

# Machine Learning Graphene Oxide

*This question is important for optimizing the properties of the carbon material in real-world applications, and researchers at CSIRO in Australia have now tried to answer it using machine learning. [27]*

*Reporting their findings in the open-access journal npj Computational Materials, the researchers show that their ML method, involving "transfer learning," enables the discovery of materials with desired properties even from an exceedingly small data set. [26]*

*The analysis of sensor data of machines, plants or buildings makes it possible to detect anomalous states early and thus to avoid further damage. [25]*

*Physicists in the US have used machine learning to determine the phase diagram of a system of 12 idealized quantum particles to a higher precision than ever before. [24]*

*The research group took advantage of a system at SLAC's Stanford Synchrotron Radiation Lightsource (SSRL) that combines machine learning—a form of artificial intelligence where computer algorithms glean knowledge from enormous amounts of data—with experiments that quickly make and screen hundreds of sample materials at a time. [23]*

*Researchers at the UCLA Samueli School of Engineering have demonstrated that deep learning, a powerful form of artificial intelligence, can discern and enhance microscopic details in photos taken by smartphones. [22]*

*Such are the big questions behind one of the new projects underway at the MIT-IBM Watson AI Laboratory, a collaboration for research on the frontiers of artificial intelligence. [21]*

*The possibility of cognitive nuclear-spin processing came to Fisher in part through studies performed in the 1980s that reported a remarkable lithium isotope dependence on the behavior of mother rats. [20]*

*And as will be presented today at the 25th annual meeting of the Cognitive Neuroscience Society (CNS), cognitive neuroscientists increasingly are using those emerging artificial networks to enhance their understanding of one of the most elusive intelligence systems, the human brain. [19]*

*U.S. Army Research Laboratory scientists have discovered a way to leverage emerging brain-like computer architectures for an age-old number-theoretic problem known as integer factorization. [18]*

*Now researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time. [17]*

*Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning. [16]*

*Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. [15]*

*Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal *Angewandte Chemie*. [14]*

*Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. [13]*

*With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials. [12]*

*The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA. [11]*

*Quantum physicist Mario Krenn and his colleagues in the group of Anton Zeilinger from the Faculty of Physics at the University of Vienna and the Austrian Academy of Sciences have developed an algorithm which designs new useful quantum experiments. As the computer does not rely on human intuition, it finds novel unfamiliar solutions. [10]*

*Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond. [9]*

*New research demonstrates that particles at the quantum level can in fact be seen as behaving something like billiard balls rolling along a table, and not merely as the probabilistic smears that the standard interpretation of quantum mechanics suggests. But there's a catch - the tracks the particles follow do not always behave as one would expect from "realistic" trajectories, but often in a fashion that has been termed "surrealistic." [8]*

*Quantum entanglement—which occurs when two or more particles are correlated in such a way that they can influence each other even across large distances—is not an all-or-nothing phenomenon, but occurs in various degrees. The more a quantum state is entangled with its partner, the better the states will perform in quantum information applications. Unfortunately, quantifying entanglement is a difficult process involving complex optimization problems that give even physicists headaches. [7]*

*A trio of physicists in Europe has come up with an idea that they believe would allow a person to actually witness entanglement. Valentina Caprara Vivoli, with the University of Geneva, Pavel Sekatski, with the University of Innsbruck and Nicolas Sangouard, with the University of Basel, have together written a paper describing a scenario where a human subject would be able to witness an instance of entanglement—they have uploaded it to the arXiv server for review by others. [6]*

*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.*

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## 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.

## Machine learning could reveal graphene oxide's real structure

What is the actual structure of graphene oxide nanoflakes? This question is important for optimizing the properties of the carbon material in real-world applications, and researchers at CSIRO in Australia have now tried to answer it using machine learning. Their approach uses over 20,000 possible structure candidates to find truly representative models and is very different to existing predictive techniques, which are often based on single or limited numbers of model structures.

Graphene oxide (GO) is a hydrophilic, 2D oxidized form of graphene (a sheet of carbon just one atomic layer thick) with oxygen functional groups decorating and disrupting the  $sp^2$  basal plane of the material, which ranges in size from a few nanometres to a few millimetres. The first model of GO's structure, proposed in 1939, suggested that the oxygen was bound to a hexagonal carbon sheet by epoxy (1,2-ether) and had the formula  $C_2O$ . Researchers have been revising this model ever since, taking into account sheet wrinkling, for example, and the presence of axially-bound functional groups that distort the flat GO structure.

[In 1998, scientists proposed the Lerf-Klinowski model.](#) In this description of GO, all the carbon rings are perfect (six-membered), and out-of-plane spatial distortions caused by functional groups or intrinsic ripples are essentially ignored. Although instructive, this model is rather limiting, and it is also largely inconsistent with structures obtained either by computational modelling of GO or by electron microscopy images.

## Unsupervised machine learning techniques

Researchers led by [Amanda Barnard](#) of Data61 at [CSIRO](#) have now revisited the structure of GO using a new clustering algorithm developed in their laboratory and have predicted centroid structures that are truly representative of the material. To extract archetypes, they performed analyses based on the unsupervised algorithm first put forward in 1994 by Cutler and Breiman.

“Theoretically, the archetypal analysis technique finds points in the feature space of the material that are on the boundary of the convex hull of the data cloud,” explains study lead author [Benyamin Motevalli](#). “This means that all possible candidate materials can be described as linear combinations of these archetypal (pure) points. The approach can even predict archetypal structures not included in the data set.”

Clustering is also an unsupervised technique that finds patterns in the data set and group structures based on similarity, he tells *Physics World*.

### The input data

The researchers gathered their input data by creating a wide range of flake sizes, and shapes. They then varied the oxygen concentrations in the flakes and added different chemical groups, distributed in different ways.

The data set contains 20396 samples in all with surface areas ranging from 320 Å<sup>2</sup> to 2457 Å<sup>2</sup>. These samples contain hydroxyl, ether, double bonds, aliphatic (cyclohexane) groups, and significant out-of-plane distortions (caused by defects) that go beyond the Lerf-Klinowski model.

The team included four different flake morphologies: hexagonal (49.5 %), trigonal (14.3 %), rectangular (30.5 %), and rhombic (5.7 %). The total number of atoms in each sample varies from 191 to 1949 and includes C, H, and O atoms. Different ratios of armchair and zigzag edges were also incorporated into the data set.

“The density and distribution of oxygen groups have a significant role in deriving GO properties, so for each of the 24 primary pristine graphene nanoflakes, we sampled numerous O/H concentrations, each with hundreds of random distributions,” explains Motevalli. In each case the O/C ratio was between 4.05% to 52.08%, and the H/C ratio between 2.22% to 49.26%.

### 28 structures can replace 20396 samples

Using this method, the researchers identified three representative GO nanoflakes that are effectively the “average” structure in 223-dimensional space.

The say they also identified 25 “pure” GO nanoflakes structures that capture all of the complexity and diversity of the entire 20396 data set they begin with. These 25 structures can be used as linear combinations to represent the whole set.

“Together these 28 structures (the 25 structures and the three prototypes) can replace the 20396 samples with no loss of information,” says Motevalli. “They can also be used as single model structures with the right chemical composition.”

Each structure is available for download

at: <https://doi.org/10.25919/5d1304152364a>.



## A machine-learning revolution

### Removing guesswork and bias

“Our 20396 GO nanoflake structures required years of work and over 30 million core supercomputer hours to generate at the electronic structure level,” he explains. “Reducing this set to the 28 most important structures will enable other research groups to make predictions on GO that are representative and reliable in a fraction of this time.”

The approach also removes the guesswork and bias in computational models of GO and provides the consistency necessary for benchmarking, he adds. “If all researchers working on GO used the same model structures, we could then easily compare and correlate results from laboratories all around the world.”

The researchers plan to use supervised machine learning to explore GO structure and property relationships and predict how different types of samples should perform under different conditions and in different applications. “Examples include electronic charge transfer properties, or studying the role of defects and distortions and how they affect fault tolerance,” Motevalli says.

The group’s findings appear in [Nano Futures](#), which (like *Physics World*) is published by IOP Publishing. [27]



## Successful application of machine learning in the discovery of new polymers

A joint research group including Ryo Yoshida (Professor and Director of the Data Science Center for Creative Design and Manufacturing at the Institute of Statistical Mathematics [ISM], Research Organization of Information and Systems), Junko Morikawa (Professor at the School of Materials and Chemical Technology, Tokyo Institute of Technology [Tokyo Tech]), and Yibin Xu (Group Leader of Thermal Management and Thermoelectric Materials Group, Center for Materials Research by Information Integration, Research and Services Division of Materials Data and Integrated System [MaDIS], NIMS) has demonstrated the promising application of machine learning (ML)—a form of AI that enables computers to "learn" from given data—for discovering innovative materials.

Reporting their findings in the open-access journal *npj Computational Materials*, the researchers show that their ML method, involving "transfer learning," enables the discovery of materials with desired properties even from an exceedingly small data set.

The study drew on a data set of polymeric properties from PoLyInfo, the largest database of polymers in the world housed at NIMS. Despite its size, PoLyInfo has a limited amount of data on the heat transfer properties of polymers. To predict the heat transfer properties from the given limited data, ML models on proxy properties were pre-trained where sufficient data were available on the related tasks; these pre-trained models captured common features relevant to the target task. Re-purposing these types of machine-acquired features on the target task yielded outstanding prediction performance even with exceedingly small datasets—not unlike the work of highly experienced human experts with respect to rational inferences even for considerably less experienced tasks. The team combined this model with a specially designed ML algorithm for computational molecular design, which is called the iQSPR algorithm previously developed by Yoshida and his colleagues. Applying this technique enabled the identification of thousands of promising "virtual" polymers.

From this large pool of candidates, three polymers were selected based on their ease of synthesis and processing. Tests confirmed that the new polymers have a [high thermal conductivity](#) of up to 0.41 Watts per meter-Kelvin (W/mK). This figure is 80 percent higher than that of typical polyimides, a group of commonly used polymers that have been mass-produced since the 1950s for applications ranging from fuel cells to cookware.

