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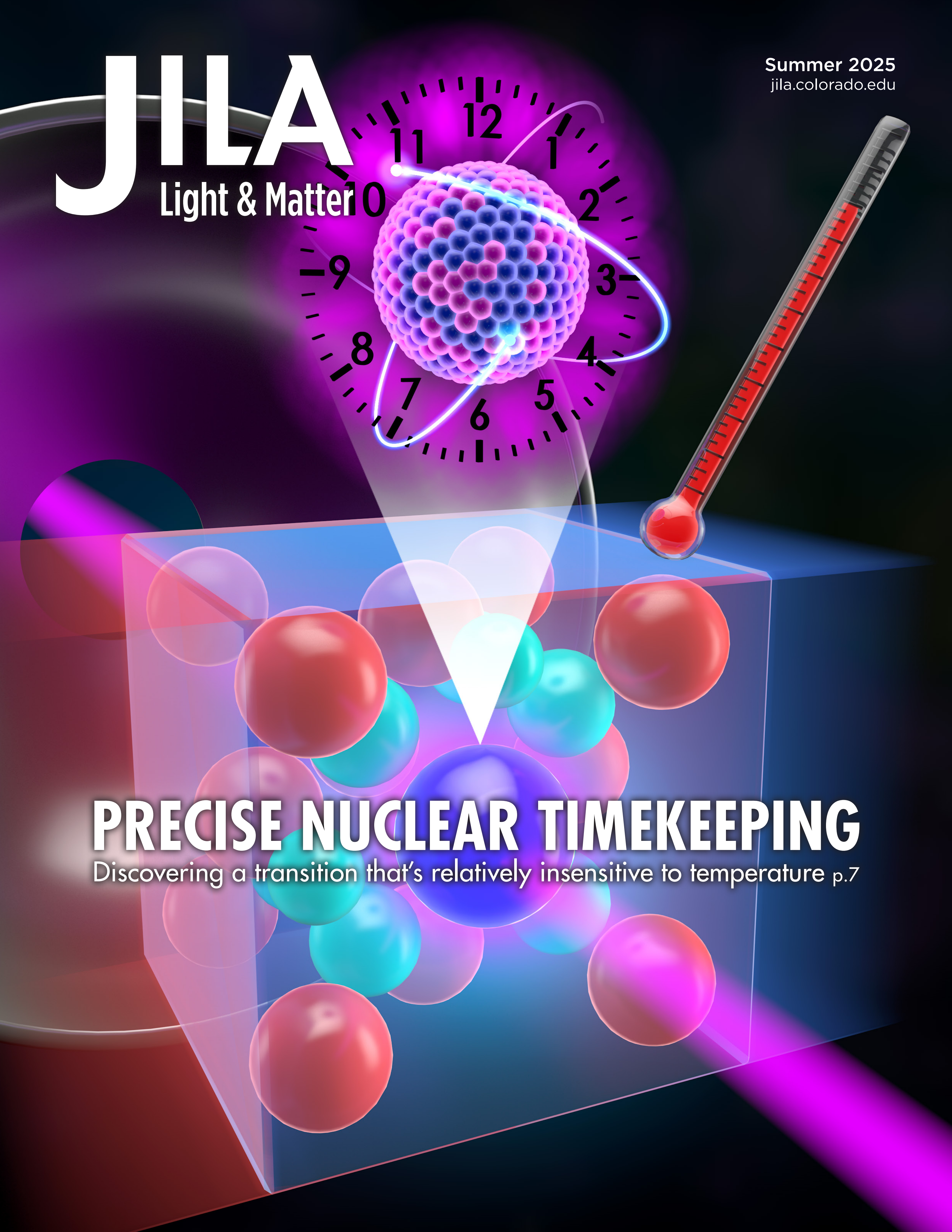

# PRECISE NUCLEAR TIMEKEEPING

Discovering a transition that's relatively insensitive to temperature p.7

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Over 100 graduate students, undergraduate students, postdoctoral researchers, staff, research scientists, and PIs attended the first **JILA Association of Graduate Students (JAGS) Industry Spotlight** on Wednesday, April 16th. This event featured a technical talk and networking with Quantinuum, a local quantum computing company with a Boulder location and a major employer of JILA alumni. The seminar's record-breaking attendance reflected both the excitement at JILA, NIST, and CU about Boulder's growing quantum industry hub and the large body of research at CU that overlaps with Quantinuum's technology.


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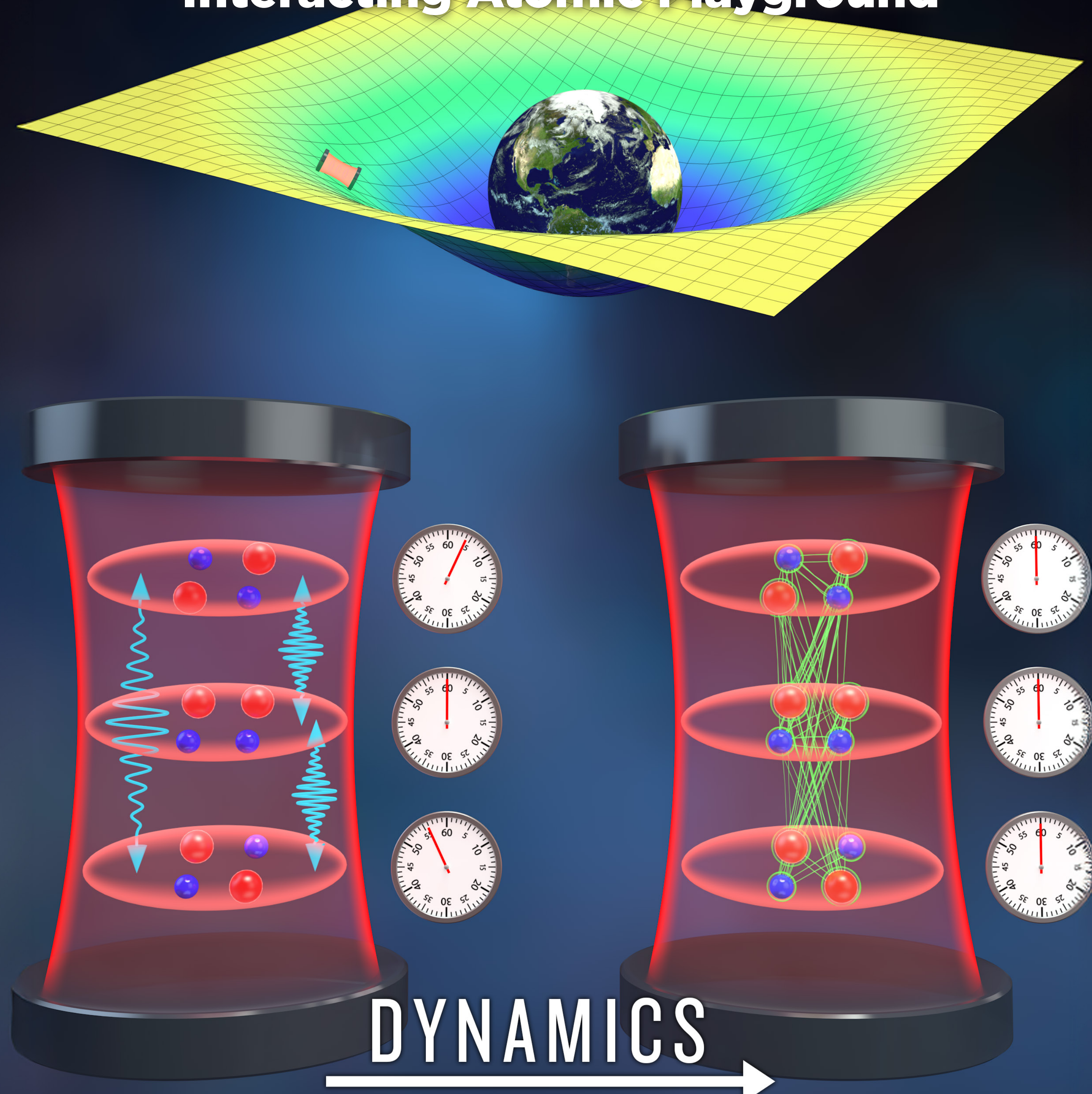
# Sneaky Clocks:

## Uncovering Einstein's Relativity in an Interacting Atomic Playground




For over a century, physicists have grappled with one of the most profound questions in science: How do the rules of quantum mechanics, which govern the smallest particles, fit with the laws of general relativity, which describe the universe on the largest scales?

The optical lattice clock, one of the most precise timekeeping devices, is becoming a powerful tool used to tackle this great challenge. Within an optical lattice clock, atoms are trapped in a "lattice" potential formed by laser beams and are manipulated with precise control of quantum coherence and interactions governed by quantum mechanics. Simultaneously, according to Einstein's laws of general relativity, time moves slower in stronger gravitational fields. This effect, known as gravitational redshift, leads to a tiny shift of atoms' internal energy levels depending on their position in gravitational fields, causing their "ticking"—the oscillations that define time in optical lattice clocks—to change.

By measuring the tiny shifts of oscillation frequency in these ultra precise clocks, researchers are able to explore the influences of Einstein's theory of relativity on quantum systems. While relativistic effects are well-understood for individual atoms, their role in many-body quantum systems, where atoms can interact and become entangled, remains largely unexplored.

Making a step forward in this direction, researchers led by JILA and NIST Fellows and University of Colorado Boulder physics professors Jun Ye and Ana Maria Rey—in collaboration with scientists at the Leibnitz University in Hanover, the Austrian Academy of Sciences, and the University of Innsbruck—proposed practical protocols to explore the effects of relativity, such as the gravitational redshift, on quantum entanglement and interactions in an optical atomic clock. Their work revealed that the interplay between gravitational effects and quantum interactions can lead to unexpected phenomena, such as atomic synchronization and quantum entanglement among particles. The results of this study were published in Physical Review Letters.

