta x position with delta p impulse and creating a wave packet of the electron. The photon gives the electromagnetic particle of the mediating force of the electrons electromagnetic field with the same distribution of wavelengths.

Atomic model

The constantly accelerating electron in the Hydrogen atom is moving on the equipotential line of the proton and it's kinetic and potential energy will be constant. Its energy will change only when it is changing its way to another equipotential line with another value of potential energy or getting free with enough kinetic energy. This means that the Rutherford-Bohr atomic model is right and only that changing acceleration of the electric charge causes radiation, not the steady acceleration. The steady acceleration of the charges only creates a centric parabolic steady electric field around the charge, the magnetic field. This gives the magnetic moment of the atoms, summing up the proton and electron magnetic moments caused by their circular motions and spins.

The Relativistic Bridge

Commonly accepted idea that the relativistic effect on the particle physics it is the fermions' spin another unresolved problem in the classical concepts. If the electric charges can move only with accelerated motions in the self maintaining electromagnetic field, once upon a time they would reach the velocity of the electromagnetic field. The resolution of this problem is the spinning particle, constantly accelerating and not reaching the velocity of light because the acceleration is radial. One origin of the Quantum Physics is the Planck Distribution Law of the electromagnetic oscillators, giving equal intensity for 2 different wavelengths on any temperature. Any of these two wavelengths will give equal intensity diffraction patterns, building different asymmetric constructions, for example proton - electron structures (atoms), molecules, etc. Since the particles are centers of diffraction patterns they also have particle – wave duality as the electromagnetic waves have. [2]

The weak interaction

The weak interaction transforms an electric charge in the diffraction pattern from one side to the other side, causing an electric dipole momentum change, which violates the CP and time reversal symmetry. The Electroweak Interaction shows that the Weak Interaction is basically electromagnetic in nature. The arrow of time shows the entropy grows by changing the temperature dependent diffraction patterns of the electromagnetic oscillators.

Another important issue of the quark model is when one quark changes its flavor such that a linear oscillation transforms into plane oscillation or vice versa, changing the charge value with 1 or -1.

This kind of change in the oscillation mode requires not only parity change, but also charge and time changes (CPT symmetry) resulting a right handed anti-neutrino or a left handed neutrino.

The right handed anti-neutrino and the left handed neutrino exist only because changing back the quark flavor could happen only in reverse, because they are different geometrical constructions, the u is 2 dimensional and positively charged and the d is 1 dimensional and negatively charged. It needs also a time reversal, because anti particle (anti neutrino) is involved.

The neutrino is a 1/2spin creator particle to make equal the spins of the weak interaction, for example neutron decay to 2 fermions, every particle is fermions with ½ spin. The weak interaction changes the entropy since more or less particles will give more or less freedom of movement. The entropy change is a result of temperature change and breaks the equality of oscillator diffraction intensity of the Maxwell–Boltzmann statistics. This way it changes the time coordinate measure and

makes possible a different time dilation as of the special relativity.

The limit of the velocity of particles as the speed of light appropriate only for electrical charged particles, since the accelerated charges are self maintaining locally the accelerating electric force. The neutrinos are CP symmetry breaking particles compensated by time in the CPT symmetry, that is the time coordinate not works as in the electromagnetic interactions, consequently the speed of neutrinos is not limited by the speed of light.

The weak interaction T-asymmetry is in conjunction with the T-asymmetry of the second law of thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes the

weak interaction, for example the Hydrogen fusion.

Probably because it is a spin creating movement changing linear oscillation to 2 dimensional oscillation by changing d to u quark and creating anti neutrino going back in time relative to the proton and electron created from the neutron, it seems that the anti neutrino fastest then the velocity of the photons created also in this weak interaction?

A quark flavor changing shows that it is a reflection changes movement and the CP- and Tsymmetry breaking!!! This flavor changing oscillation could prove that it could be also on higher level such as atoms, molecules, probably big biological significant molecules and responsible on the aging of the life.

