

QUANTXCER BI-WEEKLY NEWS LETTER



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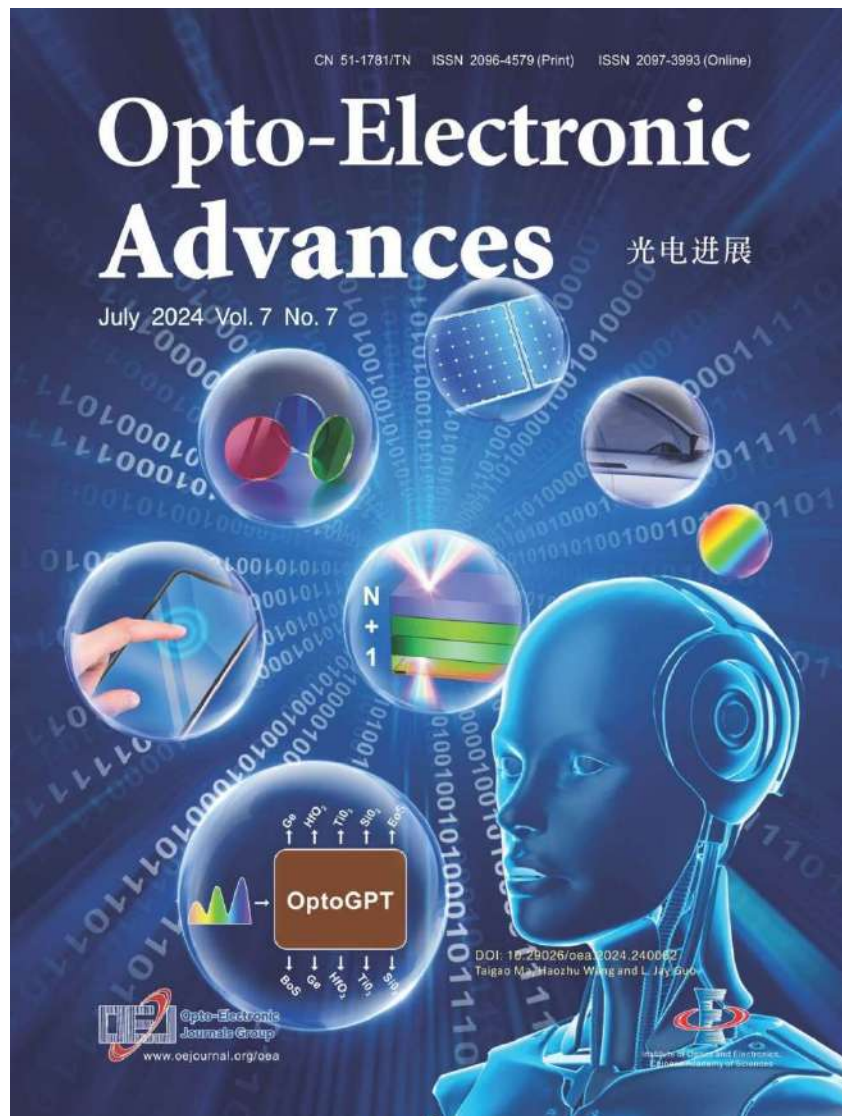
It is a quantum
fractal
algorithmic
universe

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OptoGPT For Improving Solar Cells, Smart Windows, Telescopes And More

Solar cell, telescope and other optical component manufacturers may be able to design better devices more quickly with AI.



OptoGPT is featured on the Opto-Electronic Advances journal cover for the July 2024 issue. Image credit: Opto-Electronic Advances.

OptoGPT, developed by University of Michigan engineers, harnesses the computer architecture underpinning ChatGPT to work backward from desired optical properties to the material structure that can provide them.