"One of our key findings is that interactions between atoms can help to lock them together so that now they behave as a unified system instead of ticking independently due to the gravitational redshift," explains Dr. Anjun Chu, a former JILA graduate student, now a postdoctoral researcher at the University of Chicago and the paper's first author. "This is really cool because it directly shows the interplay between quantum interactions and gravitational effects."

"The interplay between general relativity [GR] and quantum entanglement has puzzled physicists for years," Rey adds. "The challenge lies in the fact that GR corrections in most tabletop experiments are minuscule, making them extremely difficult to detect. However, atomic clocks are now reaching unprecedented precision, bringing these elusive effects within measurable range. Since these clocks simultaneously interrogate many atoms, they provide a unique platform to explore the intersection of GR and many-body quantum physics. In this work, we investigated a system where atoms interact by exchanging photons within an optical cavity. We found out that while individual interactions alone can have no direct effect on the ticking of the clock, their collective influence on the redshift can significantly modify the dynamics and even generate entanglement among the atoms."

### Distinguishing Gravitational Effects

To explore this challenge, the team devised innovative protocols to observe how gravitational redshift interferes with quantum behavior. The first issue they focused on was to uniquely distinguish gravitational effects in an optical lattice clock from other noise sources contributing to the tiny frequency shifts. They utilized a technique called a dressing protocol, which involves manipulating the internal states of particles with laser light. While dressing protocols are a standard tool in quantum optics, this is one of the first instances of the protocol being used to fine-tune gravitational effects.

The tunability is based on the mechanism known as mass-energy equivalence (from Einstein's famous equation $E=mc^2$), which means that changes in a particle's internal energy can subtly alter its mass. Based on this mechanism, an atom in the excited state has a slightly larger mass compared to the same atom in the ground state. The mass difference in gravitational potential energy is equivalent to gravitational redshift. The dressing protocol provides a flexible way to tune the mass difference, and thus the gravitational redshift, by controlling the particles to stay in a superposition of the two internal energy states. Instead of being strictly in the ground or excited state, the particles can be tuned to occupy both of the states simultaneously with a continuous change of occupation probability between these two levels. This technique provides unprecedented control of internal states, enabling the researchers to fine-tune the size of gravitational effects.

In this way, the researchers could distinguish genuine gravitational redshift effects from other influences, like magnetic field gradients, within the system.

"By changing the superpositions of internal levels of the particles you're addressing, you can change how large the gravitational effects appear," notes JILA graduate student Maya Miklos. "This is a really clever way to probe mass-energy equivalence at the quantum level."

### Seeing Synchronization and Entanglement

After providing a recipe to distinguish genuine gravitational effects, the researchers explored gravitational manifestations in quantum many-body dynamics. They made use of the photon-mediated interactions generated by placing the atoms in an optical cavity.

If one atom is in an excited state, it can relax back to the ground state by emitting a photon into the cavity. This photon doesn't necessarily escape the system but can be absorbed by another atom in the ground state, exciting it in turn. Such an exchange of energy—known as photon-mediated interactions—is key to making particles interact, even when they cannot physically touch each other.

Such types of quantum interactions can compete with gravitational effects on individual atoms inside the cavity. Typically, particles positioned at different "heights" within a gravitational field experience slight differences in how they "tick" due to gravitational redshift. Without interactions between particles, the slight difference in oscillation frequencies will cause them to fall out of sync over time.

However, when photon-mediated interactions were introduced, something remarkable happened: the particles began to synchronize, effectively "locking" their ticking together despite the differences in oscillation frequencies induced by gravity.

"It's fascinating," Chu says. "Think of each particle as its own little clock. When they interact, they start to tick in unison, even though gravity is trying to pull their timing apart."

This synchronization showcased a fascinating interplay between gravitational effects and quantum interactions, where the latter can override the natural desynchronization caused by gravitational redshift.

This synchronization wasn't just an oddity—it also led to the creation of quantum entanglement, a phenomenon where particles become interconnected, with the state of one instantly affecting the other. Remarkably, the researchers found that the speed of synchronization could also serve as an indirect measure of entanglement, offering an insight into quantifying the interplay between two effects. "Synchronization is the first phenomenon we can see that reveals this competition between gravitational redshift and quantum interactions," adds JILA postdoctoral researcher Dr. Kyungtae Kim. "It's a window into how these two forces balance each other."

### Advancing Physics Research

While this study revealed the initial interactions between these two fields of physics, the protocols developed could help refine experimental techniques, making them even more precise—with applications ranging from quantum computing to fundamental physics experiments.

"Detecting this GR-facilitated entanglement would be a groundbreaking achievement, and our theoretical calculations suggest that it is within reach of current or near-term experiments," says Rey.

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Future experiments could explore how particles behave under different conditions or how interactions can amplify gravitational effects, bringing us closer to unifying the two great pillars of modern physics.

This research was supported by the Sloan Foundation, the Simons Foundation and the Heising-Simons Foundation along with the JILA PFC.

*Written by Kenna Hughes-Castleberry.*



# Quantum Teleportation Gets an Ionic 2D Upgrade

Quantum entanglement is one of the most well-studied phenomena in quantum physics. Einstein called it "spooky action at a distance," as it enables particles to be deeply connected—such that measuring one instantly reveals information about the other, regardless of the distance between them. For decades, quantum entanglement has been used to design protocols for studying other physical processes, including quantum teleportation, which allows the transfer of quantum states without physically moving particles.

While quantum teleportation has been experimentally demonstrated in various settings, including individual photons and ions, extending this protocol to many-body systems—composed of many interacting particles—has remained a significant theoretical challenge. In contrast to isolated particles, many-body systems feature complex interdependencies where quantum information is shared across the entire ensemble. These collective behaviors give rise to rich dynamics and entanglement structures that are essential for quantum technologies but also introduce a level of complexity that makes teleportation more difficult to design and implement.

Now, in a recent study published in Physical Review Research, researchers at JILA—led by JILA and NIST Fellow and University of Colorado Boulder physics professor Ana Maria Rey and her team, along with Klaus Molmer from the Neils Bohr Institute and John Bollinger from NIST—have developed a new protocol for teleporting quantum information stored in collective spin states of ions within a two-dimensional crystal. This approach bridges concepts from atomic physics, quantum optics, and quantum information science, opening new avenues for building modular, scalable systems for quantum information processing.

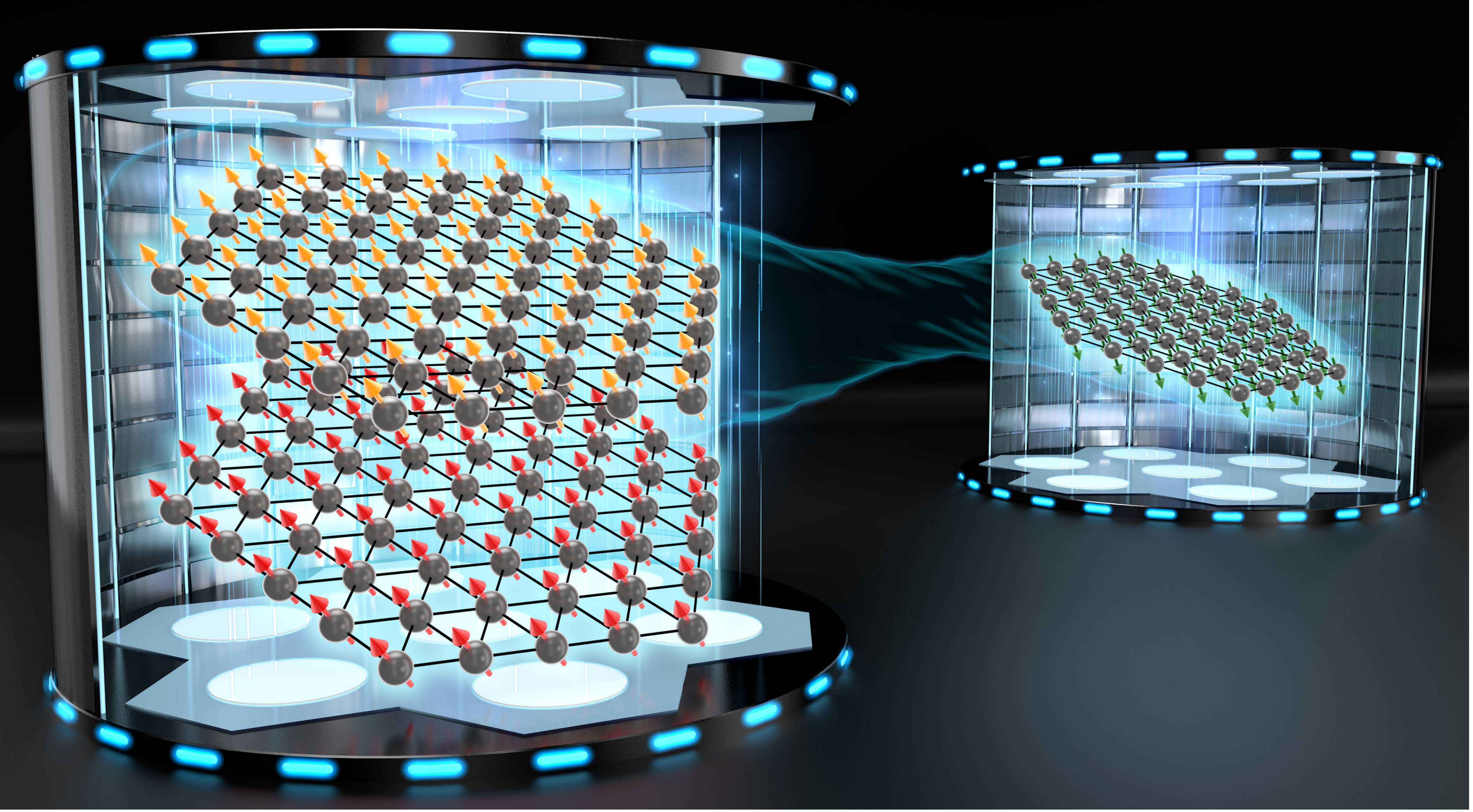
"Fundamentally, we generate Einstein-Podolsky-Rosen correlations—entanglement—between collective spin systems, using tools experimentally accessible in trapped ions," explains theorist Muhammad Miskeen Khan, who recently completed his postdoc from JILA and is now a postdoctoral researcher at Saint Louis University. "Then came up with a protocol that used that entanglement as a resource to teleport many-body collective spin states between energetically distinct ensembles."