Important to mention that the weak interaction is always contains particles and antiparticles, where the neutrinos (antineutrinos) present the opposite side. It means by Feynman's interpretation that these particles present the backward time and probably because this they seem to move faster than the speed of light in the reference frame of the other side.

Finally since the weak interaction is an electric dipole change with ½ spin creating; it is limited by the velocity of the electromagnetic wave, so the neutrino's velocity cannot exceed the velocity of light.

The General Weak Interaction

The Weak Interactions T-asymmetry is in conjunction with the T-asymmetry of the Second Law of Thermodynamics, meaning that locally lowering entropy (on extremely high temperature) causes for example the Hydrogen fusion. The arrow of time by the Second Law of Thermodynamics shows the increasing entropy and decreasing information by the Weak Interaction, changing the temperature dependent diffraction patterns. A good example of this is the neutron decay, creating more particles with less known information about them.

The neutrino oscillation of the Weak Interaction shows that it is a general electric dipole change and it is possible to any other temperature dependent entropy and information changing diffraction pattern of atoms, molecules and even complicated biological living structures. We can generalize the weak interaction on all of the decaying matter constructions, even on the biological too. This gives the limited lifetime for the biological constructions also by the arrow of time. There should be a new research space of the Quantum Information Science the 'general neutrino oscillation' for the greater then subatomic matter structures as an electric dipole change. There is also connection between statistical physics and evolutionary biology, since the arrow of time is working in the biological evolution also.

The Fluctuation Theorem says that there is a probability that entropy will flow in a direction opposite to that dictated by the Second Law of Thermodynamics. In this case the Information is growing that is the matter formulas are emerging from the chaos. So the Weak Interaction has two directions, samples for one direction is the Neutron decay, and Hydrogen fusion is the opposite direction.

Fermions and Bosons

The fermions are the diffraction patterns of the bosons such a way that they are both sides of the same thing.

Van Der Waals force

Named after the Dutch scientist Johannes Diderik van der Waals – who first proposed it in 1873 to explain the behaviour of gases – it is a very weak force that only becomes relevant when atoms and molecules are very close together. Fluctuations in the electronic cloud of an atom mean that it will have an instantaneous dipole moment. This can induce a dipole moment in a nearby atom, the result being an attractive dipole–dipole interaction.

Electromagnetic inertia and mass

Electromagnetic Induction

Since the magnetic induction creates a negative electric field as a result of the changing acceleration, it works as an electromagnetic inertia, causing an electromagnetic mass. [1]

Relativistic change of mass

The increasing mass of the electric charges the result of the increasing inductive electric force acting against the accelerating force. The decreasing mass of the decreasing acceleration is the result of the inductive electric force acting against the decreasing force. This is the relativistic mass

change explanation, especially importantly explaining the mass reduction in case of velocity decrease.

The frequency dependence of mass

Since E = hv and $E = mc^2$, $m = hv/c^2$ that is the m depends only on the v frequency. It means that the mass of the proton and electron are electromagnetic and the result of the electromagnetic induction, caused by the changing acceleration of the spinning and moving charge! It could be that the m_o inertial mass is the result of the spin, since this is the only accelerating motion of the electric charge. Since the accelerating motion has different frequency for the electron in the atom and the proton, they masses are different, also as the wavelengths on both sides of the diffraction pattern, giving equal intensity of radiation.

Electron – Proton mass rate

The Planck distribution law explains the different frequencies of the proton and electron, giving equal intensity to different lambda wavelengths! Also since the particles are diffraction patterns they have some closeness to each other – can be seen as a gravitational force. [2]

There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

Gravity from the point of view of quantum physics

The Gravitational force

The gravitational attractive force is basically a magnetic force.

The same electric charges can attract one another by the magnetic force if they are moving parallel in the same direction. Since the electrically neutral matter is composed of negative and positive charges they need 2 photons to mediate this attractive force, one per charges. The Bing Bang caused parallel moving of the matter gives this magnetic force, experienced as gravitational force.

Since graviton is a tensor field, it has spin = 2, could be 2 photons with spin = 1 together.

You can think about photons as virtual electron – positron pairs, obtaining the necessary virtual mass for gravity.