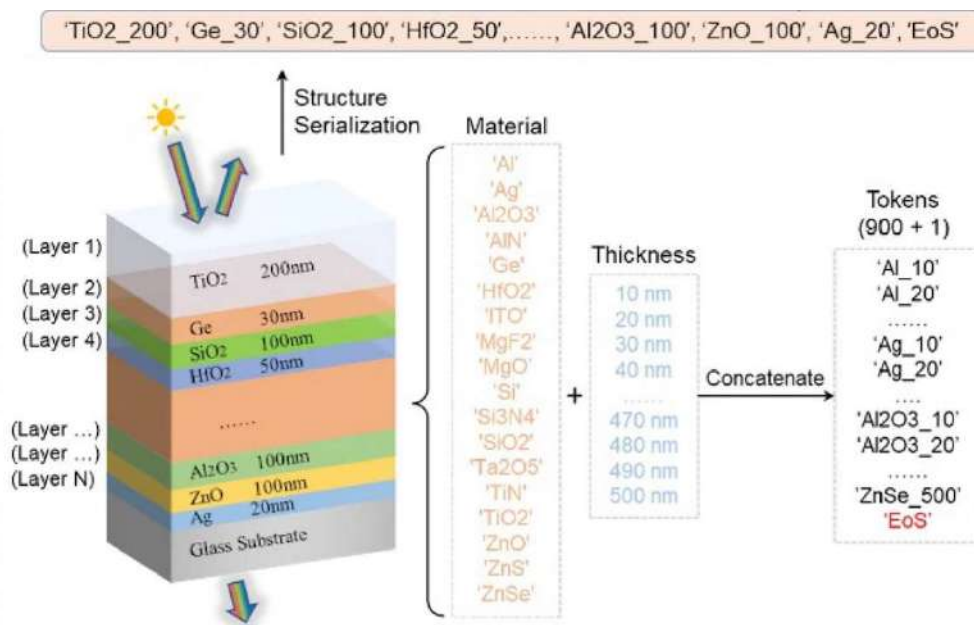
The new algorithm designs optical multilayer film structures—stacked thin layers of different materials—that can serve a variety of purposes. Well-designed multilayer structures can maximize light absorption in a solar cell or optimize reflection in a telescope. They can improve semiconductor manufacturing with extreme UV light, and make buildings better at regulating heat with smart windows that become more transparent or more reflective depending on temperature.

OptoGPT produces designs for multilayer film structures within 0.1 seconds, almost instantaneously. In addition, OptoGPT’s designs contain six fewer layers on average compared to previous models, meaning its designs are easier to manufacture.

“Designing these structures usually requires extensive training and expertise as identifying the best combination of materials, and the thickness of each layer, is not an easy task,” said L. Jay Guo, U-M professor of electrical and computer engineering and corresponding author of the study published in Opto-Electronic Advances.

For someone new to the field, it’s difficult to know where to start. To automate the design process for optical structures, the research team tailored a transformer architecture—the machine learning framework used in large language models like OpenAI’s ChatGPT and Google’s Bard—for their own purposes.

“In a sense, we created artificial sentences to fit the existing model structure,” Guo said. The model treats materials at a certain thickness as words, also encoding their associated optical properties as inputs. Seeking out correlations between these “words,” the model predicts the next word to create a “phrase”—in this case a design for an optical multilayer film structure—that achieves the desired property such as high reflection.



The schematic shows Opto-GPT’s process, combining an undetermined layer’s possible materials and thicknesses into a format that can be run through the program to choose the best possible combination. Image credit: L. Jay Guo Laboratory, Michigan Engineering.

Researchers tested the new model's performance using a validation dataset containing 1,000 known design structures including their material composition, thickness and optical properties. When comparing OptoGPT's designs to the validation set, the difference between the two was only 2.58%, lower than the closest optical properties in the training dataset at 2.96%.

Similar to how large language models are able to respond to any text-based question, OptoGPT is trained on a large amount of data and able to respond well to general optical design tasks across the field.

If researchers are focused on a task, like designing a high-efficiency coating for radiative cooling, they can use local optimization—adjusting variables within bounds to achieve the best possible outcome—to further fine-tune the thickness to improve accuracy.

During testing, the researchers found fine-tuning improves accuracy by 24%, reducing the difference between the validation dataset and OptoGPT responses to 1.92%.

Taking analysis a step further, the researchers used a statistical technique to map out associations that OptoGPT makes.