"Our proposed teleportation protocol leverages both phonon-mediated collective spin-spin interactions among three energetically separated spin-ensembles in a two-dimensional trapped ions crystal together with measurements and local operations on these ensembles," Rey says. "We have taken advantage of different nuclear spin levels accessible in the system. Although in the current proposal the suggested protocol depends on spin ensembles that are energetically separated but spatially overlapping, future advancements could be gained from implementing our proposed protocols in spatially separated ensembles, for example, using 3D ion crystals."

### Individual Ions to Collective Spin Ensembles

In quantum experiments, spin refers to the internal angular momentum of particles such as electrons or atomic nuclei. Like each goose in a flock facing one direction so that the whole flock is facing the same direction, in a system of many atoms, their spins can be treated as a collective spin—a combined property that captures the net behavior of the ensemble. Such collective spin states are helpful in precision measurements and quantum computing, especially when they exhibit quantum correlations such as squeezing or entanglement.

The JILA team designed a teleportation protocol in which these collective states—rather than individual ions—are transferred between ion subgroups within a Penning trap, a system used to trap large systems of ions via a set of electrodes and a strong magnetic field. The system they studied consists of a 2D array of trapped beryllium ions in a crystal, which vibrate coherently through shared vibrations, or phonon modes, which can be used to individually manipulate nuclear and electronic spin states of these ions by driving them with lasers and microwave fields. Instead of spatially separated ion ensembles, the researchers separated the ensembles by using distinct nuclear spin levels (or internal ion levels) within the crystal, which have large energy splittings in the strong



magnetic field used in the Penning trap to confine the ions. The investigators used three levels to emulate three independent quantum subsystems: Alice, Bob, and Charlie.

First, Alice and Bob—two ion groups—are linked together through a phonon mode of the entire crystal. This phonon mode acts like a mediator, allowing the spins in Alice and Bob to become entangled and form a correlated quantum state.

Next, the third sub-ensemble or nuclear spin energy level, Charlie, holds a quantum state that the researchers want to teleport. This state is gently combined with Alice's state to mix their information coherently without measuring it directly—like blending two sound waves before analyzing them.

Finally, both Alice and Charlie quantum states are measured. These measurements don't reveal the full quantum state but provide enough information, which is sent to adjust Bob's group to end up in the same quantum state that Charlie originally had. The result is that Charlie's state appears in Bob's ions, effectively teleporting the quantum information across the system.

The protocol, adapted from continuous-variable teleportation schemes in quantum optics, was successfully numerically simulated in systems containing up to 300 ions per ensemble. The simulation also showed the possibility of achieving a high-fidelity teleportation of classical and non-classical spin states, including spin-coherent, spin-squeezed, and Dicke states, under current experimental conditions. Spin-squeezed and Dicke states are particularly interesting because they exhibit entanglement and are helpful for quantum-enhanced sensing, quantum information processing, and computation.



Demonstrating the teleportation of these states suggests that the protocol could one day serve as a mechanism for distributing entanglement and quantum information processing in quantum networks of ions.

"Typically, teleportation circuits are applied to spin-coherent states, which are relatively easy to prepare and simulate," Khan notes. "We showed that the same protocol can be extended to non-trivial, entangled states, which had not been clearly demonstrated before in a collective spin setting."

***"We showed that the same protocol can be extended to non-trivial, entangled states, which had not been clearly demonstrated before in a collective spin setting," Kahn notes.***

This theoretical protocol is also experimentally realistic. The proposed platform leverages existing techniques in Penning traps, where ion crystals are cooled, entangled, and interrogated with a high degree of control. The phonon modes in the trap are long-lived, robust to noise, and capable of coupling hundreds of ions simultaneously, making them ideal for entanglement distribution.

## Protocols with Many Applications

Teleportation protocols like these could serve as building blocks for special types of quantum devices, where quantum information is moved from one register to another without physical transport. It also lays the groundwork for distributed quantum sensing, where entangled states are shared across separate sensors to improve measurement precision.

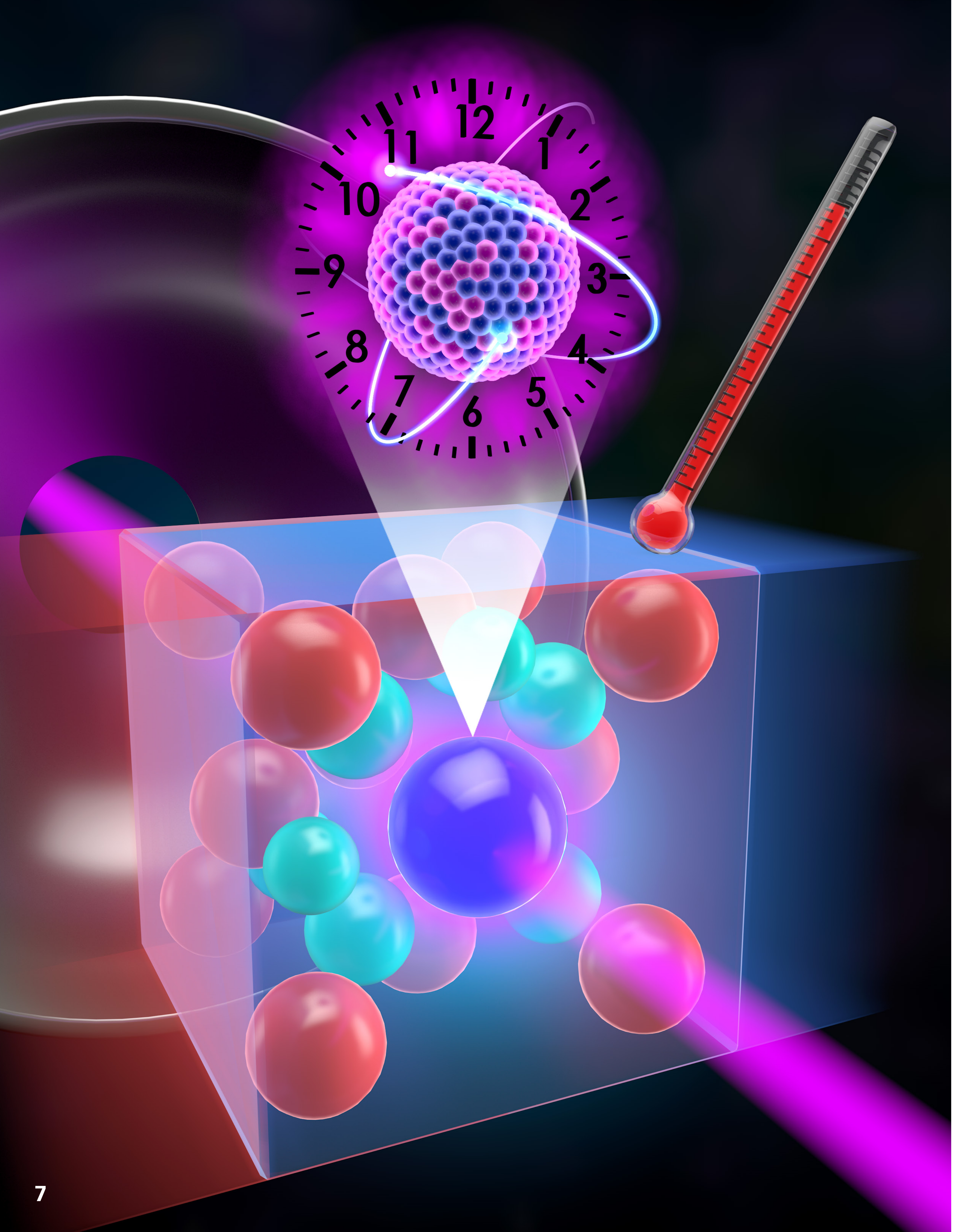
Beyond practical applications, this work could be the starting point for implementing schemes relevant to simulating quantum gravity in the lab and quantum information scrambling.

"Currently, we are working on some quantum information protocols implementable in the NIST Penning trap inspired by black hole physics," JILA graduate student Edwin Chaparro says. "Black holes are believed to be the fastest-scrambling objects in nature. We want to leverage the capability to generate scrambling in ion arrays to perform quantum teleportation and information recovery protocols and quantum metrology applications."

Looking ahead, the researchers hope to extend the protocol to spatially separated systems, potentially using a new generation of trapped ion crystals that live in three special dimensions instead of two. They also plan to explore how similar schemes could be implemented in other physical platforms, such as neutral atom arrays or polar molecules.

This work was supported by the U.S. Department of Energy's Office of Science, National Quantum Information Science Research Centers, the Quantum Systems Accelerator, the JILA Physics Frontier Center, and NIST.