The mass as seen before a result of the diffraction, for example the proton – electron mass rate Mp=1840 Me. In order to move one of these diffraction maximum (electron or proton) we need to intervene into the diffraction pattern with a force appropriate to the intensity of this diffraction maximum, means its intensity or mass.

The Big Bang caused acceleration created radial currents of the matter, and since the matter is composed of negative and positive charges, these currents are creating magnetic field and attracting forces between the parallel moving electric currents. This is the gravitational force experienced by the matter, and also the mass is result of the electromagnetic forces between the charged particles. The positive and negative charged currents attracts each other or by the magnetic forces or by the much stronger electrostatic forces!?

The gravitational force attracting the matter, causing concentration of the matter in a small space and leaving much space with low matter concentration: dark matter and energy. There is an asymmetry between the mass of the electric charges, for example proton and electron, can understood by the asymmetrical Planck Distribution Law. This temperature dependent energy distribution is asymmetric around the maximum intensity, where the annihilation of matter and antimatter is a high probability event. The asymmetric sides are creating different frequencies of electromagnetic radiations being in the same intensity level and compensating each other. One of these compensating ratios is the electron – proton mass ratio. The lower energy side has no compensating intensity level, it is the dark energy and the corresponding matter is the dark matter.

The Higgs boson

By March 2013, the particle had been proven to behave, interact and decay in many of the expected ways predicted by the Standard Model, and was also tentatively confirmed to have + parity and zero spin, two fundamental criteria of a Higgs boson, making it also the first known scalar particle to be discovered in nature, although a number of other properties were not fully proven and some partial results do not yet precisely match those expected; in some cases data is also still awaited or being analyzed.

Since the Higgs boson is necessary to the W and Z bosons, the dipole change of the Weak interaction and the change in the magnetic effect caused gravitation must be conducted. The Wien law is also important to explain the Weak interaction, since it describes the T_{max} change and the diffraction patterns change. [2]

Higgs mechanism and Quantum Gravity

The magnetic induction creates a negative electric field, causing an electromagnetic inertia. Probably it is the mysterious Higgs field giving mass to the charged particles? We can think about the photon as an electron-positron pair, they have mass. The neutral particles are built from negative and positive charges, for example the neutron, decaying to proton and electron. The wave – particle duality makes sure that the particles are oscillating and creating magnetic induction as an inertial mass, explaining also the relativistic mass change. Higher frequency creates stronger magnetic induction, smaller frequency results lesser magnetic induction. It seems to me that the magnetic induction is the secret of the Higgs field. In particle physics, the Higgs mechanism is a kind of mass generation mechanism, a process that gives mass to elementary particles. According to this theory, particles gain mass by interacting with the Higgs field that permeates all space. More precisely, the Higgs mechanism endows gauge bosons in a gauge theory with mass through absorption of Nambu–Goldstone bosons arising in spontaneous symmetry breaking.

The simplest implementation of the mechanism adds an extra Higgs field to the gauge theory. The spontaneous symmetry breaking of the underlying local symmetry triggers conversion of components of this Higgs field to Goldstone bosons which interact with (at least some of) the other fields in the theory, so as to produce mass terms for (at least some of) the gauge bosons. This mechanism may also leave behind elementary scalar (spin-0) particles, known as Higgs bosons.

In the Standard Model, the phrase "Higgs mechanism" refers specifically to the generation of masses for the W[±], and Z weak gauge bosons through electroweak symmetry breaking. The Large Hadron Collider at CERN announced results consistent with the Higgs particle on July 4, 2012 but stressed that further testing is needed to confirm the Standard Model.

What is the Spin?

So we know already that the new particle has spin zero or spin two and we could tell which one if we could detect the polarizations of the photons produced. Unfortunately this is difficult and neither ATLAS nor CMS are able to measure polarizations. The only direct and sure way to confirm that the particle is indeed a scalar is to plot the angular distribution of the photons in the rest frame of the centre of mass. A spin zero particles like the Higgs carries no directional information away from the original collision so the distribution will be even in all directions. This test will be possible when a much larger number of events have been observed. In the mean time we can settle for less certain indirect indicators.