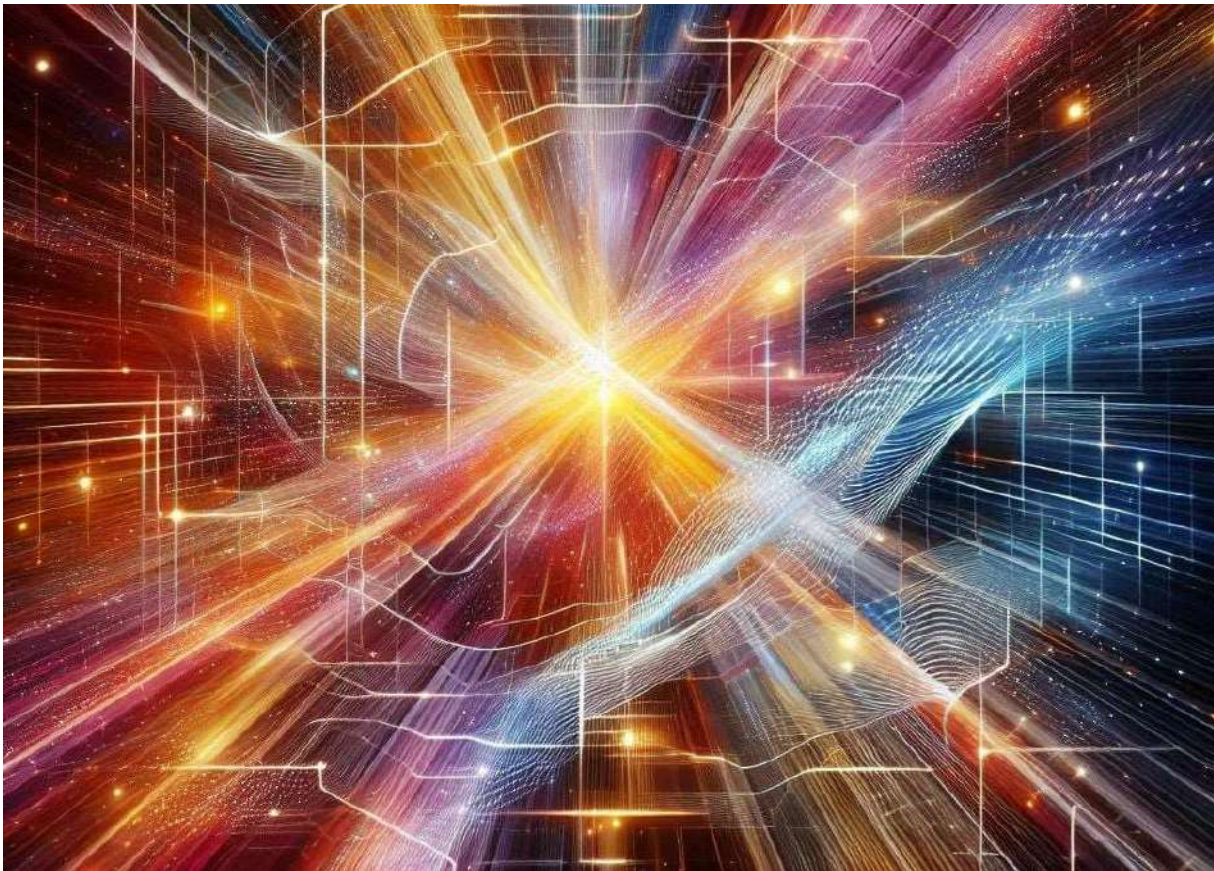
“The high-dimensional data structure of neural networks is a hidden space, too abstract to understand. We tried to poke a hole in the black box to see what was going on,” Guo said.

When mapped in a 2D space, materials cluster by type such as metals and dielectric materials, which are electrically insulating but can support an internal electric field. All dielectrics, including semiconductors, converge upon a central point as the thickness approaches 10 nanometers. From an optics perspective, the pattern makes sense as light behaves similarly regardless of material as they approach such small thicknesses, helping further validate OptoGPT's accuracy.

Known as an inverse design algorithm because it starts with the desired effect and works backward to a material design, OptoGPT offers more flexibility than previous inverse design algorithm approaches, which were developed for specific tasks. It enables researchers and engineers to design optical multilayer film structures for a wide breadth of applications.

Quantum Light Unlocks Nature's Tiny Secrets

Researchers at the University of Michigan have found a way to examine tiny structures, such as bacteria and genes, with reduced damage compared to traditional light sources.



Photonics – artistic impression. Image credit: Copilot Designer / Alius Noreika

The new technique involves spectroscopy, the study of how matter absorbs and emits light and other forms of radiation. It takes advantage of quantum mechanics to study the structure and dynamics of molecules in ways that are not possible using conventional light sources.

“This research examined a quantum light spectroscopy technique called entangled two-photon absorption that takes advantage of entanglement to reveal the structures of molecules and how ETPA acts at ultrafast speeds to determine properties that cannot be seen with classical spectroscopy,” said study senior author Theodore Goodson, U-M professor of chemistry and of macromolecular science and engineering.

Entangled two-photon absorption allows researchers to study molecules by using two photons that are interconnected through a quantum phenomenon known as entanglement.