By verifying the heat transfer properties of the computationally designed polymers, the study represents a key breakthrough for fast, cost-effective, ML-supported methods for materials design. It also demonstrates the team's combined expertise in data science, organic synthesis and advanced measurement technologies.

Yoshida comments that many aspects remain to be explored, such as "training" computational systems to work with limited data by adding more suitable descriptors. "Machine learning for [polymer](#) or soft material design is a challenging but promising field as these materials have properties that differ from metals and ceramics, and are not yet fully predicted by the existing theories," he says.

The study is a starting point for the discovery of other innovative materials, as Morikawa adds: "We would like to try to create an ML-driven high-throughput computational system to design next-generation soft materials for applications going beyond the 5G era. Through our project, we aim to pursue not only the development of materials informatics but also contribute to fundamental advancement of materials science, especially in the field of phonon engineering." [26]

## Using machine learning for the early detection of anomalies helps to avoid damage

The analysis of sensor data of machines, plants or buildings makes it possible to detect anomalous states early and thus to avoid further damage. For this purpose, the monitoring data is searched for anomalies. By means of machine learning, anomaly detection can already be partially automated.

Machine learning methods first require a stable learning phase in which they get to know all possible kinds of regular states. For [wind turbines](#) or bridges, this is only possible to a very limited extent, as they are, for example, exposed to highly fluctuating weather conditions. In addition, there is usually only little information available on anomalous events. As a result, it is difficult for the system to identify and categorize exceptional states. However, this knowledge is important in order to find out how precarious the respective deviations from the norm really are. These problems are to be addressed in the project "Machine Learning Procedures for Stochastic-Deterministic Multi-Sensor Signals" (MADESI).

Numerical simulations can run through all conceivable scenarios. For example, it is possible to simulate what happens if strong squalls hit a wind turbine. The [monitoring](#) system can then be trained with data generated by these simulations and afterwards detect and interpret anomalies autonomously.

The researchers in the MADESI project develop methods that enable the utilization of simulation data in [machine learning](#). Here, the monitoring system needs to be designed in such a way that it can be trained using real sensor data and [simulation](#) data. Moreover, the consortium intends to increase the interpretability of the monitoring data. "For this purpose, we at SCAI work on data mining methods which can recognize patterns in the scenario data," explains project manager Prof. Dr. Jochen Garcke, head of the department "Numerical Data-Driven Prediction" at Fraunhofer SCAI. "Here, we also look for characteristic features of specific damages of wind turbine gear boxes or for ice on the rotor blades of a wind [turbine](#)." [25]

## Machine learning reveals quantum phases of matter

Physicists in the US have used machine learning to determine the phase diagram of a system of 12 idealized quantum particles to a higher precision than ever before. The work was done by [Eun-Ah Kim](#) of Cornell University and colleagues who say that they are probably the first to use machine learning algorithms to uncover "information beyond conventional knowledge" of condensed matter physics.

So far, machine learning has only been used to confirm established condensed matter results in proof-of-principle demonstrations, says [Roger Melko](#) of the University of Waterloo in Canada, who was not involved in the work. For example, Melko has used machine learning to sort various magnetic states of matter that had already been previously classified. Instead, Kim and colleagues have made new predictions about their system's phases that are unattainable with other methods. "This is an example of machines beating prior work by humans," says Melko.

Kim's group studied the physics of 12 idealized electrons interacting according to the Ising model – which describes the interaction between the spins of neighbouring particles. Although their 12-particle model is simplistic compared to real-life materials, this system can just barely be simulated by supercomputers. This is because the complexity of quantum simulations grows exponentially with every additional particle.

The team was particularly interested in understanding the many body localization (MBL) phases that can arise in quantum systems. These phases occur when particles are out of equilibrium and do not behave as a collection of non-interacting particles nor as an ensemble. Physicists struggle to describe MBL phases because statistical concepts like temperature and pressure are ill-defined. "They challenge our understanding of quantum statistical mechanics and quantum chaos," says Kim.

### **90% classification accuracy**

The team taught the machine learning algorithm to draw a phase diagram that includes two different MBL phases and one conventional phase. To do this, they first generated simulated data of different configurations of the 12 quantum particles that correspond to known phases. They fed each configuration to a neural network, which classified the data as a particular phase. At this point in the machine-learning process the researchers told the neural network whether its classification was correct. Given that feedback, the neural network iteratively developed an algorithm based on matrix multiplication that could distinguish among phases. The neural network could achieve 90% classification accuracy after being trained with 1000 different particle configurations.

The next step involved using the neural network to classify particle configurations of unknown phase. By sorting these configurations, they could fill a phase diagram with boundaries that were more distinct compared to prior diagrams made from other techniques.

### **How do they learn?**

One important downside of using neural networks to predict new physics is that we do not have a clear understanding of how the systems learn. This is a broad area of current research known as the interpretability problem. Fortunately, Kim's neural network is relatively simple. Many neural networks, such as those that power speech and image recognition algorithms, involve feeding input data through multiple iterations of matrix multiplication called "hidden layers" before they produce an output. These hidden layers are the most opaque parts of the learning process, and Kim's neural network only has one hidden layer. Her group is now trying to pick apart what exactly that hidden layer is doing. "It's possible to look inside a simple, custom-built neural network and figure out how it's making its decisions," says Kim.

## A quantum boost for machine learning

In addition, Kim wants to see if the team can apply a more sophisticated type of machine learning, known as unsupervised learning, to condensed matter problems. Unlike supervised learning, where the algorithm is given the correct answer as feedback, an unsupervised learning algorithm does not receive such feedback.

Condensed matter problems are particularly well-suited for machine learning because they involve many interacting particles, and therefore lots of data, says Melko. The field is moving fast, he says. “Just like you pick up your phone and take for granted that Siri works, in a few years I think everyone’s going to take for granted that there’s some integration of AI technology in these very complex quantum experiments,” he says.

A paper describing the research has been accepted for publication in [Physical Review Letters](#) and a [preprint](#) is available on *arXiv*. [24]

## Artificial intelligence accelerates discovery of metallic glass

Blend two or three metals together and you get an alloy that usually looks and acts like a metal, with its atoms arranged in rigid geometric patterns.

But once in a while, under just the right conditions, you get something entirely new: a futuristic alloy called metallic glass that's amorphous, with its atoms arranged every which way, much like the atoms of the glass in a window. Its glassy nature makes it stronger and lighter than today's best steel, plus it stands up better to corrosion and wear.

Even though metallic glass shows a lot of promise as a protective coating and alternative to steel, only a few thousand of the millions of possible combinations of ingredients have been evaluated over the past 50 years, and only a handful developed to the point that they may become useful.

Now a group led by scientists at the Department of Energy's SLAC National Accelerator Laboratory, the National Institute of Standards and Technology (NIST) and Northwestern University has reported a shortcut for discovering and improving metallic glass—and, by extension, other elusive materials—at a fraction of the time and cost.

The research group took advantage of a system at SLAC's Stanford Synchrotron Radiation Lightsource (SSRL) that combines machine learning—a form of artificial intelligence where computer algorithms glean knowledge from enormous amounts of data—with experiments that quickly make and screen hundreds of sample materials at a time. This allowed the team to discover three new blends of ingredients that form metallic glass, and to do this 200 times faster than it could be done before, they reported today in *Science Advances*.

"It typically takes a decade or two to get a material from discovery to commercial use," said Northwestern Professor Chris Wolverton, an early pioneer in using computation and AI to predict new materials and a co-author of the paper. "This is a big step in trying to squeeze that time down. You could start out with nothing more than a list of properties you want in a material and, using AI, quickly narrow the huge field of potential materials to a few good candidates."

The ultimate goal, he said, is to get to the point where a scientist could scan hundreds of sample materials, get almost immediate feedback from machine learning models and have another set of samples ready to test the next day—or even within the hour.

Over the past half century, scientists have investigated about 6,000 combinations of ingredients that form metallic glass, added paper co-author Apurva Mehta, a staff scientist at SSRL: "We were able to make and screen 20,000 in a single year."

