# JILA Light & Matter

Summer 2012

## The Anniversary Issue

# RNA Folding: The Rest of the Story

$Mg^{2+}$ ions (blue) help RNA molecules fold by neutralizing negative charges in the RNA. It's easier for RNA to capture $Mg^{2+}$ ions when ion concentrations are higher.

Credit: The Nesbitt group and Brad Baxley , JILA

The Nesbitt group has been investigating RNA folding since the early 2000s. The group's goal has been to gain a detailed understanding of the relationship between structure and function in this important biomolecule. One challenge has been figuring out how unfolded RNA molecules assume the proper three-dimensional (3D) shape to perform their biological activities. To accomplish this, the researchers have shown how biologically active RNA is able to neutralize negative charges that end up in close proximity to each other after folding into a 3D structure.

To understand how RNA folds, the Nesbitt group makes small pieces of RNA that contain one site critical to 3D folding and studies how this site (called a tetraloop) lightly binds, or docks, to a receptor region. The docking and undocking process is somewhat like fastening and peeling apart molecular Velcro.

The Nesbitt group immobilizes a single piece of RNA on a slide. The RNA contains both a single tetraloop and its receptor. The group uses a laser to observe how the RNA structure changes in response to changing concentrations of ions such as magnesium ($Mg^{2+}$) or sodium ($Na^+$). For several years, the group has known that RNA stays folded longer with increasing amounts of $Mg^{2+}$. The conventional explanation for this observation was that the $Mg^{2+}$ ions were neutralizing the negative charges on the RNA tetraloop, making it easier for the tetraloop to dock into the receptor and stay that way.

Former graduate student Julie Fiore, graduate student Erik Holmstrom, and Fellow David Nesbitt recently looked at the folding process in greater detail. They confirmed that as the concentration of $Mg^{2+}$ ions increases, the RNA tetraloop stays folded longer. But, when they raised the temperature (which tends to unfold RNA), they found that the tetraloop didn't unfold as much if more $Mg^{2+}$ was present. This result suggested that there was more to the story of $Mg^{2+}$ ion and RNA folding than just neutralizing the negative charges in the RNA molecule.

According to Holmstrom, the rest of the story goes like this: When there's more $Mg^{2+}$ around, it gets easier for the RNA tetraloop to pull $Mg^{2+}$ ions close to it. That's why it folds better — it's simply much easier to get the exact number needed for it to fold and be able to link to its docking site.

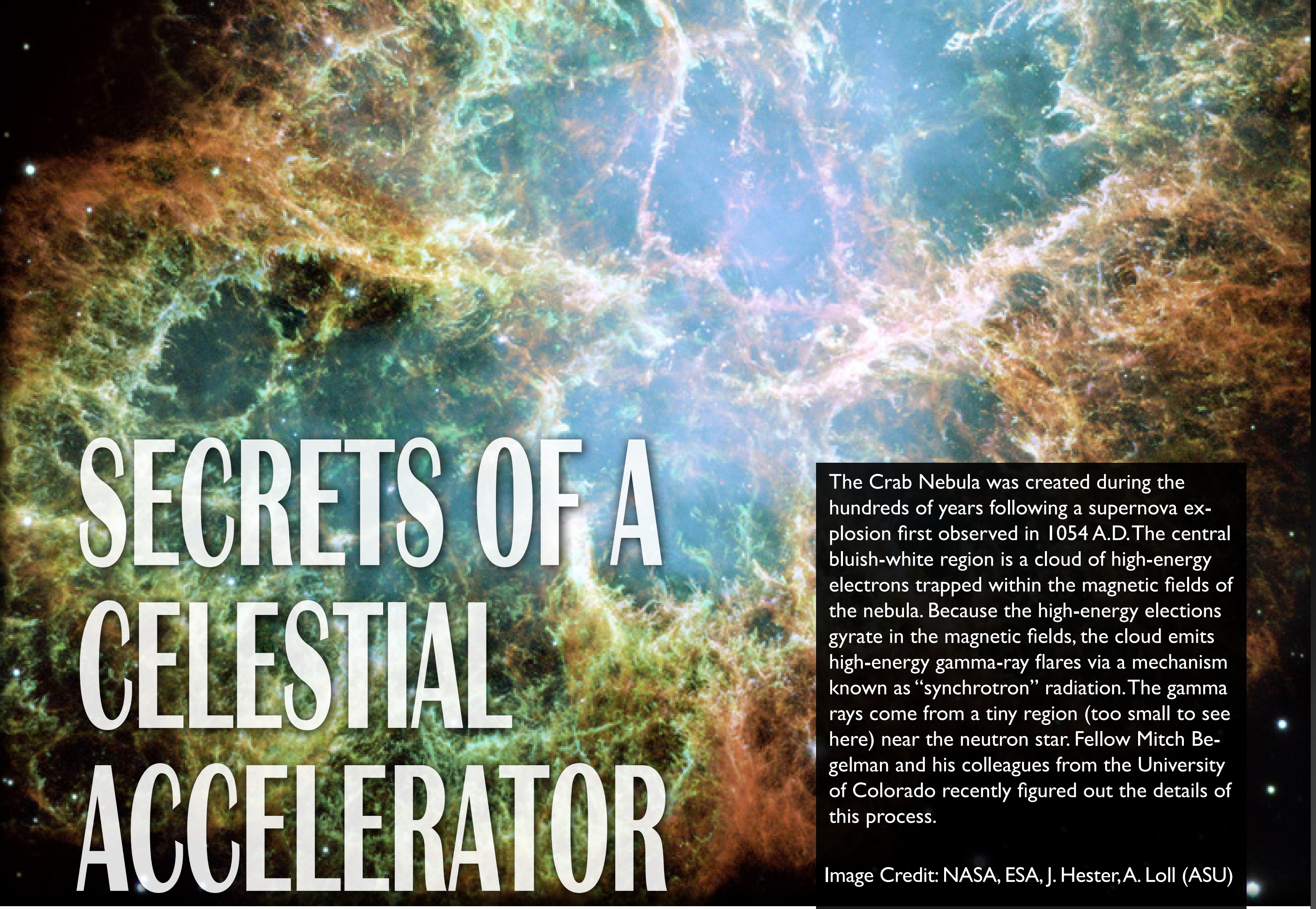
It turns out that the RNA tetraloop must capture about two $Mg^{2+}$ ions to be able to dock the tetraloop into the receptor. When there's a lot of $Mg^{2+}$ around, the capture process gets easier. It gets easier because taking a few $Mg^{2+}$ away from a solution with lots of ions doesn't change the amount of disorder, or entropy, in the system very much. That's because there are still too many $Mg^{2+}$ ions left in the solution for them to be able to move farther apart.