Photons are the smallest possible particles of electromagnetic energy and, therefore, also the smallest particles of light, allowing details about the molecule’s structure to be visible—which cannot be shown with regular light. Quantum light spectroscopy is very fast and can reveal properties that are usually hidden.

The discovery opens opportunities for non-invasive, low-intensity imaging and sensing applications with minimal photodamage to delicate biological samples like proteins, DNA, and living cells.

“Measurements with entangled photons may enable sensing biological signatures with high selectivity and at very low light levels to protect against photodamage,” said lead author Oleg Varnavski, a research lab specialist in the U-M Department of Chemistry.

The research, published in the Proceedings of the National Academy of Sciences, used an organic molecule called zinc tetraphenyl porphyrin to study the phenomenon of two-photon absorption—where a molecule simultaneously absorbs two particles of light instead of one.

Researchers found that using pairs of photons that were quantumly entangled, the ZnTPP molecule exhibited absorption in the red spectrum. With two untangled photons, the ZnTPP molecules showed absorption in a blue spectrum.

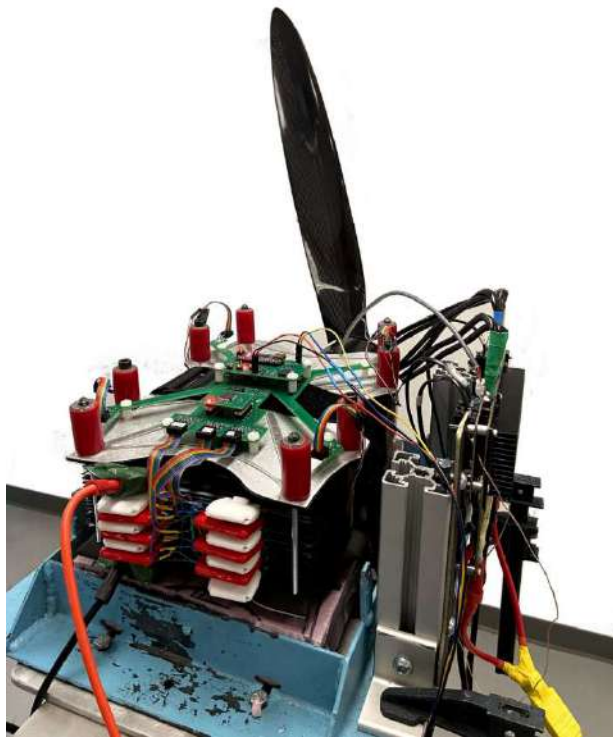
A laser produced pairs of entangled photons through a process called spontaneous parametric down-conversion. These photons were then focused onto a cuvette containing the ZnTPP solution. The transmission was measured using a highly sensitive single-photon detector.

This work paves the way for the advancement of quantum light-based spectroscopy and microscopy, potentially leading to much higher efficiency of ETPA sensors and low-intensity detection schemes. The ability to access unique molecular states with entangled photons could improve the sensing of biological signatures with significant selectivity and sensitivity even at minimum light levels to prevent photodamage.

“This provides the opportunity to study states of molecules with nonclassical light that have fundamentally different properties than are accessible with classical light,” Varnavski said.

Electric Aviation: Batteries That Stay Strong For The Flight Duration

According to a study led by Lawrence Berkeley National Laboratory with expertise from the University of Michigan, a battery component innovation could help keep power delivery high when electric aircraft land at a low charge.



Tested at the single cell level, the new electrolyte developed at Lawrence Berkeley National Laboratory maintains the power-to-energy ratio needed to support electric flight for four times longer than conventional batteries. The next step is for 24M to build the cells into a battery and send them for testing on And Battery Aero's propeller stand, running the battery through realistic flight missions. U-M aerospace engineering associate professor Venkat Viswanathan co-founded and Battery Aero. Image credit: And Battery Aero.

The research provides a solution to a problem identified in 2018 in a study led by Venkat Viswanathan, professor of aerospace engineering at U-M and a co-author of the new work published in *Joule*.

“Both takeoff and landing require high power, and landing is more challenging because you’re not fully charged,” Viswanathan said. “To get high power you have to bring all the resistances down. Anything that affects the ability to deliver that power.”

The team emphasized that this is distinct from the needs of EV batteries, which mainly need to maintain their ranges.

“In an electric vehicle, you focus on capacity fade over time,” said study lead author Youngmin Ko, a postdoctoral researcher at Berkeley Lab’s Molecular Foundry. “But for aircraft, the power fade is critical—the ability to consistently achieve high power for takeoff and landing.”