*Written by Kenna Hughes-Castleberry.*






# Dialing in the Temperature Needed for Precise Nuclear Timekeeping

For decades, atomic clocks have been the pinnacle of precision timekeeping, enabling GPS navigation, cutting-edge physics research, and tests of fundamental theories. But researchers at JILA, led by JILA and NIST Fellow and University of Colorado Boulder physics professor Jun Ye, in collaboration with the Technical University of Vienna, are pushing beyond atomic transitions to something potentially even more stable: a nuclear clock. This clock could revolutionize timekeeping by using a uniquely low-energy transition within the nucleus of a thorium-229 atom. This transition is less sensitive to environmental disturbances than modern atomic clocks and has been proposed for tests of fundamental physics beyond the Standard Model.

This idea isn't new in Ye's laboratory. In fact, work in the lab on nuclear clocks began with a landmark experiment, the results of which were published as the cover article of Nature last year, where the team made the first frequency-based, quantum-state-resolved measurement of the thorium-229 nuclear transition in a thorium-doped host crystal. This achievement confirmed that thorium's nuclear transition could be measured with enough precision to be used as a timekeeping reference.

However, to build a precise clock, researchers must fully characterize how the transition responds to external conditions, including temperature. That's where this new investigation—an "Editor's Choice" paper published in Physical Review Letters—comes in, as the team studied the energy shifts in the thorium nuclei as the crystal containing the atoms was heated to different temperatures.

"This is the first step toward characterizing the systematics of the nuclear clock," says JILA postdoctoral researcher Dr. Jacob Higgins, the study's first author. "We have found a transition that's relatively insensitive to temperature, which is exactly what we want for a precision timekeeping device."

"A solid-state nuclear clock has a great potential to become a robust and portable timing device that is highly precise," notes Jun Ye. "We are searching for the parameter space for a compact nuclear clock to maintain 10-18 fractional frequency stability for continuous operation."

## The Precision of Nuclear Clocks

Because the nucleus of an atom is less affected by environmental disturbances than its electrons, a nuclear clock could retain accuracy under conditions where atomic clocks would falter, as the clock is more resistant to noise. Among all other nuclei, thorium-229 is particularly well-suited for this because it has a nuclear transition with unusually low energy, making it possible to probe with ultraviolet laser light rather than high-energy gamma rays.

As opposed to measuring thorium in a trapped ion system, the Ye lab has taken a different approach: embedding thorium-229 into a solid-state host—a calcium fluoride ($CaF_2$) crystal. This method, developed by their collaborators at the Technical University of Vienna, allows for a much higher density of thorium nuclei than traditional ion-trap techniques. More nuclei means stronger signals and better stability for measuring the nuclear transition.

## Heating a Nuclear Clock

To look at how temperature affects this nuclear transition, the researchers both cooled and heated the thorium-doped crystal to three different temperatures: 150K (-123°C) with liquid nitrogen, 229K (-44°C) with a dry ice-methanol mixture, and 293K (around room temperature). Using a frequency comb laser, they measured how the nuclear transition frequency shifted at each temperature, revealing two competing physical effects within the crystal.

For one effect, as the crystal warmed, it expanded, subtly altering the atomic lattice and shifting the electric field gradients experienced by the thorium nuclei. This electric field gradient caused the thorium transition to split into multiple spectral lines, which shifted in different directions as temperature changed. The second effect: the lattice expansion also changed the charge density of electrons in the crystal, modifying the electrons' interaction strength with the nucleus and causing spectral lines to move in the same direction.

As these two effects fought for control of the thorium atoms, one particular transition was observed to be far less temperature-sensitive than the others, as the two effects mostly canceled each other out. Across the full temperature range examined, this transition shifted by only 62 kilohertz, a shift at least 30 times smaller than in the other transitions.

"This transition is behaving in a way that's really promising for clock applications," adds Chuankun Zhang, a JILA graduate student. "If we can stabilize it further, it could be a real game-changer in precision timekeeping."

As a next step, the team plans to look for a temperature 'sweet spot' where the nuclear transition remains almost completely independent of temperature. Their initial data suggests that somewhere between 150K and 229K, the transition frequency would be even easier to temperature stabilize, providing an ideal operating condition for a future nuclear clock.

### Customizing a Nuclear Clock System

Building an entirely new type of clock requires one-of-a-kind-designed equipment, much of which doesn't exist to the level of customization required. Thanks to JILA's instrument shop—with its machinists and engineers—the team was able to create critical components for their experiment.

"Kim Hagan and the whole instrument shop have been super helpful throughout this process," Higgins notes. "They machined the crystal mount, which holds the thorium-doped crystal, and built parts of the cold trap system that allowed us to control the temperature precisely."

Having in-house machining expertise allowed the researchers to quickly iterate on designs and ensure that even small changes could be done with ease.

"If we only had used off-the-shelf parts, we wouldn't have had the same level of confidence in our setup," adds JILA graduate student Tian Ooi. "The custom-built pieces from the instrument shop save us so much time."

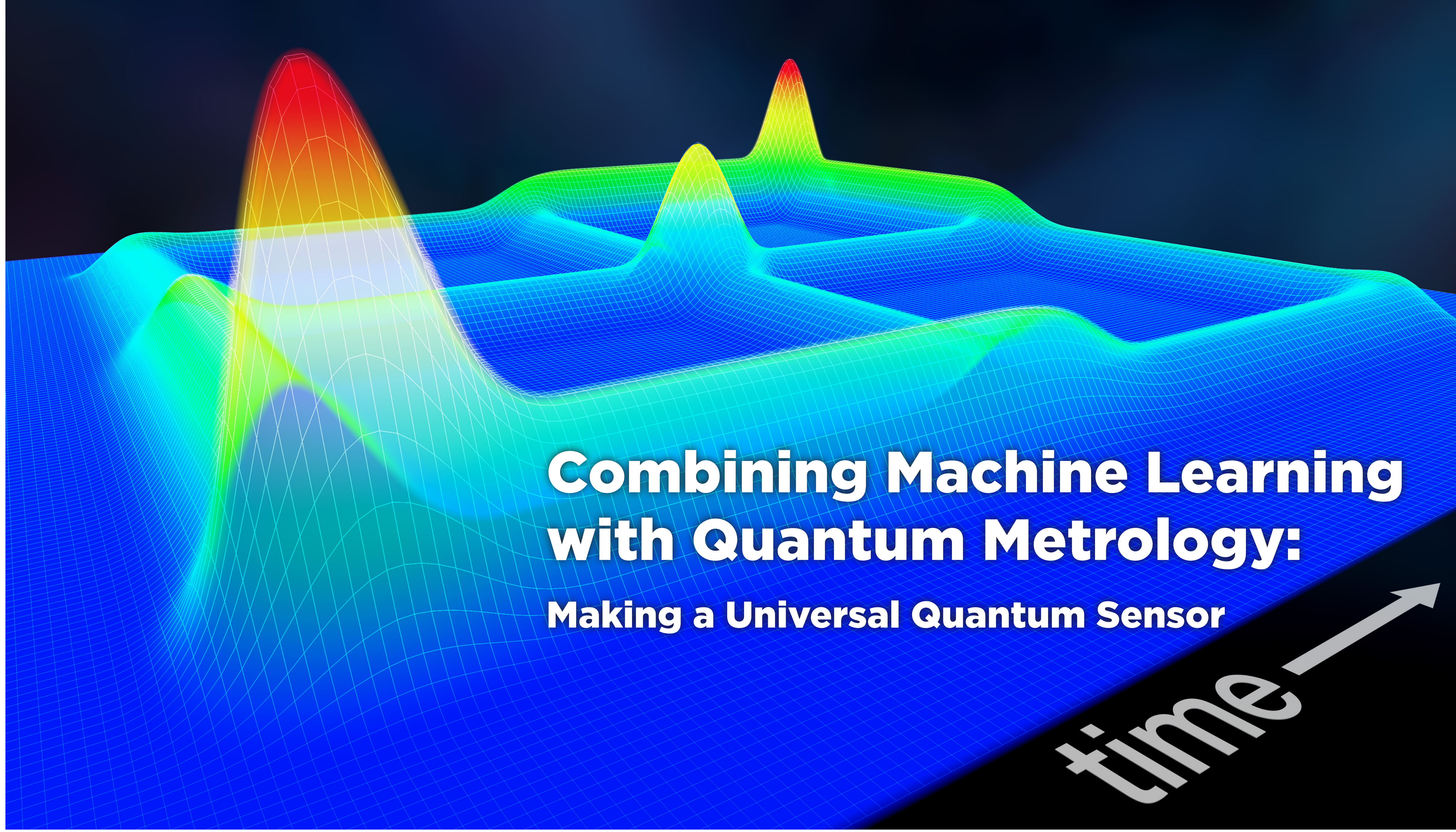
### Sensing Beyond Time

While the primary goal of this research is to develop a more stable nuclear clock, its implications go beyond timekeeping. The thorium nuclear transition is very insensitive to disturbances in its environment, but highly sensitive to variations in fundamental forces—any unexpected shift in frequency could indicate new physics, such as the presence of dark matter.

"The nuclear transition's sensitivity could allow us to probe new physics," Higgins explains. "Beyond just making a better clock, this could open doors to entirely new ways of studying the universe."

This research was supported by the Army Research Office, the Air Force Office of Scientific Research, the National Science Foundation, the Quantum System Accelerator, and NIST.

*Written by Kenna Hughes-Castleberry.*




# Combining Machine Learning with Quantum Metrology:

## Making a Universal Quantum Sensor

Atom interferometry, a technique that leverages the wavelike nature of atoms, has been pivotal in precision measurements, including satellite navigation and measuring the Earth's roundness. Traditional atom interferometry setups, however, often lack flexibility, requiring hardware modifications for performing different measurement tasks.