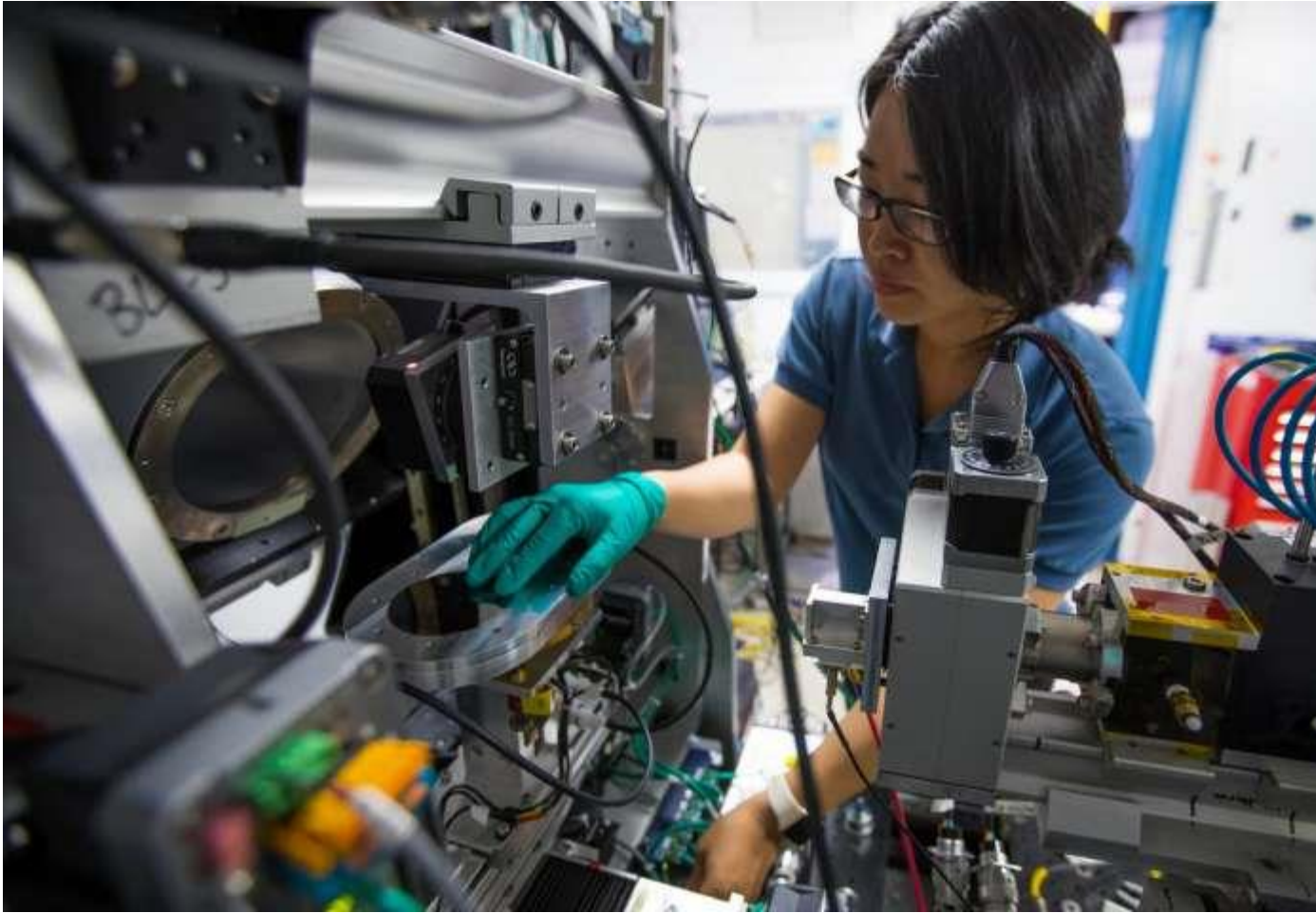
### **Just Getting Started**

While other groups have used machine learning to come up with predictions about where different kinds of metallic glass can be found, Mehta said, "The unique thing we have done is to rapidly verify our predictions with experimental measurements and then repeatedly cycle the results back into the next round of machine learning and experiments."

There's plenty of room to make the process even speedier, he added, and eventually automate it to take people out of the loop altogether so scientists can concentrate on other aspects of their work that require human intuition and creativity. "This will have an impact not just on synchrotron users, but on the whole materials science and chemistry community," Mehta said.

The team said the method will be useful in all kinds of experiments, especially in searches for materials like metallic glass and catalysts whose performance is strongly influenced by the way they're manufactured, and those where scientists don't have theories to guide their search. With machine learning, no previous understanding is needed. The algorithms make connections and draw conclusions on their own, and this can steer research in unexpected directions.

"One of the more exciting aspects of this is that we can make predictions so quickly and turn experiments around so rapidly that we can afford to investigate materials that don't follow our normal rules of thumb about whether a material will form a glass or not," said paper co-author Jason Hatrick-Simpers, a materials research engineer at NIST. "AI is going to shift the landscape of how materials science is done, and this is the first step."



Fang Ren, who developed algorithms to analyze data on the fly while a postdoctoral scholar at SLAC, at a Stanford Synchrotron Radiation Lightsource beamline where the system has been put to use. Credit: Dawn Harmer/SLAC National Accelerator Laboratory

### **Strength in Numbers**

The paper is the first scientific result associated with a DOE-funded pilot project where SLAC is working with a Silicon Valley AI company, Citrine Informatics, to transform the way new materials are discovered and make the tools for doing that available to scientists everywhere.

Founded by former graduate students from Stanford and Northwestern universities, Citrine has created a materials science data platform where data that had been locked away in published papers, spreadsheets and lab notebooks is stored in a consistent format so it can be analyzed with AI specifically designed for materials.

"We want to take materials and chemical data and use them effectively to design new materials and optimize manufacturing," said Greg Mulholland, founder and CEO of the company. "This is the power of artificial intelligence: As scientists generate more data, it learns alongside them, bringing hidden trends to the surface and allowing scientists to identify high-performance materials much faster and more effectively than relying on traditional, purely human-driven materials development."

Until recently, thinking up, making and assessing new materials was painfully slow. For instance, the authors of the metallic glass paper calculated that even if you could cook up and examine five potential types of metallic glass a day, every day of the year, it would take more than a thousand years to plow through every possible combination of metals. When they do discover a metallic glass, researchers struggle to overcome problems that hold these materials back. Some have toxic or expensive ingredients, and all of them share glass's brittle, shatter-prone nature.

Over the past decade, scientists at SSRL and elsewhere have developed ways to automate experiments so they can create and study more novel materials in less time. Today, some SSRL users can get a preliminary analysis of their data almost as soon as it comes out with AI software developed by SSRL in conjunction with Citrine and the CAMERA project at DOE's Lawrence Berkeley National Laboratory.

"With these automated systems we can analyze more than 2,000 samples per day," said Fang Ren, the paper's lead author, who developed algorithms to analyze data on the fly and coordinated their integration into the system while a postdoctoral scholar at SLAC.

### **Experimenting with Data**

In the metallic glass study, the research team investigated thousands of alloys that each contain three cheap, nontoxic metals.

They started with a trove of materials data dating back more than 50 years, including the results of 6,000 experiments that searched for metallic glass. The team combed through the data with advanced machine learning algorithms developed by Wolverton and graduate student Logan Ward at Northwestern.

Based on what the algorithms learned in this first round, the scientists crafted two sets of sample alloys using two different methods, allowing them to test how manufacturing methods affect whether an alloy morphs into a glass.

Both sets of alloys were scanned by an SSRL X-ray beam, the data fed into the Citrine database, and new machine learning results generated, which were used to prepare new samples that underwent another round of scanning and machine learning.

By the experiment's third and final round, Mehta said, the group's success rate for finding metallic glass had increased from one out of 300 or 400 samples tested to one out of two or three samples tested. The metallic glass samples they identified represented three different combinations of ingredients, two of which had never been used to make metallic glass before. [23]

### **Deep learning transforms smartphone microscopes into laboratory-grade devices**

Researchers at the UCLA Samueli School of Engineering have demonstrated that deep learning, a powerful form of artificial intelligence, can discern and enhance microscopic details in photos taken

by smartphones. The technique improves the resolution and color details of smartphone images so much that they approach the quality of images from laboratory-grade microscopes.

The advance could help bring high-quality medical diagnostics into resource-poor regions, where people otherwise do not have access to high-end diagnostic technologies. And the technique uses attachments that can be inexpensively produced with a 3-D printer, at less than \$100 a piece, versus the thousands of dollars it would cost to buy laboratory-grade equipment that produces images of similar quality.

Cameras on today's smartphones are designed to photograph people and scenery, not to produce high-resolution microscopic images. So the researchers developed an attachment that can be placed over the smartphone lens to increase the resolution and the visibility of tiny details of the images they take, down to a scale of approximately one millionth of a meter.

But that only solved part of the challenge, because no attachment would be enough to compensate for the difference in quality between smartphone cameras' image sensors and lenses and those of high-end lab equipment. The new technique compensates for the difference by using [artificial intelligence](#) to reproduce the level of resolution and color details needed for a laboratory analysis.

The research was led by Aydogan Ozcan, Chancellor's Professor of Electrical and Computer Engineering and Bioengineering, and Yair Rivenson, a UCLA postdoctoral scholar. Ozcan's research group has introduced several innovations in mobile microscopy and sensing, and it maintains a particular focus on developing field-portable medical diagnostics and sensors for resource-poor areas.

"Using deep learning, we set out to bridge the gap in image quality between inexpensive mobile phone-based microscopes and gold-standard bench-top microscopes that use high-end lenses," Ozcan said. "We believe that our approach is broadly applicable to other low-cost microscopy systems that use, for example, inexpensive lenses or cameras, and could facilitate the replacement of high-end bench-top microscopes with cost-effective, mobile alternatives."

He added that the new technique could find numerous applications in global health, telemedicine and diagnostics-related applications.

The researchers shot images of lung tissue samples, blood and Pap smears, first using a standard laboratory-grade microscope, and then with a [smartphone](#) with the 3-D-printed [microscope](#) attachment. The researchers then fed the pairs of corresponding images into a computer system that "learns" how to rapidly enhance the mobile phone images. The process relies on a deep-learning-based computer code, which was developed by the UCLA researchers.

To see if their technique would work on other types of lower-quality images, the researchers used deep learning to successfully perform similar transformations with images that had lost some detail because they were compressed for either faster transmission over a computer network or more efficient storage.

The study was published in *ACS Photonics*, a journal of the American Chemical Society. It builds upon previous studies by Ozcan's group that used [deep learning](#) to reconstruct holograms and improve microscopy. [22]



## Training computers to recognize dynamic events

A person watching videos that show things opening—a door, a book, curtains, a blooming flower, a yawning dog—easily understands the same type of action is depicted in each clip.

"Computer models fail miserably to identify these things. How do humans do it so effortlessly?" asks Dan Gutfreund, a principal investigator at the MIT-IBM Watson AI Laboratory and a staff member at IBM Research. "We process information as it happens in space and time. How can we teach computer models to do that?"

Such are the big questions behind one of the new projects underway at the MIT-IBM Watson AI Laboratory, a collaboration for research on the frontiers of artificial intelligence. Launched last fall, the lab connects MIT and IBM researchers together to work on AI algorithms, the application of AI to industries, the physics of AI, and ways to use AI to advance shared prosperity.

The [Moments in Time dataset](#) is one of the projects related to AI algorithms that is funded by the lab. It pairs Gutfreund with Aude Oliva, a principal research scientist at the MIT Computer Science and Artificial Intelligence Laboratory, as the project's principal investigators. Moments in Time is built on a collection of 1 million annotated videos of dynamic events unfolding within three seconds. Gutfreund and Oliva, who is also the MIT executive director at the MIT-IBM Watson AI Lab, are using these clips to address one of the next big steps for AI: teaching machines to recognize actions.

## Learning from dynamic scenes

The goal is to provide deep-learning algorithms with large coverage of an ecosystem of visual and auditory moments that may enable models to learn information that isn't necessarily taught in a supervised manner and to generalize to novel situations and tasks, say the researchers.