The Graviton

In physics, the graviton is a hypothetical elementary particle that mediates the force of gravitation in the framework of quantum field theory. If it exists, the graviton is expected to be massless (because the gravitational force appears to have unlimited range) and must be a spin-2 boson. The spin follows from the fact that the source of gravitation is the stress-energy tensor, a second-rank tensor (compared to electromagnetism's spin-1 photon, the source of which is the four-current, a first-rank tensor). Additionally, it can be shown that any massless spin-2 field would give rise to a force indistinguishable from gravitation, because a massless spin-2 field must couple to (interact with) the stress-energy tensor in the same way that the gravitational field does. This result suggests that, if a massless spin-2 particle is discovered, it must be the graviton, so that the only experimental verification needed for the graviton may simply be the discovery of a massless spin-2 particle. [3]

Conclusions

The accelerated charges self-maintaining potential shows the locality of the relativity, working on the quantum level also. [1]

The Secret of Quantum Entanglement that the particles are diffraction patterns of the electromagnetic waves and this way their quantum states every time is the result of the quantum state of the intermediate electromagnetic waves. [2]

One of the most important conclusions is that the electric charges are moving in an accelerated way and even if their velocity is constant, they have an intrinsic acceleration anyway, the so called spin, since they need at least an intrinsic acceleration to make possible they movement . The bridge between the classical and quantum theory is based on this intrinsic acceleration of the spin, explaining also the Heisenberg Uncertainty Principle. The particle – wave duality of the electric charges and the photon makes certain that they are both sides of the same thing. Basing the gravitational force on the accelerating Universe caused magnetic force and the Planck Distribution Law of the electromagnetic waves caused diffraction gives us the basis to build a Unified Theory of the physical interactions.

References

[1] The Magnetic field of the Electric current and the Magnetic induction

http://academia.edu/3833335/The Magnetic field of the Electric current

- [2] 3 Dimensional String Theory <u>http://academia.edu/3834454/3 Dimensional String Theory</u>
- [3] Graviton Production By Two Photon and Electron-Photon Processes In Kaluza-Klein Theories

With Large Extra Dimensions http://arxiv.org/abs/hep-ph/9909392 [4] Quantum Entanglement

http://en.wikipedia.org/wiki/Quantum_entanglement

[5] Space-based experiment could test gravity's effects on quantum entanglement

http://phys.org/news/2014-05-space-based-gravity-effects-quantum-entanglement.html

[6] Common Interpretation of Heisenberg's Uncertainty Principle Is Proved False

<u>http://www.scientificamerican.com/article/common-interpretation-of-heisenbergs-</u> <u>uncertaintyprinciple-is-proven-false/</u>

[7] Particle Measurement Sidesteps the Uncertainty Principle

<u>http://www.scientificamerican.com/article/particle-measurement-sidesteps-the-</u> uncertaintyprinciple/

[8] Tricking the uncertainty principle <u>http://phys.org/news/2014-05-uncertainty-principle.html</u> [9]

Small entropy changes allow quantum measurements to be nearly reversed

http://phys.org/news/2015-09-small-entropy-quantum-reversed.html [10] Physicists put the

arrow of time under a quantum microscope

http://physicsworld.com/cws/article/news/2015/nov/12/physicists-put-the-arrow-of-time-underaquantum-microscope

[11] Physicists confirm thermodynamic irreversibility in a quantum system

http://phys.org/news/2015-12-physicists-thermodynamic-irreversibility-quantum.html

[12] What is quantum in quantum thermodynamics?