Both capacity fade and power fade typically occur when lithium ions can no longer move easily in and out of the electrodes.

While the key for capacity fade is the quantity of lithium ions that can move between the electrodes, the main factor for power fade is speed. The problem is that corrosion builds up on the electrodes, taking up space that could have housed lithium ions and making it harder for the lithium to reach available spaces.

Under the leadership of Brett Helms, corresponding author of the study and a senior staff scientist at Berkeley Lab’s Molecular Foundry, the team explored the interactions among the electrodes and electrolyte using an approach borrowed from biology. In studies of life, the field generally called “omics” looks for clues in the constituents of cells—what genes are being read, what proteins are being made, and so on.

In this case, the team tried different electrolyte chemistries, looking at subtle changes that occurred within the electrolyte at different locations in the battery during charging and discharging. Prior research has typically attributed power fade to problems arising at the battery’s negative side, as lithium metal is very reactive.

However, the team observed that damaging molecules were forming near the positive side—nickel-manganese-cobalt oxide in this case. Reacting with those molecules caused the particles of the positive electrode to crack and corrode over time, hindering the movement of lithium and reducing power delivery.

“It was a non-obvious outcome,” Ko said. “We found that mixing salts in the electrolyte could suppress the reactivity of typically reactive species, which formed a stabilizing, corrosion-resistant coating.”

The company 24M then built a test cell with this chemistry and sent it to And Battery Aero—a startup that Viswanathan co-founded with his former Ph.D. student Shashank Sripad, a co-author of this study and the one from 2018.



Tested at the single cell level, the new electrolyte developed at Lawrence Berkeley National Laboratory maintains the power-to-energy ratio needed to support electric flight for four times longer than conventional batteries. The next step is for 24M to build the cells into a full-size aviation battery, like the one pictured, for further testing at And Battery Aero, which was co-founded by U-M aerospace engineering associate professor Venkat Viswanathan. Image credit: And Battery Aero.

Sripad tested the cell by repeatedly drawing power from it in a realistic sequence of takeoff, flight and landing, as if the cell were part of a complete battery module powering an electric aircraft. When compared to conventional batteries, the new cell maintained the power-to-energy ratio needed for electric flight for four times longer.

“Heavy transport sectors, including aviation, have been underexplored in terms of electrification,” Helms said. “Our work redefines what’s possible, pushing the boundaries of battery technology to enable deeper decarbonization.”

Next, 24M will build a complete battery that And Battery Aero will test on a propeller stand, running the propeller through the flight sequence repeatedly. Then, next year, the team intends to attempt to perform an electric flight test with those batteries.

The team—which includes scientists at the University of California, Berkeley—also plans to expand the use of omics in battery research, exploring the interactions of various electrolyte components to further understand and tailor the performance of batteries for current and emerging use-cases in transportation and the grid.

New Technique Pinpoints Nanoscale ‘Hot Spots’ In Electronics To Improve Their Longevity

Rochester engineers have developed a way to spot tiny, overheated components that degrade electronics’ performance by borrowing methods from biological imaging.



NOBEL NOD: Materials science PhD student Benjamin Harrington uses a wire bonder to add electrical connections to an electrical heater structure. The structure was designed as a test subject for a new heat mapping technique that leverages Nobel Prize in Chemistry–winning optical super-resolution fluorescence microscopy techniques. Image credit: University of Rochester / J. Adam Fenster

When electronic devices like laptops or smartphones overheat, they suffer from a nanoscale heat transfer problem. Pinpointing that problem's source can be like finding a needle in a haystack.