"As we grow up, we look around, we see people and objects moving, we hear sounds that people and object make. We have a lot of visual and auditory experiences. An AI system needs to learn the same way and be fed with videos and dynamic information," Oliva says.

For every action category in the dataset, such as cooking, running, or opening, there are more than 2,000 videos. The short clips enable computer models to better learn the diversity of meaning around specific actions and events.

"This dataset can serve as a new challenge to develop AI models that scale to the level of complexity and abstract reasoning that a human processes on a daily basis," Oliva adds, describing the factors involved. Events can include people, objects, animals, and nature. They may be symmetrical in time—for example, opening means closing in reverse order. And they can be transient or sustained.

Oliva and Gutfreund, along with additional researchers from MIT and IBM, met weekly for more than a year to tackle technical issues, such as how to choose the action categories for annotations, where to find the videos, and how to put together a wide array so the AI system learns without bias.

The team also developed machine-learning models, which were then used to scale the data collection. "We aligned very well because we have the same enthusiasm and the same goal," says Oliva.

### Augmenting human intelligence

One key goal at the lab is the development of AI systems that move beyond specialized tasks to tackle more complex problems and benefit from robust and continuous learning. "We are seeking new algorithms that not only leverage big data when available, but also learn from limited data to augment human intelligence," says Sophie V. Vandebroek, chief operating officer of IBM Research, about the collaboration.

In addition to pairing the unique technical and scientific strengths of each organization, IBM is also bringing MIT researchers an influx of resources, signaled by its \$240 million investment in AI efforts over the next 10 years, dedicated to the MIT-IBM Watson AI Lab. And the alignment of MIT-IBM interest in AI is proving beneficial, according to Oliva.

"IBM came to MIT with an interest in developing new ideas for an artificial intelligence system based on vision. I proposed a project where we build data sets to feed the model about the world. It had not been done before at this level. It was a novel undertaking. Now we have reached the milestone of 1 million videos for visual AI training, and people can go to our website, download the dataset and our deep-learning computer models, which have been taught to recognize actions."

Qualitative results so far have shown models can recognize moments well when the action is well-framed and close up, but they misfire when the category is fine-grained or there is background clutter, among other things. Oliva says that MIT and IBM researchers have submitted an article describing the performance of neural network models trained on the dataset, which itself was deepened by shared viewpoints. "IBM researchers gave us ideas to add action categories to have more richness in areas like health care and sports. They broadened our view. They gave us ideas about how AI can make an impact from the perspective of business and the needs of the world," she says.

This first version of the Moments in Time dataset is one of the largest human-annotated video datasets capturing visual and audible short events, all of which are tagged with an action or activity label among 339 different classes that include a wide range of common verbs. The researchers intend to produce more datasets with a variety of levels of abstraction to serve as stepping stones toward the development of learning algorithms that can build analogies between things, imagine and synthesize novel events, and interpret scenarios.

In other words, they are just getting started, says Gutfreund. "We expect the Moments in Time dataset to enable models to richly understand actions and dynamics in videos." [21]

## Are we quantum computers? International collaboration will investigate the brain's potential for quantum computation

Much has been made of quantum computing processes using ultracold atoms and ions, superconducting junctions and defects in diamonds, but could we be performing them in our own brains?

It's a question UC Santa Barbara theoretical physicist [Matthew Fisher](#) has been asking for years. Now, as scientific director of the new Quantum Brain Project (QuBrain), he is seeking to put this inquiry through rigorous experimental tests.

"Might we, ourselves, be [quantum](#) computers, rather than just clever robots who are designing and building quantum computers?" Fisher asks.

Some functions the [brain](#) performs continue to elude neuroscience—the substrate that "holds" very long-term memories and how it operates, for example. Quantum mechanics, which deals with the behavior of nature at atomic and subatomic levels, may be able to unlock some clues. And that in turn could have major implications on many levels, from quantum computing and materials sciences to biology, mental health and even what it is to be human.

The idea of [quantum computing](#) in our brains is not a new one. In fact, it has been making the rounds for a while with some scientists, as well as those with less scientific leanings. But Fisher, a world-renowned expert in the field of quantum mechanics, has identified a precise—and unique—set of biological components and key mechanisms that could provide the basis for quantum processing in the brain. With \$1.2 million in grant funding over three years from the Heising-Simons Foundation, Fisher will launch the QuBrain collaboration at UCSB. Composed of an international team of leading scientists spanning quantum physics, molecular biology, biochemistry, colloid science and behavioral neuroscience, the project will seek explicit experimental evidence to answer whether we might in fact be quantum computers.

"We are extremely grateful to the Heising-Simons Foundation for the bold vision in granting this project at the very frontier of quantum- and neuroscience," said UC Santa Barbara Chancellor Henry T. Yang. "Professor Matthew Fisher is an exceptional quantum physicist as evidenced by the Oliver E. Buckley Prize he shared in 2015 for his research on quantum phase transitions. Now he is stepping out of his traditional theoretical research framework, assembling an international team of experts to develop an experimentally based research program that will determine if quantum processes exist in the brain. Their research could shed new light on how the brain works, which might lead to novel mental health treatment protocols. As such, we eagerly anticipate the results of QuBrain's collaborative research endeavors in the years to come."

"If the question of whether quantum processes take place in the brain is answered in the affirmative, it could revolutionize our understanding and treatment of brain function and human

cognition," said Matt Helgeson, a UCSB professor of chemical engineering and associate director at QuBrain.

### Biochemical Qubits

The hallmarks of quantum computers lie in the behaviors of the infinitesimal systems of atoms and ions, which can manifest "qubits" (e.g. "spins") that exhibit quantum entanglement. Multiple qubits can form networks that encode, store and transmit information, analogous to the digital bits in a conventional computer. In the quantum computers we are trying to build, these effects are generated and maintained in highly controlled and isolated environments and at low temperatures. So the warm, wet brain is not considered a conducive environment to exhibit quantum effects as they should be easily "washed out" by the thermal motion of atoms and molecules.

However, Fisher asserts that nuclear spins (at the core of the atom, rather than the surrounding electrons) provide an exception to the rule.

"Extremely well-isolated nuclear spins can store—and perhaps process—quantum information on human time scales of hours or longer," he said. Fisher posits that phosphorus atoms—one of the most abundant elements in the body—have the requisite nuclear spin that could serve as a biochemical qubit. One of the experimental thrusts of the collaboration will be to monitor the quantum properties of phosphorus atoms, particularly entanglement between two phosphorus nuclear spins when bonded together in a molecule undergoing biochemical processes.

Meanwhile, Helgeson and Alexej Jerschow, a professor of chemistry at New York University, will investigate the dynamics and nuclear spin of Posner molecules—spherically shaped calcium phosphate nano-clusters—and whether they have the ability to protect the nuclear spins of the phosphorus atom qubits, which could promote the storage of quantum information. They will also explore the potential for non-local quantum information processing that could be enabled by pair-binding and disassociation of Posner molecules.

### Entangled Neurons

In another set of experiments, Tobias Fromme, a scientist at the Technical University of Munich, will study the potential contribution of mitochondria to entanglement and their quantum coupling to neurons. He will determine if these cellular organelles—responsible for functions such as metabolism and cell signaling—can transport Posner molecules within and between neurons via their tubular networks. Fusing and fissioning of mitochondria could allow for establishment of non-local intra- and intercellular quantum entanglement. Subsequent disassociation of Posner molecules could trigger release of calcium, correlated across the mitochondrial network, activating neurotransmitter release and subsequent synaptic firing across what would essentially be a quantum coupled network of neurons—a phenomena that Fromme will seek to emulate in vitro.

The possibility of cognitive nuclear-spin processing came to Fisher in part through studies performed in the 1980s that reported a remarkable lithium isotope dependence on the behavior of mother rats. Though given the same element, their behavior changed dramatically depending on the number of neutrons in the lithium nuclei. What to most people would be a negligible difference was to a quantum physicist like Fisher a fundamentally significant disparity, suggesting the importance of [nuclear spins](#). Aaron Ettenberg, UCSB Distinguished Professor of Psychological &

Brain Sciences, will lead investigations that seek to replicate and extend these lithium isotope experiments.

"However likely you judge Matthew Fisher's hypothesis, by testing it through QuBrain's collaborative research approach we will explore neuronal function with state-of-the-art technology from completely new angles and with enormous potential for discovery," said Fromme. Similarly, according to Helgeson, the research conducted by QuBrain has the potential for breakthroughs in the fields of biomaterials, biochemical catalysis, [quantum entanglement](#) in solution chemistry and mood disorders in humans, regardless of whether or not quantum processes indeed take place in the brain. [20]

## **Dissecting artificial intelligence to better understand the human brain**

In the natural world, intelligence takes many forms. It could be a bat using echolocation to expertly navigate in the dark, or an octopus quickly adapting its behavior to survive in the deep ocean. Likewise, in the computer science world, multiple forms of artificial intelligence are emerging - different networks each trained to excel in a different task. And as will be presented today at the 25th annual meeting of the Cognitive Neuroscience Society (CNS), cognitive neuroscientists increasingly are using those emerging artificial networks to enhance their understanding of one of the most elusive intelligence systems, the human brain.

"The fundamental questions cognitive neuroscientists and computer scientists seek to answer are similar," says Aude Oliva of MIT. "They have a complex system made of components - for one, it's called [neurons](#) and for the other, it's called units - and we are doing experiments to try to determine what those components calculate."

In Oliva's work, which she is presenting at the CNS symposium, neuroscientists are learning much about the role of contextual clues in human image recognition. By using "artificial neurons" - essentially lines of code, software - with neural [network](#) models, they can parse out the various elements that go into recognizing a specific place or object.

"The brain is a deep and complex neural network," says Nikolaus Kriegeskorte of Columbia University, who is chairing the symposium. "Neural network models are brain-inspired models that are now state-of-the-art in many artificial intelligence applications, such as computer vision."

In one recent study of more than 10 million images, Oliva and colleagues taught an artificial network to recognize 350 different places, such as a kitchen, bedroom, park, living room, etc. They expected the network to learn objects such as a bed associated with a bedroom. What they didn't expect was that the network would learn to recognize people and animals, for example dogs at parks and cats in living rooms.