http://phys.org/news/2015-10-quantum-thermodynamics.html

[13] Researchers posit way to locally circumvent Second Law of Thermodynamics

http://phys.org/news/2016-10-posit-locally-circumvent-law-thermodynamics.html

[14] Physicists read Maxwell's Demon's mind https://phys.org/news/2017-07-physicists-maxwell-

demon-mind.html [15] Maxwell's demon extracts work from quantum measurement

https://phys.org/news/2017-07-maxwell-demon-quantum.html

[16] Controlling heat and particle currents in nanodevices by quantum observation

https://phys.org/news/2017-07-particle-currents-nanodevices-quantum.html

[17] Fast heat flows in warm, dense aluminum <u>https://phys.org/news/2017-09-fast-</u>

dense-aluminum.html

[18] A new efficient and portable electrocaloric cooling device

https://phys.org/news/2017-09-efficient-portable-electrocaloric-cooling-device.html

[19] Converting heat into electricity with pencil and paper

https://phys.org/news/2018-02-electricity-pencil-paper.html

[20] Researchers develop heat switch for electronics

https://phys.org/news/2018-03-electronics.html

[21] Breakthrough in circuit design makes electronics more resistant to damage and defects

https://phys.org/news/2018-03-breakthrough-circuit-electronics-resistant-defects.html

[22] The quantum states on the surface of conducting materials can strongly interact with light

https://phys.org/news/2018-03-quantum-states-surface-materials-strongly.html

[23] Revolutionizing computer memory—with magnets

https://phys.org/news/2018-03-revolutionizing-memorywith-magnets.html

[24] Terahertz computer chip now within reach

https://phys.org/news/2018-03-terahertz-chip.html

[25] Researchers developing materials for quantum computing

https://phys.org/news/2018-03-materials-quantum.html

[26] Researchers develop nanoparticle films for high-density data storage

https://phys.org/news/2018-04-nanoparticle-high-density-storage.html

[27] Nanoparticles form supercrystals under pressure

https://phys.org/news/2018-09-nanoparticles-supercrystals-pressure.html

[28] Researchers decipher the dynamics of electrons in perovskite crystals

https://phys.org/news/2018-09-decipher-dynamics-electrons-perovskite-crystals.html

[29] Perovskite semiconductors seeing right through next generation X-ray detectors

https://phys.org/news/2018-09-perovskite-semiconductors-x-ray-detectors.html

[30] Supercomputer predicts optical and thermal properties of complex hybrid materials

https://phys.org/news/2018-10-supercomputer-optical-thermal-properties-complex.html

[31] Researchers switch material from one state to another with a single flash of light

https://phys.org/news/2018-10-material-state.html

[32] Researchers validate 80-year-old ferroelectric theory

https://phys.org/news/2018-10-validate-year-old-ferroelectric-theory.html

[33] Nanosized ferroelectrics become a reality

https://phys.org/news/2018-10-nanosized-ferroelectrics-reality.html

[34] Research team discovers perfectly imperfect twist on nanowire growth

https://phys.org/news/2019-04-team-perfectly-imperfect-nanowire-growth.html

[35] Scientists explore the unknown behaviour of gold nanoparticles with neutrons

https://phys.org/news/2019-04-scientists-explore-unknown-behaviour-gold.html

[36] Research reveals liquid gold on the nanoscale

https://phys.org/news/2019-06-reveals-liquid-gold-nanoscale.html

[37] Using carbon nanotubes to strengthen graphene-based membranes used for desalination

https://phys.org/news/2019-06-carbon-nanotubes-graphene-based-membranes-desalination.html

[38] Researchers create uniform-shape polymer nanocrystals

https://phys.org/news/2019-06-uniform-shape-polymer-nanocrystals.html

[39] Opposite piezoresistant effects of rhenium disulfide in two principle directions

https://phys.org/news/2019-06-piezoresistant-effects-rhenium-disulfide-principle.html

[40] Plot twist: Straightening single-molecule conductors improves their performance

https://phys.org/news/2019-06-plot-straightening-single-molecule-conductors.html

[41] Solvent pH controls interactions of gold nanoclusters, offers potential applications in drugs and imaging

https://phys.org/news/2019-06-solvent-ph-interactions-gold-nanoclusters.html

[42] Study reveals new structure of gold at extremes

https://phys.org/news/2019-07-reveals-gold-extremes.html

[43] Actively swimming gold nanoparticles

https://phys.org/news/2019-07-gold-nanoparticles.html