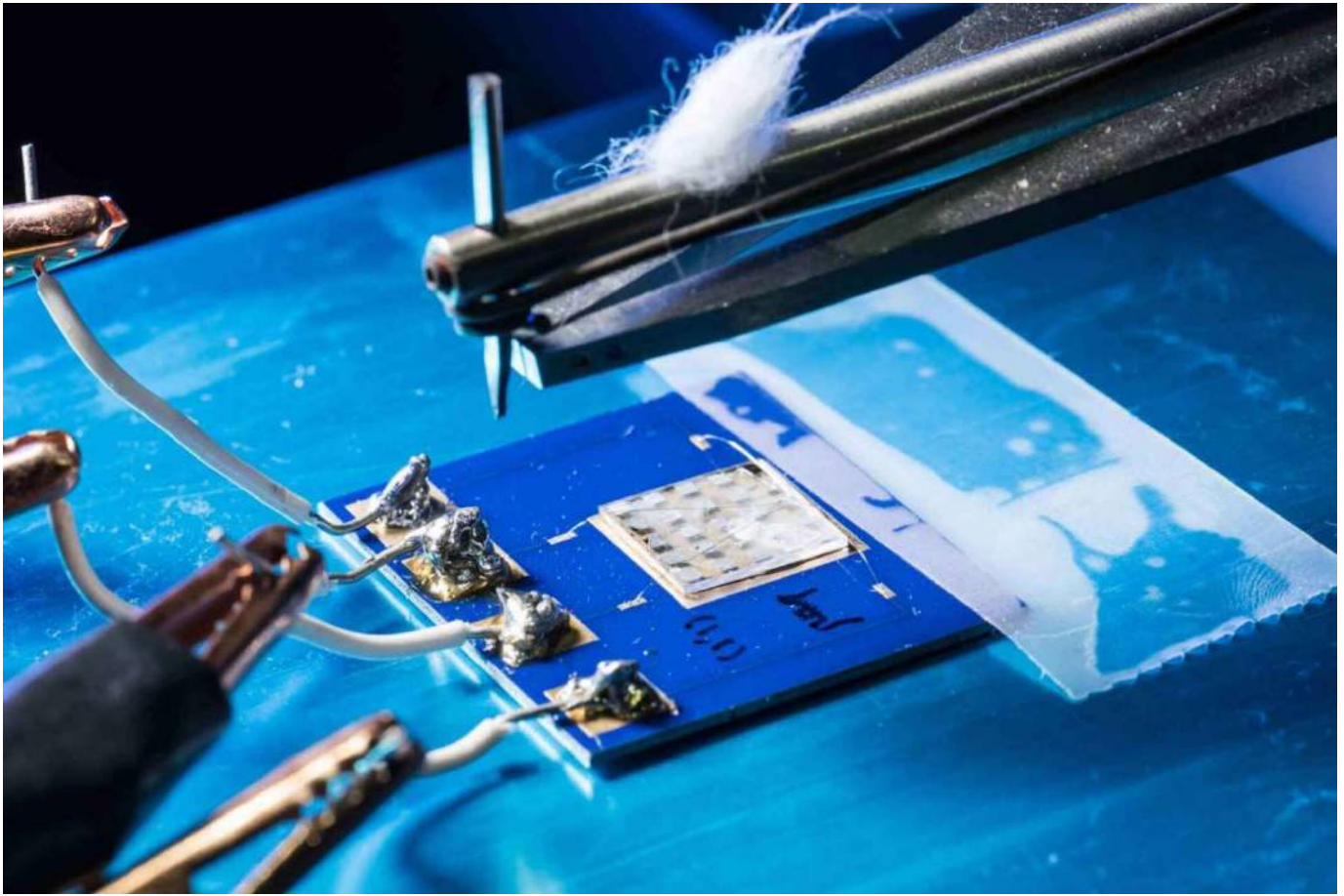
"The building blocks of our modern electronics are transistors with nanoscale features, so to understand which parts of overheating, the first step is to get a detailed temperature map," says Andrea Pickel, an assistant professor from the University of Rochester's Department of Mechanical Engineering and a scientist with the Laboratory for Laser Energetics. "But you need something with nanoscale resolution to do that."

Existing optical thermometry techniques are impractical because they have fundamental limits on the spatial resolution they can achieve. So Pickel and her materials science PhD students Ziyang Ye and Benjamin Harrington engineered a new approach to overcome these limitations by leveraging Nobel Prize in Chemistry–winning optical super-resolution fluorescence microscopy techniques used in biological imaging. In a new *Science Advances* study, the researchers outline their process for mapping heat transfer using luminescent nanoparticles.

By applying highly doped upconverting nanoparticles to a device's surface, the researchers achieved super-high resolution thermometry at the nanoscale level from up to 10 millimeters away. According to Pickel, that distance is extremely far in the world of super-resolution microscopy and that the biological imaging techniques they used for inspiration typically operate less than one millimeter away.

Pickel says that while the biological imaging techniques provide great inspiration, applying them to electronics had significant hurdles because they involve such different materials.

"Our requirements are very different from biologists because they're looking at things like cells and water-based materials," she says. "Often, they might have a liquid like water or an oil between their objective lens and their sample. That's great for biological imaging, but if you're working with an electronic device, that's the last thing you want."