The machine [intelligence](#) programs learn very quickly when given lots of data, which is what enables them to parse contextual learning at such a fine level, Oliva says. While it is not possible to dissect human neurons at such a level, the computer [model](#) performing a similar task is entirely transparent. The [artificial neural networks](#) serve as "mini-brains that can be studied, changed, evaluated, compared against responses given by human neural networks, so the cognitive neuroscientists have some sort of sketch of how a real brain may function."

Indeed, Kriegeskorte says that these models have helped neuroscientists understand how people can recognize the objects around them in the blink of an eye. "This involves millions of signals emanating from the retina, that sweep through a sequence of layers of neurons, extracting semantic information, for example that we're looking at a street scene with several people and a dog," he says. "Current neural network models can perform this kind of task using only computations that biological neurons can perform. Moreover, these neural network models can predict to some extent how a neuron deep in the brain will respond to any image."

Using computer science to understand the human brain is a relatively new field that is expanding rapidly thanks to advancements in computing speed and power, along with neuroscience imaging tools. The artificial networks cannot yet replicate human visual abilities, Kriegeskorte says, but by modeling the human brain, they are furthering understanding of both cognition and [artificial intelligence](#). "It's a uniquely exciting time to be working at the intersection of neuroscience, cognitive science, and AI," he says.

Indeed, Oliva says; "Human cognitive and computational neuroscience is a fast-growing area of research, and knowledge about how the [human brain](#) is able to see, hear, feel, think, remember, and predict is mandatory to develop better diagnostic tools, to repair the [brain](#), and to make sure it develops well." [19]

## **Army's brain-like computers moving closer to cracking codes**

U.S. Army Research Laboratory scientists have discovered a way to leverage emerging brain-like computer architectures for an age-old number-theoretic problem known as integer factorization.

By mimicking the brain functions of mammals in computing, Army scientists are opening up a new solution space that moves away from traditional computing architectures and towards devices that are able to operate within extreme size-, weight-, and power-constrained environments.

"With more computing power in the battlefield, we can process information and solve computationally-hard problems quicker," said Dr. John V. "Vinnie" Monaco, an ARL computer scientist. "Programming the type of devices that fit these criteria, for example, brain-inspired computers, is challenging, and cracking crypto codes is just one application that shows we know how to do this."

The problem itself can be stated in simple terms. Take a composite integer  $N$  and express it as the product of its prime components. Most people have completed this task at some point in grade school, often an exercise in elementary arithmetic. For example, 55 can be expressed as  $5 \cdot 11$  and 63 as  $3 \cdot 3 \cdot 7$ . What many didn't realize is they were performing a task that if completed quickly enough for large numbers, could break much of the modern day internet.

Public key encryption is a method of secure communication used widely today, based on the RSA algorithm developed by Rivest, Shamir, and Adleman in 1978. The security of the RSA algorithm relies on the difficulty of factoring a large composite integer  $N$ , the public key, which is distributed by the receiver to anyone who wants to send an encrypted message. If  $N$  can be factored into its prime components, then the private key, needed to decrypt the message, can be recovered. However, the difficulty in factoring large integers quickly becomes apparent.

As the size of  $N$  increases by a single digit, the time it would take to factor  $N$  by trying all possible combinations of prime factors is approximately doubled. This means that if a number with ten digits takes 1 minute to factor, a number with twenty digits will take about 17 hours and a number with 30 digits about two years, an exponential growth in effort. This difficulty underlies the security of the RSA algorithm.

Challenging this, Monaco and his colleague Dr. Manuel Vindiola, of the lab's Computational Sciences Division, demonstrated how brain-like computers lend a speedup to the currently best known algorithms for factoring integers.

The team of researchers have devised a way to factor large composite integers by harnessing the massive parallelism of novel computer architectures that mimic the functioning of the mammalian brain. So called [neuromorphic computers](#) operate under vastly different principles than conventional computers, such as laptops and mobile devices, all based on an architecture described by John von Neumann in 1945.

In the von Neumann architecture, memory is separate from the central processing unit, or CPU, which must read and write to memory over a bus. This bus has a limited bandwidth, and much of the time, the CPU is waiting to access memory, often referred to as the von Neumann bottleneck.

Neuromorphic computers, on the other hand, do not suffer from a von Neumann bottleneck. There is no CPU, memory, or bus. Instead, they incorporate many individual computation units, much like neurons in the brain.

These units are connected by physical or simulated pathways for passing data around, analogous to synaptic connections between neurons. Many neuromorphic devices operate based on the physical response properties of the underlying material, such as graphene lasers or magnetic tunnel junctions. Because of this, these devices consume orders of magnitude less energy than their von Neumann counterparts and can operate on a molecular time scale. As such, any algorithm capable of running on these devices stands to benefit from their capabilities.

The speedup acquired by the ARL researchers is due to the formulation of a method for integer factorization with the help of a neuromorphic co-processor. The current fastest algorithms for factoring integers consist primarily of two stages, sieving and a matrix reduction, and the sieving stage comprises most of the computational effort.

Sieving involves searching for many integers that satisfy a certain property called B-smooth, integers that don't contain a prime factor greater than  $B$ . Monaco and Vindiola were able to construct a neural network that discovers B-smooth numbers quicker and with greater accuracy than on a von Neumann architecture. Their algorithm leverages the massive parallelism of brain-inspired computers and the innate ability of individual neurons to perform arithmetic operations, such as addition. As neuromorphic architectures continue to increase in size and speed, not limited by Moore's Law, their ability to tackle larger integer factorization problems also grows. In their work, it's estimated that 1024-bit keys could be broken in about a year, a task once thought to be out of reach. For comparison, the current record, a 232 decimal digit number (RSA-768) took about 2,000 years of computing time over the course of several years.

From a broader perspective, this discovery pushes us to question how a shift in computing paradigm might affect some of our most basic security assumptions. As emerging devices shift to incorporate massive parallelism and harness material physics to compute, the computational hardness underlying some security protocols may be challenged in ways not previously imagined. This work also opens the door to new research areas of emerging computer architectures, in terms of algorithm design and function representation, alongside low-power machine learning and artificial intelligence applications.

"Encrypted messages in warfare often have an expiration date, when their contents become un-actionable," Monaco said. "There is an urgency to decrypt enemy communications, especially those at the field level, since these expire the quickest, compared to communication at higher echelons. In field conditions, power and connectivity are extremely limited. This is a strong motivating factor for using a brain-inspired computer for such a task where conventional computers are not practical."  
[18]

## Teaching computers to guide science: Machine learning method sees forests and trees

While it may be the era of supercomputers and "big data," without smart methods to mine all that data, it's only so much digital detritus. Now researchers at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and UC Berkeley have come up with a novel machine learning method that enables scientists to derive insights from systems of previously intractable complexity in record time.

In a paper published recently in the *Proceedings of the National Academy of Sciences (PNAS)*, the researchers describe a technique called "iterative Random Forests," which they say could have a transformative effect on any area of science or engineering with complex systems, including biology, precision medicine, materials science, environmental science, and manufacturing, to name a few.

"Take a human cell, for example. There are  $10^{170}$  possible molecular interactions in a single cell. That creates considerable computing challenges in searching for relationships," said Ben Brown, head of Berkeley Lab's Molecular Ecosystems Biology Department. "Our method enables the identification of interactions of high order at the same computational cost as main effects - even when those interactions are local with weak marginal effects."

Brown and Bin Yu of UC Berkeley are lead senior authors of "Iterative Random Forests to Discover Predictive and Stable High-Order Interactions." The co-first authors are Sumanta Basu (formerly a joint postdoc of Brown and Yu and now an assistant professor at Cornell University) and Karl Kumbier (a Ph.D. student of Yu in the UC Berkeley Statistics Department). The paper is the culmination of three years of work that the authors believe will transform the way science is done. "With our method we can gain radically richer information than we've ever been able to gain from a learning machine," Brown said.



The needs of [machine learning](#) in science are different from that of industry, where machine learning has been used for things like playing chess, making self-driving cars, and predicting the stock market.

"The machine learning developed by industry is great if you want to do high-frequency trading on the [stock market](#)," Brown said. "You don't care why you're able to predict the stock will go up or down. You just want to know that you can make the predictions."

But in science, questions surrounding why a process behaves in certain ways are critical. Understanding "why" allows scientists to model or even engineer processes to improve or attain a desired outcome. As a result, machine learning for science needs to peer inside the black box and understand why and how computers reached the conclusions they reached. A long-term goal is to use this kind of information to model or engineer systems to obtain desired outcomes.

In highly complex systems - whether it's a single cell, the human body, or even an entire ecosystem - there are a large number of variables interacting in nonlinear ways. That makes it difficult if not impossible to build a model that can determine cause and effect. "Unfortunately, in biology, you come across interactions of order 30, 40, 60 all the time," Brown said. "It's completely intractable with traditional approaches to statistical learning."

The method developed by the team led by Brown and Yu, iterative Random Forests (iRF), builds on an algorithm called random forests, a popular and effective predictive modeling tool, translating the internal states of the black box learner into a human-interpretable form. Their approach allows researchers to search for complex interactions by decoupling the order, or size, of interactions from the computational cost of identification.

"There is no difference in the computational cost of detecting an interaction of order 30 versus an interaction of order two," Brown said. "And that's a sea change."

In the PNAS paper, the scientists demonstrated their method on two genomics problems, the role of gene enhancers in the fruit fly embryo and alternative splicing in a human-derived cell line. In both cases, using iRF confirmed previous findings while also uncovering previously unidentified higher-order interactions for follow-up study.

Brown said they're now using their method for designing phased array laser systems and optimizing sustainable agriculture systems.

"We believe this is a different paradigm for doing science," said Yu, a professor in the departments of Statistics and Electrical Engineering & Computer Science at UC Berkeley. "We do prediction, but we introduce stability on top of prediction in iRF to more reliably learn the underlying structure in the predictors."

"This enables us to learn how to engineer systems for goal-oriented optimization and more accurately targeted simulations and follow-up experiments," Brown added.