Addressing this limitation, JILA Fellow and University of Colorado Boulder physics professor Murray Holland and his team, along with CU Boulder Engineering Professor Marco Nicotra, developed a platform that combines machine learning with atom interferometry. Recently published in Physical Review Research, their work establishes a programmable framework for quantum sensing, where, using universal programmable atom-optic "gates," a single device can be reconfigured via software to perform a wide range of precision measurements—such as acceleration, rotation, and gravity gradients—without hardware changes.

This innovation not only advances the flexibility and efficiency of quantum sensors but also lays the groundwork for a new wave of quantum engineering in which future quantum technologies integrate AI-driven control to provide extra precision and functionality.

"Understanding the superposition and interference of particles has been at the heart of quantum for more than a century, but just now we are just beginning to develop the experimental tools to really exploit the ideas and build new future technologies," Holland says.

## Following JILA's Legacy of Laser Stability

JILA has long been recognized as a global leader in precision measurement, particularly in laser stability and atomic control. Building on this tradition, Holland, along with JILA postdoctoral researcher Catie LeDesma and graduate student Kendall Mehling, used ultra-stable lasers as the foundation for their system. These lasers create the optical lattice that traps and manipulates a Bose-Einstein condensate—an ultracold cloud of atoms behaving as a single quantum wave.

Each gate operation—such as splitting, reflecting, or stopping the atom wave-packets—was executed through carefully choreographed shifts in the lattice position. These gates acted like programmable "tiles" that could be arranged sequentially, like LEGO bricks, to build complex atom interferometer circuits. By snapping these elements together in different combinations, the team could effectively program the quantum sensor to perform various measurement tasks—all within the same physical setup.

## Adding Machine Learning

What sets this project apart is how the team used machine learning to design the gates or "tiles" in their system. Instead of relying on manually tuned parameters or hard-to-find solutions of mathematical equations, the researchers turned to artificial intelligence to solve the complex problem of finding the precise lattice modulations needed to implement each gate. They used optimization algorithms to train a computer to discover how to dynamically position the optical lattice in just the right way to achieve high-fidelity quantum state transformations. This approach not only streamlined the design process but also uncovered solutions that might be non-intuitive to human inventors.

"Artificial intelligence is a trending theme in the science of today, and our experiment is no exception, where the computers find solutions to our design tasks that would be impossible to envisage without their help," says LeDesma.

## Validating Their Setup

To prove their system worked, the team ran a series of experiments with a Bose-Einstein condensate (BEC) of rubidium atoms trapped in the optical lattice. Using precision imaging, they captured the motion of the atoms in real time as each gate was applied, watching as the atom cloud split, reflected, or froze in place according to the programmed instructions. These visual results were then matched with time-of-flight measurements, where the atoms are released and their wave-functions allowed to expand, revealing their momentum distribution—an essential tool for verifying the implementation of the state transformations.

The comparison between experimental data and the machine learning simulations showed remarkable agreement. Gates designed purely through computational optimization were realized in the lab with high fidelity, often exceeding 90% accuracy. This confirmed that the AI-designed protocols were viable and could be executed with precision in a real-world quantum system—a significant achievement in quantum control engineering.

## Creating Versatile Quantum Sensors

By creating a universal gate platform for atom interferometry, Holland's team has laid the groundwork for software-defined quantum sensors—devices that can switch functions with a new program rather than a new piece of hardware. What's more, the fusion of AI and quantum hardware offers a pathway to optimizing these sensors for changing environments. In principle, a future sensor could learn in real time, adjusting its gate sequences on the fly to compensate for noise or to prioritize different measurement axes—opening the door to adaptive, intelligent quantum metrology.

This work is also part of NASA's Quantum Pathways Institute (QPI), a multi-institutional effort to develop deployable quantum technologies. NASA's vision includes mobilizing quantum sensors for use in space, where traditional systems may be too rigid or sensitive to operate effectively. The universal gate framework aligns perfectly with this goal—enabling sensors that can be reprogrammed mid-mission to adapt to new objectives or conditions in orbit, on planetary surfaces, or even deep-space missions.

"We think this technology solution that bridges quantum physics and AI will allow us to build new kinds of applications that will bring the fuzzy quantum world out of the lab and into everyday life," Holland says.

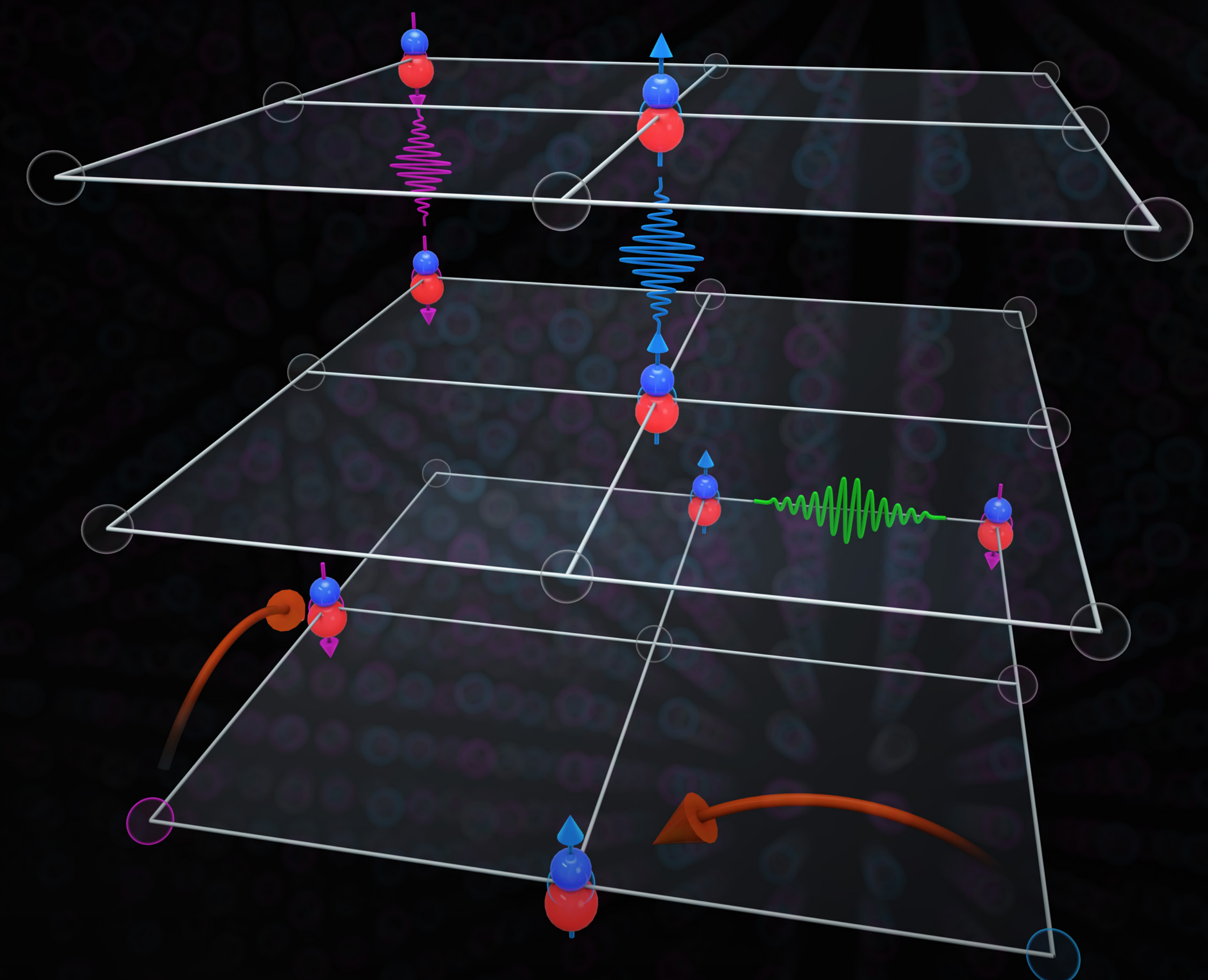
This research was supported by NASA and the National Science Foundation.

*Written by Kenna Hughes-Castleberry*



# Where Motion Meets Spin:

## A Quantum Leap in Simulating Magnetism



The strange behaviors of high-temperature superconductors—materials that conduct electricity without resistance above the boiling point of liquid nitrogen—and other systems with unusual magnetic properties have fascinated scientists for decades. While researchers have developed mathematical models for these systems, much of the underlying quantum dynamics and phases remain a mystery because of the immense computational difficulty of solving these models.

In a new study published in Science, researchers from JILA, led by JILA and NIST Fellows and University of Colorado Boulder physics professors Jun Ye and Ana Maria Rey and JILA and CU Boulder physics professor John Bohn, used ultracold molecules to realize these models with an unprecedented level of control. Their work bridges the fields of atomic, molecular, and optical (AMO) physics with condensed matter physics, opening new doors for quantum simulations and advances in quantum technologies.

"It is very exciting that experiments with polar molecules are now reaching the point where these models can be implemented in the lab," Rey says. "While currently, we are exploring dynamics at low filling fractions where theory effort can still have some predicting capabilities, very soon experiments will reach dense regimes intractable by theory, fulfilling the dream of quantum simulation."

## A Decade in the Making

JILA has long been celebrated as a hub where experimentalists and theorists collaborate to tackle some of the most challenging questions in physics. Indeed, over two decades of collaboration among JILA researchers, first with the experimentalists Ye and the late JILA Fellow Deborah Jin, later joined by theory colleagues Rey and Bohn, pioneered ultracold molecule research and laid the foundation for this work.

In this study, the researchers from Ye's group collaborated with theorists in Rey's and Bohn's groups to understand the data from several new experiments exploring different regimes of molecular motion and dipolar interactions.