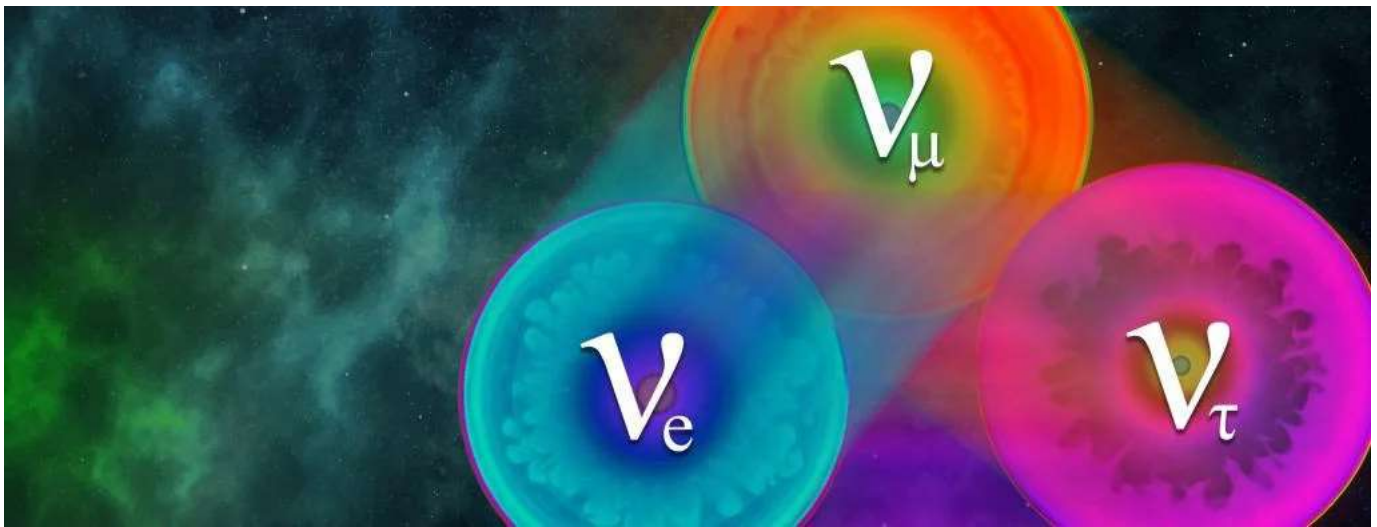


DOWN TO THE WIRE: Rochester researchers demonstrated their super-high resolution thermometry techniques on an electrical heater structure that the team designed to produce sharp temperature gradients. Image credit: University of Rochester photo / J. Adam Fenster

The paper demonstrates the technique using an electrical heater structure that the team designed to produce sharp temperature gradients, but Pickel says their method can be used by manufacturers to improve a wide array of electrical components. To further improve the process, the team hopes to lower the laser power used and refine the methods for applying layers of nanoparticles to the devices.

Untangling The Entangled: Quantum Study Shines Fresh Light On How Neutrinos Fuel Supernovae

Researchers used quantum simulations to obtain new insights into the nature of neutrinos — the mysterious subatomic particles that abound throughout the universe — and their role in the deaths of massive stars.



Researchers used quantum simulations made possible by ORNL's Quantum Computing User Project to model the flavor oscillations of neutrinos in a supernova. Neutrinos come in three "flavors," or types, that each correspond to a partner particle: an electron (e), a muon (μ), or a tau (τ). Credit: ORNL, U.S. Dept. of Energy

The study relied on support from the Quantum Computing User Program, or QCUP, and the Quantum Science Center, a national Quantum Information Science Research Center, at the Department of Energy's Oak Ridge National Laboratory.

"This understanding was something new that hasn't come out of classical computing systems," said Martin Savage, the study's senior author and a professor of physics at the University of Washington. "We recognized for the first time we could study how entanglement between multiple neutrinos is induced over time, and these results are within the error bars of what we'd expect from a classical computer. It's a step in the direction of better, more accurate and more scalable quantum simulations."

Neutrinos result from nuclear reactions — from the huge reactions that cause the sun to shine, to the tiny reactions that enable radioactive tracers for medical tests. These extremely light particles appear everywhere, carry no electric charge and seldom interact with other matter.

But during the collapse and explosion of a star — a process better known as a supernova — neutrinos exchange energy and momentum with not just each other but with everything around them.