In a [PNAS commentary](#) on the technique, Danielle Denisko and Michael Hoffman of the University of Toronto wrote: "iRF holds much promise as a new and effective way of detecting interactions in a variety of settings, and its use will help us ensure no branch or leaf is ever left unturned." [17]

## Rise of the quantum thinking machines

Quantum computers can be made to utilize effects such as quantum coherence and entanglement to accelerate machine learning.

Although we typically view information as being an abstract or virtual entity, information, of course, must be stored in a physical medium. Information processing devices such as computers and phones are therefore fundamentally governed by the laws of physics. In this way, the fundamental physical limits of an agent's ability to learn are governed by the laws of physics. The best known theory of physics is quantum theory, which ultimately must be used to determine the absolute physical limits of a machine's ability to learn.

A quantum algorithm is a stepwise procedure performed on a quantum computer to solve a problem such as searching a database. Quantum machine learning software makes use of quantum algorithms to process information in ways that classical computers cannot. These quantum effects open up exciting new avenues which can, in principle, outperform the best known classical algorithms when solving certain machine learning problems. This is known as quantum enhanced machine learning.

Machine learning methods use mathematical algorithms to search for certain patterns in large data sets. Machine learning is widely used in biotechnology, pharmaceuticals, particle physics and many other fields. Thanks to the ability to adapt to new data, machine learning greatly exceeds the ability of people. Despite this, machine learning cannot cope with certain difficult tasks.

Quantum enhancement is predicted to be possible for a host of machine learning tasks, ranging from optimization to quantum enhanced deep learning.

In the new paper published in Nature, a group of scientists led by Skoltech Associate Professor Jacob Biamonte produced a feasibility analysis outlining what steps can be taken for practical quantum enhanced machine learning.

The prospects of using quantum computers to accelerate machine learning has generated recent excitement due to the increasing capabilities of quantum computers. This includes a commercially available 2000 spin quantum accelerated annealing by the Canada-based company D-Wave Systems Inc. and a 16 qubit universal quantum processor by IBM which is accessible via a (currently free) cloud service.

The availability of these devices has led to increased interest from the machine learning community. The interest comes as a bit of a shock to the traditional quantum physics community, in which researchers have thought that the primary applications of quantum computers would be using quantum computers to simulate chemical physics, which can be used in the pharmaceutical industry for drug discovery. However, certain quantum systems can be mapped to certain machine learning models, particularly deep learning models. Quantum machine learning can be used to work in tandem with these existing methods for quantum chemical emulation, leading to even greater capabilities for a new era of quantum technology.

"Early on, the team burned the midnight oil over Skype, debating what the field even was—our synthesis will hopefully solidify topical importance. We submitted our draft to Nature, going forward subject to significant changes. All in all, we ended up writing three versions over eight months with nothing more than the title in common," said lead study author Biamonte. [16]

## **A Machine Learning Systems That Called Neural Networks Perform Tasks by Analyzing Huge Volumes of Data**

Neural networks learn how to carry out certain tasks by analyzing large amounts of data displayed to them. These machine learning systems continually learn and readjust to be able to carry out the task set out before them. Understanding how neural networks work helps researchers to develop better applications and uses for them.

At the 2017 Conference on Empirical Methods on Natural Language Processing earlier this month, MIT researchers demonstrated a new general-purpose technique for making sense of neural networks that are able to carry out natural language processing tasks where they attempt to extract data written in normal text opposed to something of a structured language like database-query language.

The new technique works great in any system that reads the text as input and produces symbols as the output. One such example of this can be seen in an automatic translator. It works without the need to access any underlying software too. Tommi Jaakkola is Professor of Electrical Engineering and Computer Science at MIT and one of the authors on the paper. He says, "I can't just do a simple randomization. And what you are predicting is now a more complex object, like a sentence, so what does it mean to give an explanation?"

As part of the research, Jaakkola, and colleague David Alvarez-Melis, an MIT graduate student in electrical engineering and computer science and first author on the paper, used a black-box neural net in which to generate test sentences to feed black-box neural nets. The duo began by teaching the network to compress and decompress natural sentences. As the training continues the encoder and decoder get evaluated simultaneously depending on how closely the decoder's output matches up with the encoder's input.

Neural nets work on probabilities. For example, an object-recognition system could be fed an image of a cat, and it would process that image as it saying 75 percent probability of being a cat, while still having a 25 percent probability that it's a dog. Along with that same line, Jaakkola and Alvarez-Melis' sentence compressing network has alternative words for each of those in a decoded sentence along with the probability that each is correct. So, once the system has generated a list of closely related sentences they're then fed to a black-box natural language processor. This then allows the researchers to analyze and determine which inputs have an effect on which outputs.

During the research, the pair applied this technique to three different types of a natural language processing system. The first one inferred the way in which words were pronounced; the second was a set of translators, and the third was a simple computer dialogue system which tried to provide adequate responses to questions or remarks. In looking at the results, it was clear and pretty obvious that the translation systems had strong dependencies on individual words of both the input and output sentences. A little more surprising, however, was the identification of gender

biases in the texts on which the machine translation systems were trained. The dialogue system was too small to take advantage of the training set.

“The other experiment we do is in flawed systems,” says Alvarez-Melis. “If you have a black-box model that is not doing a good job, can you first use this kind of approach to identify problems? A motivating application of this kind of interpretability is to fix systems, to improve systems, by understanding what they’re getting wrong and why.” [15]

## **Active machine learning for the discovery and crystallization of gigantic polyoxometalate molecules**

Who is the better experimentalist, a human or a robot? When it comes to exploring synthetic and crystallization conditions for inorganic gigantic molecules, actively learning machines are clearly ahead, as demonstrated by British Scientists in an experiment with polyoxometalates published in the journal *Angewandte Chemie*.

Polyoxometalates form through self-assembly of a large number of metal atoms bridged by oxygen atoms. Potential uses include catalysis, electronics, and medicine. Insights into the self-organization processes could also be of use in developing functional chemical systems like "molecular machines".

Polyoxometalates offer a nearly unlimited variety of structures. However, it is not easy to find new ones, because the aggregation of complex inorganic molecules to gigantic molecules is a process that is difficult to predict. It is necessary to find conditions under which the building blocks aggregate and then also crystallize, so that they can be characterized.

A team led by Leroy Cronin at the University of Glasgow (UK) has now developed a new approach to define the range of suitable conditions for the synthesis and crystallization of polyoxometalates. It is based on recent advances in machine learning, known as active learning. They allowed their trained machine to compete against the intuition of experienced experimenters. The test example was  $\text{Na}(6)[\text{Mo}(120)\text{Ce}(6)\text{O}(366)\text{H}(12)(\text{H}(2)\text{O})(78)] \cdot 200 \text{H}(2)\text{O}$ , a new, ring-shaped polyoxometalate cluster that was recently discovered by the researchers' automated chemical robot.

In the experiment, the relative quantities of the three necessary reagent solutions were to be varied while the protocol was otherwise prescribed. The starting point was a set of data from successful and unsuccessful crystallization experiments. The aim was to plan ten experiments and then use the results from these to proceed to the next set of ten experiments - a total of one hundred crystallization attempts.

Although the flesh-and-blood experimenters were able to produce more successful crystallizations, the far more "adventurous" machine algorithm was superior on balance because it covered a significantly broader domain of the "crystallization space". The quality of the prediction of whether an experiment would lead to crystallization was improved significantly more by the machine than the human experimenters. A series of 100 purely random experiments resulted in no improvement. In addition, the machine discovered a range of conditions that led to crystals which would not have been expected based on pure intuition. This "unbiased" automated method makes the discovery of

novel compounds more probably than reliance on human intuition. The researchers are now looking for ways to make especially efficient "teams" of man and machine. [14]

## Using machine learning to understand materials

Whether you realize it or not, machine learning is making your online experience more efficient. The technology, designed by computer scientists, is used to better understand, analyze, and categorize data. When you tag your friend on Facebook, clear your spam filter, or click on a suggested YouTube video, you're benefitting from machine learning algorithms.

Machine learning algorithms are designed to improve as they encounter more data, making them a versatile technology for understanding large sets of photos such as those accessible from Google Images. Elizabeth Holm, professor of materials science and engineering at Carnegie Mellon University, is leveraging this technology to better understand the enormous number of research images accumulated in the field of materials science. This unique application is an interdisciplinary approach to machine learning that hasn't been explored before.

"Just like you might search for cute cat pictures on the internet, or Facebook recognizes the faces of your friends, we are creating a system that allows a computer to automatically understand the visual data of materials science," explains Holm.

The field of materials science usually relies on human experts to identify research images by hand. Using machine learning algorithms, Holm and her group have created a system that automatically recognizes and categorizes microstructural images of materials. Her goal is to make it more efficient for materials scientists to search, sort, classify, and identify important information in their visual data.

"In materials science, one of our fundamental data is pictures," explains Holm. "Images contain information that we recognize, even when we find it difficult to quantify numerically."

Holm's machine learning system has several different applications within the materials science field including research, industry, publishing, and academia. For example, the system could be used to create a visual search of a scientific journal archives so that a researcher could find out whether a similar image had ever been published. Similarly, the system can be used to automatically search and categorize image archives in industries or research labs. "Big companies can have archives of 600,000 or more research images. No one wants to look through those, but they want to use that data to better understand their products," explains Holm. "This system has the power to unlock those archives."

Holm and her group have been working on this research for about three years and are continuing to grow the project, especially as it relates to the metal 3-D printing field. For example, they are beginning to compile a database of experimental and simulated metal powder micrographs in order to better understand what types of raw materials are best suited for 3-D printing processes.

Holm published an article about this research in the December 2015 issue of Computational Materials Science titled "A computer vision approach for automated analysis and classification of microstructural image data." [13]

## Artificial intelligence helps in the discovery of new materials

With the help of artificial intelligence, chemists from the University of Basel in Switzerland have computed the characteristics of about two million crystals made up of four chemical elements. The researchers were able to identify 90 previously unknown thermodynamically stable crystals that can be regarded as new materials.

They report on their findings in the scientific journal *Physical Review Letters*.