"We wanted to understand how motion and magnetism are coupled in quantum systems," says Annette Carroll, a JILA graduate student in the Ye laboratory and the paper's first author. "The molecules offer a unique platform to study this interplay, thanks to their long-range dipolar interactions."

These dipolar interactions were key to the experiment's success. While neutral atoms have been widely used in quantum studies due to their ease of cooling and control, their typical short-range interactions often limit their ability to simulate magnetism. Ultracold molecules, with their natural long-range dipolar interactions, offer a richer platform for exploring exotic quantum phases but are complicated to control.

## Focusing on Framework

In the experiment, an array of ultracold potassium-rubidium molecules were used to emulate the behavior of electrons in a solid state crystal. Electrons tunnel between nearby ion cores in a crystal at a rate "t".

To imitate the fact that electrons are like tiny magnets, which can point in two directions, spin up or spin down, molecules were prepared in two accessible internal (rotational) states. Electrons are charged particles and see each other at a distance, but due to the ion cores and other electrons in the system, they strongly screen each other, and effectively, one electron only sees another electron when they are at the same lattice site. In this setup, two nearby molecules (simulating electrons), one with spin up and one with spin down, can flip their spins but to do that, for example, the spin up electron needs to hop into the site where the down electron is, interact just for a glimpse to reduce the large energy cost to be at the same site, and then hop back to its original site now as a spin down.

This process is called superexchange and happens at a rate "J." The behavior of electrons hopping and exchanging their spins is called "t-J" model and it is believed to have all the necessary ingredients to explain the emergence of high temperature superconductivity. But, this is not yet well understood.

"Polar molecules have the advantage that they carry a dipole moment, and this means that two molecules can exchange the spins far from the distance without needing to move where the other is. This has great consequences," elaborates Rey. "It allows us to simulate the 't-J' model in a broader parameter regime since the exchange rate J can be controlled in the lab. It opens exciting opportunities for the exploration of magnetism and superconductivity in new regimes."

"The t-J model captures the interplay between motion and spin interactions," adds Sean Muleady, a former JILA graduate student in Rey's theory group now at the Joint Center for Quantum Information and Computer Science (QuICS) and the Joint Quantum Institute (JQI), who was also involved in this study. "These dynamics are critical to understanding phenomena like magnetism in strongly-correlated systems and, in certain regimes, even superconductivity. But studying these effects in real materials is notoriously difficult."

To overcome these challenges, Rey, Muleady, and postdoctoral researcher David Wellnitz worked with Bohn and his graduate student Reuben Wang to develop mathematical tools to simulate the spin dynamics of moving dipolar particles within different lattice arrangements set up by the researchers within Ye's experimental group.

"Using dipolar interactions adds an entirely new dimension," says Bohn. "This is a more generalized version of the t-J model, incorporating features that condensed matter physicists could only theorize about."

## Combining Theory and Experiment

For the researchers in Ye's laboratory, the team focused on ultracold potassium-rubidium molecules trapped in an optical lattice—a grid of laser light designed to confine the molecules to specific locations. This lattice structure served as a simulated crystal, mimicking the confinement of electrons in real materials. By applying electric fields, the researchers



precisely controlled the strength and nature of the molecules' dipolar interactions and, by tuning the strength of the optical lattice, tuned their ability to move within the lattice.

The experimentalists studied the dynamics between two distinct motional extremes: one where the molecules were "frozen" in place and another where they could move freely within two-dimensional planes without any transverse lattice confinement. By tuning the transverse lattice depth between these two extremes, the researchers explored a large range of behaviors governed by the t-J model, from interactions between frozen spins to dynamic coupling between spin and motion. In all setups, the researchers prepared the molecules in a superposition of rotational states, simulating magnetic spins all pointing in the same direction, and measured how quickly the spins lost their initial magnetization because of their interactions.

Interpreting these behaviors, however, required an equally flexible theoretical approach. Two theoretical groups, led by JILA Fellows Ana Maria Rey and John Bohn, collaborated to combine their unique expertise. Rey's group specialized in lattice-based models, while Bohn's group brought insights into molecular collisions and scattering processes.

"These were two very different schools of thought," says Muleady. "Bringing them together was critical because the experiment operates in a middle ground that neither approach alone could fully describe."

The collaboration resulted in novel theoretical frameworks that bridged the gap between frozen and dynamic motional regimes, enabling a comprehensive interpretation of the experimental data.

## Connecting Magnetism and Motion

Through their collaboration, the team made several significant discoveries, including that the spins stayed aligned much longer at a particular electric field when the interaction between the spins is independent of their orientation. Observing coherence in this context is crucial because the spins maintain their alignment over time, which is rare. Long coherence times are important for preserving quantum entanglement, a behavior where particles' quantum states are interdependent.

"At this special point, the spins of the molecules align perfectly, leading to slower decay of quantum coherence than at any other point," explains Cal Miller, a JILA graduate student in the Ye group. "This is something that had been theorized but never observed in an experiment until now."

This finding confirmed theoretical predictions about the behavior of spin systems and demonstrated the precise tunability of interactions between molecules.

However, the experimentalists observed other dynamics that required new theoretical modeling. The researchers systematically explored how the coherence between the spins depends on molecular motion, developing for the first time a model of how collisions between molecules allowed to move freely within 2D layers lead to the decoherence of the spins.

"At first, we couldn't explain why the decoherence behaved this way," explains Junyu Lin, a postdoctoral researcher in Ye's group. "It took many discussions. Finally, when we saw the model from Reuben and John, and it matched our data, we thought: 'Oh, that's the mechanism."

Moreover, when the molecules were allowed to move freely, the researchers observed a striking new phenomenon in the spin alignment.

"We saw a fascinating 'stretched exponential' behavior in the decay of spin alignment," says Wang. "It's a result of the molecules' motion and their spin alignment—a combination that's difficult to describe using traditional methods."

The key understanding from the work is how motion, which can be regulated by optical lattices, affects the magnetization dynamics of strongly interacting dipoles. The researchers observed more complex spin orientation dynamics by allowing the molecules to move. The coupling between spin and motion modifies the rate at which interacting spins evolve.

## Pushing New Frontiers in Experiment & Theory

Understanding these experimental discoveries would not have been possible without the team's new advances in theoretical modeling.

"This project pushed our tools to the limit," explains Wellnitz. "We had to develop new methods to bridge the gap between systems where molecules are frozen and those where they're moving freely."

The collaboration also highlighted the challenges and rewards of interdisciplinary research within theoretical physics.

"One of the most exciting parts of this work was finding a shared language between the different theoretical approaches," says Muleady. "Each group brought something unique to the table, and the experiment provided a real-world test for our models."

For the experimentalists, these results may bring new interest to the t-J model from multiple different subfields of physics.

"While the condensed matter community is already interested in this model, I think the AMO community will also be more interested in our work because we're approaching things differently," adds Lin.

While the results of this study have uncovered vital information about the rich dynamics of long-range interacting spin systems, the researchers are already looking toward the project's next steps.

For the experimentalists, future work will focus on achieving even colder temperatures and higher densities of molecules.

"We're working toward regimes where the molecules' interactions are strong enough to create new quantum phases," says Carroll. "These are the conditions where we might observe rich phenomena like superfluidity."

For others, the results of this project suggest major implications for the future development of quantum devices.

"By advancing our understanding of spin-motion coupling, this work could inform the design of new quantum technologies," notes Wellnitz. "It's an exciting time to be in this field."

This research is supported by the National Science Foundation, the US Department of Energy's Office of Science, National Quantum Information Science Research Centers, the Quantum Systems Accelerator, the Air Force Office and Office of Science and Research, and the JILA Physics Frontier Center.

*Written by Kenna Hughes-Castleberry.*

# Molecular Lock and Key:

## Decoding the Secrets of Ion Binding

Understanding how molecules interact with ions is a cornerstone of chemistry, with applications from pollution detection and cleanup to drug delivery. In a series of new studies led by JILA Fellow and University of Colorado Boulder chemistry professor Mathias Weber, researchers explored how a specific ion receptor called octamethyl calix[4]pyrrole (omC4P) binds to different anions, such as fluoride or nitrate. These findings, published in The Journal of the American Chemical Society, The Journal of Physical Chemistry Letters, and The Journal of Physical Chemistry B, provide fundamental insights about molecular binding that could help advance fields such as environmental science and synthetic chemistry.

"The main issue with understanding these interactions is that there is a competition between an ion binding to a certain receptor and that same ion wanting to be surrounded by solvent molecules," Weber explains. "This competition impacts how effective and specific an ion receptor can be, and we currently don't understand it sufficiently well to design better ion receptors for applications. This has been a problem for decades, and we can now try to solve it by taking a different perspective."

### Looking at Ion Receptors

The test molecule in question, omC4P, is a prototypical anion receptor that has received much interest for nearly 30 years, a macrocyclic molecule with a cup-like structure designed to capture negatively charged ions (anions). Its rigid yet adaptable cavity contains four NH groups that form hydrogen bonds with incoming ions, making it an ideal system for investigating how different anions interact with molecular hosts.

What makes omC4P especially interesting is its specificity. Because its binding pocket has a particular size and shape, simple anions like fluoride or chloride fit quite snugly. However, when larger or more complex anions enter, like nitrate or formate, their shapes can disrupt the pocket structure, and the ions stick out into the surrounding solvent . At the same

time, some ions bind strongly to omC4P even though they are relatively large, because they bind tightly to the NH groups.

Understanding these variations in binding is crucial for designing selective receptors. If a receptor can differentiate between closely related anions, it could help significantly in advancing applications such as water purification, medical diagnostics, or industrial sensing.

"These studies help us figure out what makes a receptor highly selective," elaborates JILA graduate student Lane Terry, the papers' first author. "If we can fine-tune its structure, we can create targeted ion sensors for real-world applications."