“At this point, the neutrinos go from passive particles — almost bystanders — to major elements that help drive the collapse,” Savage said. “Supernovae are interesting for a variety of reasons, including as sites that produce heavy elements such as gold and iron. If we can better understand neutrinos and their role in the star’s collapse, then we can better determine and predict the rate of events such as a supernova.”

Scientists seldom observe a supernova close-up, but researchers have used classical supercomputers such as ORNL’s Summit to model aspects of the process. Those tools alone wouldn’t be enough to capture the quantum nature of neutrinos.

“These neutrinos are entangled, which means they’re interacting not just with their surroundings and not just with other neutrinos but with themselves,” Savage said. “It’s extremely difficult to simulate this kind of system, because entanglement’s an intrinsically quantum-mechanical property beyond what we can capture and approximate in classical computing. That’s why we need a quantum computer that uses calculations based on quantum physics to model what’s happening.”

Savage and his co-author Marc Illa of the University of Washington’s InQubator for Quantum Simulation obtained an allocation of time on Quantinuum’s H1-1 quantum computer via QCUP, part of the Oak Ridge Leadership Computing Facility, which awards time on privately owned quantum processors around the country to support research projects. The Quantinuum computer uses trapped ions as qubits, one of several quantum computing approaches.

Classical computers store information in bits equal to either 0 or 1. In other words, a classical bit, like a light switch, exists in one of two states: on or off.

Quantum computers store information in qubits, the quantum equivalent of bits. Qubits, unlike classical bits, can exist in more than one state simultaneously via quantum superposition — more like a dial with a wider range of more detailed settings than an on/off switch. That difference enables qubits to carry more information than classical bits. Scientists hope to use this increased capacity to fuel a quantum computing revolution built on a new generation of devices.

That capacity allowed Savage and the research team to simulate an approximation of the quantum-mechanical interactions between a supernova’s neutrinos. An actual supernova

would involve a minimum of a septendecillion, or 10^{54} , neutrinos. Savage and Illa began their simulation using a simpler model with a system of 12 neutrinos.

Each neutrino “flavor,” or type, found in nature corresponds to a “partner” particle: an electron, muon or tau. The model used in the study focused on just two flavors.

Quantum circuits – the quantum equivalent of traditional digital circuits – allowed the team to model the complicated connections and interactions between the particles so that each neutrino could interact with each of the others, not just its nearest neighbors.

The results offered a realistic approximation of how neutrinos become entangled at the quantum level, so that changing the properties of one also changes the properties of another. During a supernova, neutrinos can change flavor from an electron flavor to a muon flavor or to a tau flavor as the neutrinos begin to interact with each other and their surroundings. The detail provided by the simulations enabled the team to measure the evolution from one flavor to another over time of various entangled neutrinos.

Why track the flavor conversion? Because the mu and tau flavors of neutrinos interact differently with matter than their electron-flavored brethren. These interactions can impact the amounts and types of heavier elements produced in the supernova explosion.

“These circuits turned out to approximate the neutrinos’ behavior very well,” Savage said. “We discovered we could use these simulations to measure neutrino entanglement in a statistically significant way and that we could identify a significant scaling in size as the number of neutrinos increased. This was the first time this kind of study had been done.”

The primary hurdle for useful quantum simulations has been the relatively high error rate caused by noise that degrades qubit quality. The problem’s so common the current generation of quantum computers has become known as noisy intermediate-scale quantum, or NISQ. Various programming methods can help reduce these errors, but Savage and Illa didn’t need those methods to conduct their study thanks to the high quality of the Quantinuum computer’s qubits and gates. The computer’s 12-qubit circuits proved to be sufficient for almost 200 of the 2-qubit gates.

“We found the systematic errors on the quantum hardware were less than the statistical errors,” Savage said. “We still have a long way to go to predict the behavior of large neutrino systems with precision, and we don’t know whether the current generation of NISQ devices can take us there. But this technique should be portable to other types of quantum computers, and the results help us set protocols that can be used to simulate larger systems of neutrinos.”

Next steps include simulating a system of as many as 50 neutrinos. Savage hopes to model such systems in a variety of environments.

“We want to understand the implications of different thermal states, of states in and out of equilibrium,” he said. “We’re excited to see what we can explore.”

Support for this research came from the DOE Office of Science's Advanced Scientific Computing Research program, the DOE Quantum Science Center and the DOE Nuclear Physics InQubator for Quantum Simulation. The OLCF is a DOE Office of Science user facility at ORNL.

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