Elpasolite is a glassy, transparent, shiny and soft mineral with a cubic crystal structure. First discovered in El Paso County (Colorado, USA), it can also be found in the Rocky Mountains, Virginia and the Apennines (Italy). In experimental databases, elpasolite is one of the most frequently found quaternary crystals (crystals made up of four chemical elements). Depending on its composition, it can be a metallic conductor, a semi-conductor or an insulator, and may also emit light when exposed to radiation.

These characteristics make elpasolite an interesting candidate for use in scintillators (certain aspects of which can already be demonstrated) and other applications. Its chemical complexity means that, mathematically speaking, it is practically impossible to use quantum mechanics to predict every theoretically viable combination of the four elements in the structure of elpasolite.

## Machine learning aids statistical analysis

Thanks to modern artificial intelligence, Felix Faber, a doctoral student in Prof. Anatole von Lilienfeld's group at the University of Basel's Department of Chemistry, has now succeeded in solving this material design problem. First, using quantum mechanics, he generated predictions for thousands of elpasolite crystals with randomly determined chemical compositions. He then used the results to train statistical machine learning models (ML models). The improved algorithmic strategy achieved a predictive accuracy equivalent to that of standard quantum mechanical approaches.

ML models have the advantage of being several orders of magnitude quicker than corresponding quantum mechanical calculations. Within a day, the ML model was able to predict the formation energy – an indicator of chemical stability – of all two million elpasolite crystals that theoretically can be obtained from the main group elements of the periodic table. In contrast, performance of the calculations by quantum mechanical means would have taken a supercomputer more than 20 million hours.

## Unknown materials with interesting characteristics

An analysis of the characteristics computed by the model offers new insights into this class of materials. The researchers were able to detect basic trends in formation energy and identify 90 previously unknown crystals that should be thermodynamically stable, according to quantum mechanical predictions.

On the basis of these potential characteristics, elpasolite has been entered into the Materials Project material database, which plays a key role in the Materials Genome Initiative. The initiative was launched by the US government in 2011 with the aim of using computational support to accelerate the discovery and the experimental synthesis of interesting new materials.

Some of the newly discovered elpasolite crystals display exotic electronic characteristics and unusual compositions. "The combination of artificial intelligence, big data, quantum mechanics and supercomputing opens up promising new avenues for deepening our understanding of materials and discovering new ones that we would not consider if we relied solely on human intuition," says study director von Lilienfeld. [12]

## **Physicists are putting themselves out of a job, using artificial intelligence to run a complex experiment**

The experiment, developed by physicists from The Australian National University (ANU) and UNSW ADFA, created an extremely cold gas trapped in a laser beam, known as a Bose-Einstein condensate, replicating the experiment that won the 2001 Nobel Prize.

"I didn't expect the machine could learn to do the experiment itself, from scratch, in under an hour," said co-lead researcher Paul Wigley from the ANU Research School of Physics and Engineering.

"A simple computer program would have taken longer than the age of the Universe to run through all the combinations and work this out."

Bose-Einstein condensates are some of the coldest places in the Universe, far colder than outer space, typically less than a billionth of a degree above absolute zero.

They could be used for mineral exploration or navigation systems as they are extremely sensitive to external disturbances, which allows them to make very precise measurements such as tiny changes in the Earth's magnetic field or gravity.

The artificial intelligence system's ability to set itself up quickly every morning and compensate for any overnight fluctuations would make this fragile technology much more useful for field measurements, said co-lead researcher Dr Michael Hush from UNSW ADFA.

"You could make a working device to measure gravity that you could take in the back of a car, and the artificial intelligence would recalibrate and fix itself no matter what," he said.

"It's cheaper than taking a physicist everywhere with you."

The team cooled the gas to around 1 microkelvin, and then handed control of the three laser beams over to the artificial intelligence to cool the trapped gas down to nanokelvin.

Researchers were surprised by the methods the system came up with to ramp down the power of the lasers.

"It did things a person wouldn't guess, such as changing one laser's power up and down, and compensating with another," said Mr Wigley.

"It may be able to come up with complicated ways humans haven't thought of to get experiments colder and make measurements more precise.

The new technique will lead to bigger and better experiments, said Dr Hush.

"Next we plan to employ the artificial intelligence to build an even larger Bose-Einstein condensate faster than we've seen ever before," he said.

The research is published in the Nature group journal Scientific Reports. [11]

## **Quantum experiments designed by machines**

The idea was developed when the physicists wanted to create new quantum states in the laboratory, but were unable to conceive of methods to do so. "After many unsuccessful attempts to come up with an experimental implementation, we came to the conclusion that our intuition about these phenomena seems to be wrong. We realized that in the end we were just trying random arrangements of quantum building blocks. And that is what a computer can do as well - but thousands of times faster", explains Mario Krenn, PhD student in Anton Zeilinger's group and first author research.

After a few hours of calculation, their algorithm - which they call Melvin - found the recipe to the question they were unable to solve, and its structure surprised them. Zeilinger says: "Suppose I want build an experiment realizing a specific quantum state I am interested in. Then humans intuitively consider setups reflecting the symmetries of the state. Yet Melvin found out that the most simple realization can be asymmetric and therefore counterintuitive. A human would probably never come up with that solution."

The physicists applied the idea to several other questions and got dozens of new and surprising answers. "The solutions are difficult to understand, but we were able to extract some new experimental tricks we have not thought of before. Some of these computer-designed experiments are being built at the moment in our laboratories", says Krenn.

Melvin not only tries random arrangements of experimental components, but also learns from previous successful attempts, which significantly speeds up the discovery rate for more complex solutions. In the future, the authors want to apply their algorithm to even more general questions in quantum physics, and hope it helps to investigate new phenomena in laboratories. [10]

## **Moving electrons around loops with light: A quantum device based on geometry**

Researchers at the University of Chicago's Institute for Molecular Engineering and the University of Konstanz have demonstrated the ability to generate a quantum logic operation, or rotation of the qubit, that - surprisingly—is intrinsically resilient to noise as well as to variations in the strength or duration of the control. Their achievement is based on a geometric concept known as the Berry phase and is implemented through entirely optical means within a single electronic spin in diamond.

Their findings were published online Feb. 15, 2016, in Nature Photonics and will appear in the March print issue. "We tend to view quantum operations as very fragile and susceptible to noise, especially when compared to conventional electronics," remarked David Awschalom, the Liew Family Professor of Molecular Engineering and senior scientist at Argonne National Laboratory,



who led the research. "In contrast, our approach shows incredible resilience to external influences and fulfills a key requirement for any practical quantum technology."

### Quantum geometry

When a quantum mechanical object, such as an electron, is cycled along some loop, it retains a memory of the path that it travelled, the Berry phase. To better understand this concept, the Foucault pendulum, a common staple of science museums helps to give some intuition. A pendulum, like those in a grandfather clock, typically oscillates back and forth within a fixed plane. However, a Foucault pendulum oscillates along a plane that gradually rotates over the course of a day due to Earth's rotation, and in turn knocks over a series of pins encircling the pendulum.

The number of knocked-over pins is a direct measure of the total angular shift of the pendulum's oscillation plane, its acquired geometric phase. Essentially, this shift is directly related to the location of the pendulum on Earth's surface as the rotation of Earth transports the pendulum along a specific closed path, its circle of latitude. While this angular shift depends on the particular path traveled, Awschalom said, it remarkably does not depend on the rotational speed of Earth or the oscillation frequency of the pendulum.

"Likewise, the Berry phase is a similar path-dependent rotation of the internal state of a quantum system, and it shows promise in quantum information processing as a robust means to manipulate qubit states," he said.

### A light touch

In this experiment, the researchers manipulated the Berry phase of a quantum state within a nitrogen-vacancy (NV) center, an atomic-scale defect in diamond. Over the past decade and a half, its electronic spin state has garnered great interest as a potential qubit. In their experiments, the team members developed a method with which to draw paths for this defect's spin by varying the applied laser light. To demonstrate Berry phase, they traced loops similar to that of a tangerine slice within the quantum space of all of the potential combinations of spin states.

"Essentially, the area of the tangerine slice's peel that we drew dictated the amount of Berry phase that we were able to accumulate," said Christopher Yale, a postdoctoral scholar in Awschalom's laboratory, and one of the co-lead authors of the project.

This approach using laser light to fully control the path of the electronic spin is in contrast to more common techniques that control the NV center spin, through the application of microwave fields. Such an approach may one day be useful in developing photonic networks of these defects, linked and controlled entirely by light, as a way to both process and transmit quantum information.

### A noisy path

A key feature of Berry phase that makes it a robust quantum logic operation is its resilience to noise sources. To test the robustness of their Berry phase operations, the researchers intentionally added noise to the laser light controlling the path. As a result, the spin state would travel along its intended path in an erratic fashion.

However, as long as the total area of the path remained the same, so did the Berry phase that they measured.

"In particular, we found the Berry phase to be insensitive to fluctuations in the intensity of the laser. Noise like this is normally a bane for quantum control," said Brian Zhou, a postdoctoral scholar in the group, and co-lead author.

"Imagine you're hiking along the shore of a lake, and even though you continually leave the path to go take pictures, you eventually finish hiking around the lake," said F. Joseph Heremans, co-lead author, and now a staff scientist at Argonne National Laboratory. "You've still hiked the entire loop regardless of the bizarre path you took, and so the area enclosed remains virtually the same."

These optically controlled Berry phases within diamond suggest a route toward robust and fault-tolerant quantum information processing, noted Guido Burkard, professor of physics at the University of Konstanz and theory collaborator on the project.

"Though its technological applications are still nascent, Berry phases have a rich underlying mathematical framework that makes them a fascinating area of study," Burkard said. [9]

## **Researchers demonstrate 'quantum surrealism'**

In a new version of an old experiment, CIFAR Senior Fellow Aephraim Steinberg (University of Toronto) and colleagues tracked the trajectories of photons as the particles traced a path through one of two slits and onto a screen. But the researchers went further, and observed the "nonlocal" influence of another photon that the first photon had been entangled with.