### First Step: Simple Halides

The team's first study, published in The Journal of the American Chemical Society, focused on halide ions—fluoride, chloride, and bromide—with simple spherical shapes.

"We started with halides because they are the simplest—they act as just a single point charge," Terry explains.

To analyze how these anions interacted with omC4P, researchers used cryogenic ion vibrational spectroscopy (CIVS) to take a molecular "snapshot" showing the interactions happening in the sample. CIVS is a technique that investigates ionized molecules cooled to low temperatures, which reduces their movement and isolates their vibrations. Ions are then bombarded with infrared photons, causing the ions to absorb specific wavelengths based on how their atoms are arranged and how they vibrate. This, in combination with quantum chemical calculations, allows researchers to measure how the receptor interacts with different ions without interference from external factors like solvent molecules.

After multiple CIVS measurements, the team verified their measurements with those predicted by Density Functional Theory (DFT), a computational method that calculates the molecular structure of complexes to predict how they interact.

"DFT helps us compare our experimental data with theoretical models," Terry explains, "so we can confirm what we're seeing and refine our understanding of ion binding."

Through this process, the team discovered that fluoride formed the strongest hydrogen bonds, remaining tightly bound even in solution, whereas chloride and bromide showed weaker ion-receptor interactions due to weaker proton affinities and thus, more susceptible to solvent interaction.

"This is important because most of these ion receptors are used in aqueous environments," Terry notes. "Meaning that fluoride's binding will be more stable with these ion receptors than the other halides."

### Adding Complexity: Nitrate's Unique Binding

Building on this foundation, the team then explored the nitrate anion binding to omC4P, detailed in The Journal of Physical Chemistry Letters. Unlike halides, nitrate is polyatomic, meaning it has multiple atoms, in this case, arranged in a Y-shape.

Using the CIVS plus DFT method, the researchers found that nitrate prefers a binding mode where only one of its three oxygen atoms interacts with the omC4P's NH groups. This was a surprising result, as one might expect two oxygen atoms to bind symmetrically.

"Even though nitrate has multiple possible configurations, it strongly favors just one," Terry says. "The ion shape and charge distribution make a big difference, especially when in an aqueous environment."

### The Most Complex Case: Formate and Isomerism

The final study, published in The Journal of Physical Chemistry B, tackled the most intricate binding behavior yet—formate ($HCOO^-$), a small but more asymmetric anion binding to the omC4P. Unlike nitrate, formate was observed to have multiple binding configurations—a process known as isomerism—to the ion receptor.

"Formate actually isomerizes at a low enough energy that we detect multiple isomers, even at cryogenic temperatures," Terry explains.

The researchers observed that the formate shifted between different configurations, unlike nitrate, which settled into one stable structure. Interestingly, the most stable formate configuration was not symmetrical at all, defying conventional expectations. While highly symmetrical structures often allow for predictable, in contrast, asymmetry can lead to unexpected behaviors that influence selectivity and stability in ion receptors.

After analyzing these findings, the team is now investigating modified omC4P with added structural "walls" to deepen the binding cavity and alter ion interactions, which will add further complexity to their experiment.

### Beyond Fundamentals

While these studies focus on fundamental chemistry, their implications extend far beyond the lab. Environmental monitoring, drug delivery, and chemical sensing all rely on understanding ion interactions at the molecular level.

Terry says, "We work closely with organic chemists who design these molecules. Our findings help them build better ion receptors with improved selectivity."

Whether detecting contaminants in water or designing better drug carriers, their discoveries bring us one step closer to harnessing chemistry for the greater good.

This research was supported by the National Science Foundation, the JILA Physics Frontier Center, the University of Colorado Boulder, and Colorado State University.

*Written by Kenna Hughes-Castleberry*

# JILA NEWS & AWARDS

### JILA and NIST Fellow and University of Colorado Boulder Physics Professor Jun Ye Receives the Berthold Leibinger Zukunftspreis 2025 Award

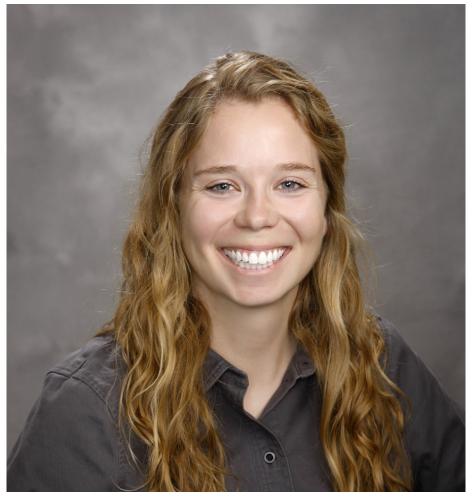
Jun Ye, a distinguished Fellow at JILA and the National Institute of Standards and Technology (NIST) and a physics professor at the University of Colorado Boulder, has been honored with the 2025 Berthold Leibinger Zukunftspreis. This prestigious biennial award, established in 2006 by the German non-profit Berthold Leibinger Stiftung, recognizes outstanding research in laser science and technology and carries a prize of €50,000.

The award acknowledges Ye's groundbreaking work in optical clocks and frequency metrology, which has significantly advanced precision measurement and timekeeping. His contributions have deepened our understanding of fundamental physics and paved the way for technological innovations in various sectors.

"I am honored and humbled by this recognition," says Ye. "Such an honor clearly reflects the scientific spirit of all the amazing people I have had the privilege working with over the years, including many of our outstanding graduate students, postdocs, and dear colleagues near and far."

The award ceremony is scheduled for June 20, 2025, in Ditzingen, Germany, where Ye will be formally presented with the prize. This accolade places him among an esteemed group of scientists who have previously received the Zukunftspreis, including Nobel laureates Gérard Mourou and Anne L'Huillier.

Ye's recognition with the Berthold Leibinger Zukunftspreis not only highlights his individual achievements but also underscores the pivotal role of laser technology research in advancing science and industry globally.



### JILA and University of Colorado Boulder Physics Alum Dr. Olivia Krohn is Awarded the 2025 APS Global Summit Thesis Prize

Dr. Olivia Krohn, a former JILA graduate student and now a postdoctoral researcher at Sandia National Laboratories, has been awarded the prestigious Justin Jankunas dissertation award, given out by the American Physical Society (APS) division of chemical physics at the APS Global Summit conference. This award recognizes exceptional doctoral research that advances the frontiers of physics. Krohn's award highlights her dissertation research, which bridges the legacy of JILA's origins in astrophysics with its current role as a global leader in atomic, molecular, and optical (AMO) physics.

Krohn's thesis, completed under the mentorship of JILA Fellow and University of Colorado Boulder physics professor Heather Lewandowski, investigates the ion-neutral gas-phase chemical reactions of interstellar relevance using cold arrays of trapped ions known as "coulomb crystals". Her work explores the fundamental processes that govern the chemistry of space—particularly focusing on the elusive ion $CCl^+$—within the controlled conditions of the laboratory.

"While 'JILA' once stood for the 'Joint Institute for Laboratory Astrophysics,' the name is now an acronym-less moniker signifying a research center that pushes the frontier of AMO physics," says Krohn. "My dissertation is a great example that these two identities of JILA are still sometimes entangled."

To trap and cool the cold ensembles into Coulumb crystals, an ultra-high vacuum (UHV) environment is needed to make the crystal. However, having the ions in UHV is not the only influence in creating Coulomb crystals. By doing this, Krohn could simulate key reactions of the interstellar medium. Her research not only provided insight into chemical networks that may help explain why $CCl^+$ has yet to be detected in space but also advanced the understanding of how chemical reactions behave at temperatures close to absolute zero—where quantum mechanics begins to dominate.

A major component of her work also involved developing methods to pair a traveling wave Stark decelerator with the ion trap, an innovation that allows precise tuning of the collision energy between ions and neutral molecules.

"At the colder end of this spectrum, at collision energies equivalent to a few Kelvin," she explains, "we can venture into regimes where quantum mechanics plays a more direct role on the chemical dynamics and push the frontier of studying fundamental chemical transformation to colder and more controlled systems."

Dr. Lewandowski praised Krohn's scientific leadership and creativity throughout her graduate career.

"This is a well-deserved recognition of the outstanding work Olivia completed for her Ph.D. dissertation," Lewandowski says. "She was a true leader in these studies, which have important implications for chemistry in the interstellar medium. I was incredibly fortunate to have the opportunity to work with her during her time at JILA."

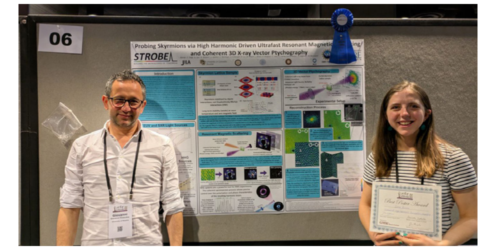
Reflecting on the award, Krohn expressed gratitude for the community that supported her research. "I was extremely humbled and grateful to receive this award," she notes. "I am thankful for the amazing guidance of Heather and for the incredible teammates I worked beside in my Ph.D. I am indebted to support from my friends and family. And of course, I learned so much from our amazing JILA shop, support staff, and colleagues. It was a privilege to conduct my dissertation research at JILA."

## Graduate Students Anya Grafov and Iona Binnie Receive Top Honors at MMM Intermag 2025 Conference

Congratulations to JILA graduate students Anya Grafov and Iona Binnie—who conduct their cutting-edge research in the laboratory of JILA Fellows and the University of Colorado Boulder professors Margaret Murnane and Henry Kapteyn—for their outstanding achievements at the MMM Intermag 2025 conference!