The results counter a long-standing criticism of an interpretation of quantum mechanics called the De Broglie-Bohm theory. Detractors of this interpretation had faulted it for failing to explain the behaviour of entangled photons realistically. For Steinberg, the results are important because they give us a way of visualizing quantum mechanics that's just as valid as the standard interpretation, and perhaps more intuitive.

"I'm less interested in focusing on the philosophical question of what's 'really' out there. I think the fruitful question is more down to earth. Rather than thinking about different metaphysical interpretations, I would phrase it in terms of having different pictures. Different pictures can be useful. They can help shape better intuitions."

At stake is what is "really" happening at the quantum level. The uncertainty principle tells us that we can never know both a particle's position and momentum with complete certainty. And when we do interact with a quantum system, for instance by measuring it, we disturb the system. So if we fire a photon at a screen and want to know where it will hit, we'll never know for sure exactly where it will hit or what path it will take to get there.

The standard interpretation of quantum mechanics holds that this uncertainty means that there is no "real" trajectory between the light source and the screen. The best we can do is to calculate a "wave function" that shows the odds of the photon being in any one place at any time, but won't tell us where it is until we make a measurement.

Yet another interpretation, called the De Broglie-Bohm theory, says that the photons do have real trajectories that are guided by a "pilot wave" that accompanies the particle. The wave is still probabilistic, but the particle takes a real trajectory from source to target. It doesn't simply "collapse" into a particular location once it's measured.

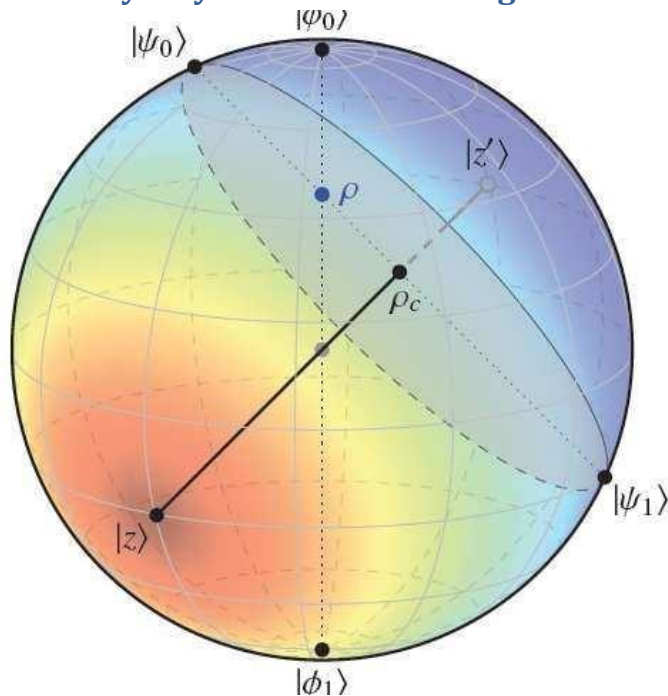
In 2011 Steinberg and his colleagues showed that they could follow trajectories for photons by subjecting many identical particles to measurements so weak that the particles were barely disturbed, and then averaging out the information. This method showed trajectories that looked similar to classical ones - say, those of balls flying through the air.

But critics had pointed out a problem with this viewpoint. Quantum mechanics also tells us that two particles can be entangled, so that a measurement of one particle affects the other. The critics complained that in some cases, a measurement of one particle would lead to an incorrect prediction of the trajectory of the entangled particle. They coined the term "surreal trajectories" to describe them.

In the most recent experiment, Steinberg and colleagues showed that the surrealism was a consequence of non-locality - the fact that the particles were able to influence one another instantaneously at a distance. In fact, the "incorrect" predictions of trajectories by the entangled photon were actually a consequence of where in their course the entangled particles were measured. Considering both particles together, the measurements made sense and were consistent with real trajectories.

Steinberg points out that both the standard interpretation of quantum mechanics and the De Broglie-Bohm interpretation are consistent with experimental evidence, and are mathematically equivalent. But it is helpful in some circumstances to visualize real trajectories, rather than wave function collapses, he says. [8]

## Physicists discover easy way to measure entanglement—on a sphere



Entanglement on a sphere: This Bloch sphere shows entanglement for the one-root state  $\rho$  and its radial state  $\rho_c$ . The color on the sphere corresponds to the value of the entanglement, which is determined by the distance from the root state  $z$ , the point at which there is no entanglement. The

closer to  $z$ , the less the entanglement (red); the further from  $z$ , the greater the entanglement (blue). Credit: Regula and Adesso. ©2016 American Physical Society

Now in a new paper to be published in Physical Review Letters, mathematical physicists Bartosz Regula and Gerardo Adesso at The University of Nottingham have greatly simplified the problem of measuring entanglement.

To do this, the scientists turned the difficult analytical problem into an easy geometrical one. They showed that, in many cases, the amount of entanglement between states corresponds to the distance between two points on a Bloch sphere, which is basically a normal 3D sphere that physicists use to model quantum states.

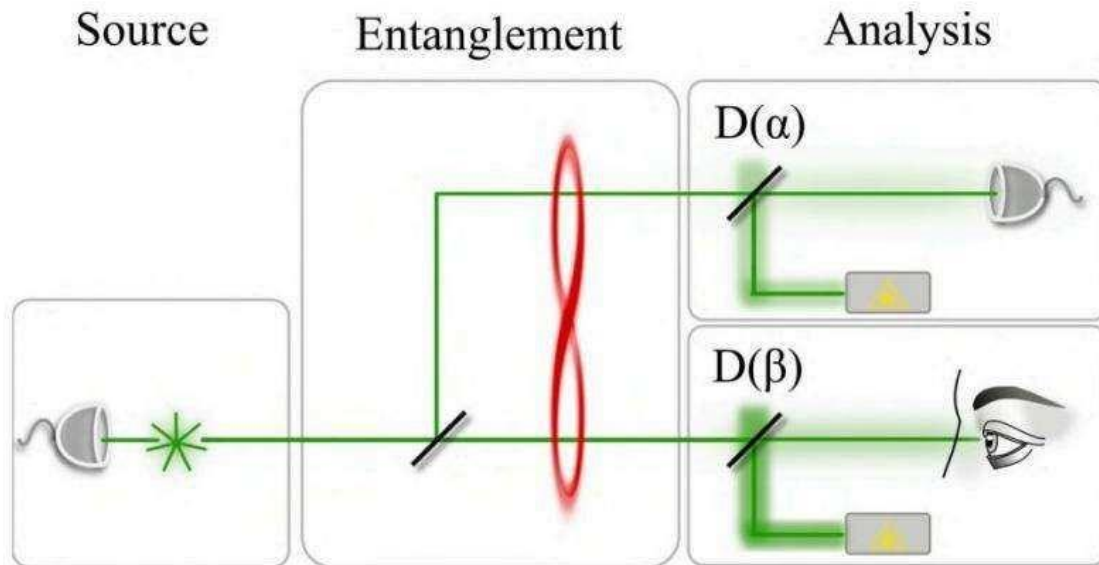
As the scientists explain, the traditionally difficult part of the math problem is that it requires finding the optimal decomposition of mixed states into pure states. The geometrical approach completely eliminates this requirement by reducing the many possible ways that states could decompose down to a single point on the sphere at which there is zero entanglement. The approach requires that there be only one such point, or "root," of zero entanglement, prompting the physicists to describe the method as "one root to rule them all."

The scientists explain that the "one root" property is common among quantum states and can be easily verified, transforming a formidable math problem into one that is trivially easy. They demonstrated that the new approach works for many types of two-, three- and four-qubit entangled states.

"This method reveals an intriguing and previously unexplored connection between the quantum features of a state and classical geometry, allowing all one-root states to enjoy a convenient visual representation which considerably simplifies the study and understanding of their properties," the researchers explained.

The simple way of measuring a state's entanglement could have applications in many technological areas, such as quantum cryptography, computation, and communication. It could also provide insight into understanding the foundations of thermodynamics, condensed matter physics, and biology. [7]

## An idea for allowing the human eye to observe an instance of entanglement



Scheme of the proposal for detecting entanglement with the human eye. Credit: arXiv:1602.01907

Entanglement, is of course, where two quantum particles are intrinsically linked to the extent that they actually share the same existence, even though they can be separated and moved apart. The idea was first proposed nearly a century ago, and it has not only been proven, but researchers routinely cause it to occur, but, to date, not one single person has ever actually seen it happen—they only know it happens by conducting a series of experiments. It is not clear if anyone has ever actually tried to see it happen, but in this new effort, the research trio claim to have found a way to make it happen—if only someone else will carry out the experiment on a willing volunteer.

The idea involves using a beam splitter and two beams of light—an initial beam of coherent photons fired at the beam splitter and a secondary beam of coherent photons that interferes with the photons in the first beam causing a change of phase, forcing the light to be reflected rather than transmitted. In such a scenario, the secondary beam would not need to be as intense as the first, and could in fact be just a single coherent photon—if it were entangled, it could be used to allow a person to see the more powerful beam while still preserving the entanglement of the original photon.

The researchers suggest the technology to carry out such an experiment exists today, but also acknowledge that it would take a special person to volunteer for such an assignment because to prove that they had seen entanglement taking place would involve shooting a large number of photons in series, into a person's eye, whereby the resolute volunteer would announce whether they had seen the light on the order of thousands of times. [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 its 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 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  $1/2$  spin creator particle to make equal the spins of the weak interaction, for example neutron decay to 2 fermions, every particle is fermions with  $1/2$  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 T-symmetry 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  $1/2$  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 than 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  $E = h\nu$  and  $E = mc^2$ ,  $m = h\nu/c^2$  that is the  $m$  depends only on the  $\nu$  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  $m_0$  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  $M_p=1840 M_e$ . 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  $W^\pm$ , 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]

### The Secret of Quantum Entanglement

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] When one of the entangled particles wave function is collapses by measurement, the intermediate photon also collapses and transforms its

state to the second entangled particle giving it the continuity of this entanglement. Since the accelerated charges are self-maintaining their potential locally causing their acceleration, it seems that they entanglement is a spooky action at a distance.

## Conclusions

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

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.

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.

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