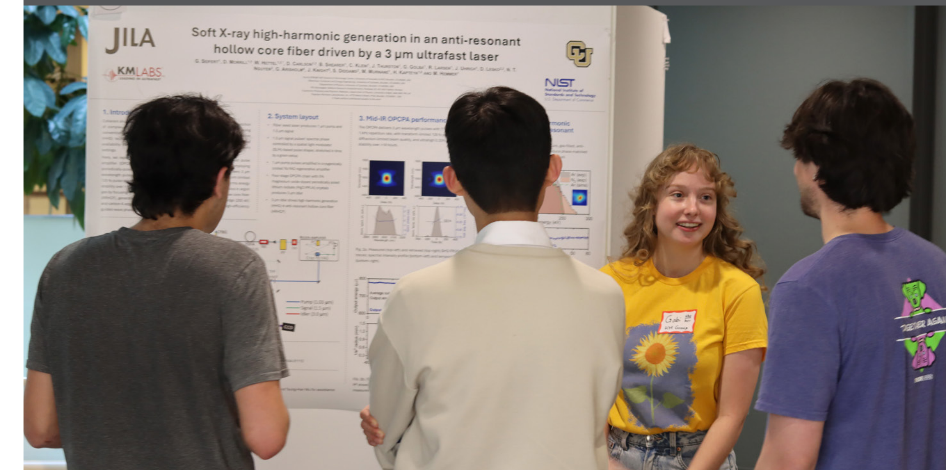
"I'm grateful to the IEEE Magnetics Society for the opportunity to share my research and honored to be recognized," said Grafov. "The Young Professionals Lightning Talks required us to present our research to a general audience in just two minutes. Ultrafast magnetism and extreme ultraviolet light science are complex topics, so explaining my entire project in such a short time was no easy task. Summarizing my project without jargon or lengthy explanations was a rewarding challenge that strengthened my science communication skills."

Grafov earned 1st Place in the Young Professionals Lightning Talks for her presentation, "Measuring Magnetic Dynamics with Extreme Ultraviolet Light," while Binnie won the Best Poster Award in her session for her poster, "Probing Skyrmions via High Harmonic Driven Ultrafast Magnetic Scattering and Coherent 3D X-ray Vector Ptychography."



"Presenting my poster was a demanding but very rewarding experience," added Binnie. "I really enjoyed the opportunity to share my research with the magnetics community, which is a different audience than I am used to. Their questions sparked new insights into my own research challenges."

Their achievements showcase the innovative work happening at JILA in the fields of ultrafast magnetism and extreme ultraviolet light science.

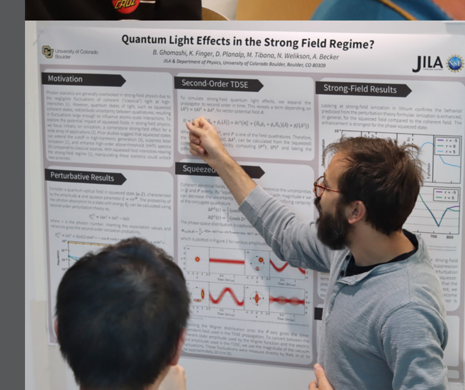



## 9th Annual PosterFest: A Celebration of Scientific Innovation

On May 1st, JILA hosted its 9th annual PosterFest, a vibrant community event that brought together graduate students, postdocs, fellows, and faculty to showcase their latest research. This year's PosterFest was particularly notable for the diverse range of topics covered, reflecting the dynamic and interdisciplinary nature of research at JILA.

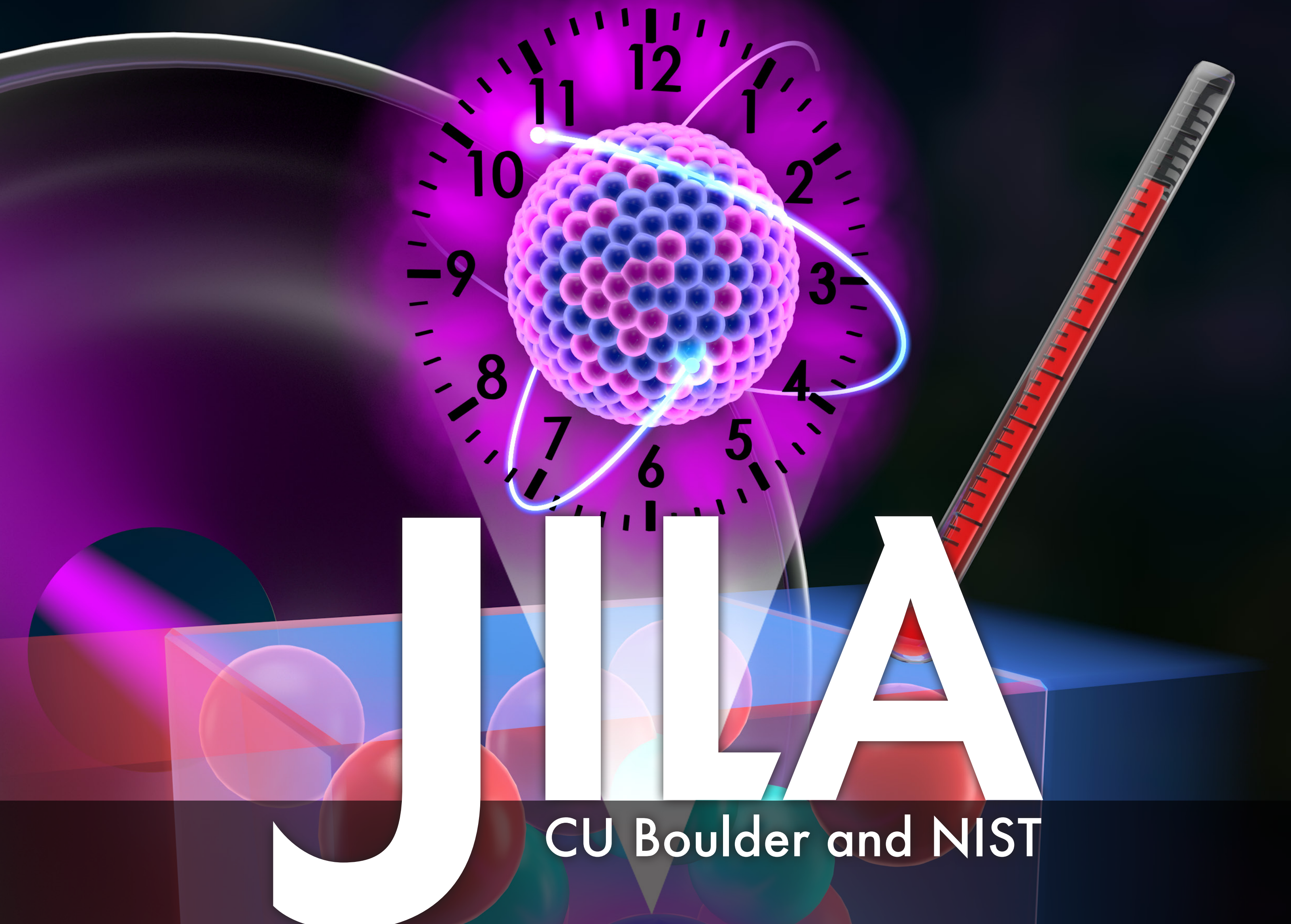
The event was structured around two 45-minute presentation intervals, allowing attendees to explore a broad array of projects and engage in meaningful discussions. The atmosphere was buzzing with excitement as presenters shared their findings and attendees networked, explored other projects, and enjoyed refreshments together.

Some of the notable presentations included: "Four-Wave Mixing for Efficient Generation of VUV Light" by the Becker and Kapteyn-Murnane groups, "Entanglement Generation in Multilevel Atomic Arrays Using Dipolar Interactions" by the Rey group, "Cavity Mediated Interactions Inside a Bragg Interferometer: From XYZ Spin Model to N-Body Interactions" by the Thompson group, and the "Th229 solid state nuclear clock" by the Ye group.




Throughout the event, attendees had the opportunity to catch up on their neighboring labs' research, fostering a collaborative and supportive atmosphere. The discussions were lively and engaging, with many students and researchers exchanging ideas and feedback.

JILA's PosterFest continues to be a cornerstone event. It's more than just a showcase of scientific advancements; it's a celebration of the collaborative spirit that defines JILA. Events like these play a crucial role in building a strong research community, where individuals can learn from each other, share their knowledge, and work together to push the boundaries of science.



# JILA

## CU Boulder and NIST

JILA was founded in 1962 as a joint institute of CU-Boulder and NIST. JILA is located at the base of the Rocky Mountains on the CU-Boulder campus in the Duane Physics complex.

JILA's faculty includes two Nobel laureates, Eric Cornell and John Hall, as well as two John D. and Catherine T. MacArthur Fellows, Margaret Murnane and Ana Maria Rey. JILA's CU members hold faculty appointments in the Departments of Physics; Astrophysical & Planetary Science; Chemistry; Biochemistry; and Molecular, Cellular, and Developmental Biology, as well as in the School of Engineering.

The wide-ranging interests of our scientists have made JILA one of the nation's leading research institutes in the physical sciences. They explore some of today's most challenging and fundamental scientific questions about quantum physics, the design of precision optical and x-ray lasers, the fundamental principles underlying the interaction of light and matter, and processes that have governed the evolution of the Universe for nearly 14 billion years. Research topics range from the small, frigid world governed by the laws of quantum mechanics through the physics of biological and chemical systems to the processes that shape the stars and galaxies. JILA science encompasses eight broad categories: Astrophysics, Atomic & Molecular Physics, Biophysics, Chemical Physics, Laser Physics, Nanoscience, Precision Measurement, and Quantum Information Science & Technology.

To learn more visit **jila.colorado.edu**

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