In the future, the Nesbitt group plans to investigate whether the effects on the tetraloop of increasing the concentration of $Na^+$ are the same as with $Mg^{2+}$. Preliminary results suggest there may be some differences: Higher concentrations of $Na^+$ may also make it easier to pull $Na^+$ into the tetraloop. However, the $Na^+$ may actually change the structure of the tetraloop — something that doesn't appear to happen with higher concentrations of $Mg^{2+}$ ions.

References

Julie L. Fiore, Erik D. Holmstrom, and David J. Nesbitt, *Proceedings of the National Academy of Sciences* **109**, 2902–2907 (2012).

Erik D. Holmstrom, Julie L. Fiore, and David J. Nesbitt, *Biochemistry* **51**, 3732–3743 (2012).



# SECRETS OF A CELESTIAL ACCELERATOR

The Crab Nebula was created during the hundreds of years following a supernova explosion first observed in 1054 A.D. The central bluish-white region is a cloud of high-energy electrons trapped within the magnetic fields of the nebula. Because the high-energy elections gyrate in the magnetic fields, the cloud emits high-energy gamma-ray flares via a mechanism known as "synchrotron" radiation. The gamma rays come from a tiny region (too small to see here) near the neutron star. Fellow Mitch Begelman and his colleagues from the University of Colorado recently figured out the details of this process.

Image Credit: NASA, ESA, J. Hester, A. Loll (ASU)

On Earth, people use enormous linear accelerators and synchrotrons for such purposes as high-energy physics experiments, chemical composition analysis, and drug research. Linear accelerators ramp up the speeds of electrons and other charged subatomic particles close to the speed of light. Synchrotrons also accelerate charged particles (in a circular track) that, when deflected through magnetic fields, create extremely bright high-energy light.

Both of these processes occur naturally inside the Crab Nebula. Throughout the nebula, linear acceleration processes boost electrons to very high energies. In one tiny area of the nebula, however, synchrotron processes also generate intense and focused beams of gamma rays. These beams are produced from particularly energetic electrons (traveling near the speed of light) that are also gyrating in a magnetic field. As the most energetic gyrating electrons calm down, they emit gamma rays with the highest energies produced anywhere in space by a synchrotron process.

The Crab Nebula's day-long gamma-ray flares were discovered by the space telescope AGILE in 2007 and confirmed by the Fermi telescope in 2010. By August of 2011, Fellow Mitch Begelman and his CU colleagues Dmitri Uzdensky and Benoît Cerutti had figured out how the flares were produced in the celestial linear accelerator. They were also able to explain why the flares had higher energies than expected.

In the energetic and chaotic environment of the Crab Nebula, multiple powerful linear accelerators ramp up the speed of electrons traveling along them — to close to the speed of light. These linear accelerators are produced by the annihilation of reversing magnetic fields, creating ideal conditions for producing synchrotron radiation. The magnetic fields lurch and twist throughout the center of the nebula, buffeted by winds produced by the pulsating neutron star (pulsar) at the center of the Crab Nebula. Inside the roiling environment of the nebula, the magnetic lines of force bump up against each other with their directions out of alignment.

When this happens, the reversing magnetic fields get weaker, allowing the accompanying electric field to get stronger. These rapid changes cause electrons funneled into this region to get even more energetic. And, as the electrons get more energetic, they are driven into a place where the magnetic field is quite small. There they can be accelerated to higher energies than was once thought possible. Eventually, the ultrahigh energy electrons calm down by releasing a powerful, but narrow, beam of gamma rays in just one direction.

Begelman and his colleagues believe that such gamma-ray flares are emitted continually from the central part of the Crab Nebula. However, we Earthlings can only "see" the ones that just happen to be aimed right at us or toward a space-based telescope.

Their new insights into the genesis of these gamma-ray flares from the Crab Nebula are helping Begelman and his colleagues to better understand similar space phenomena such as the high-energy jets produced by pulsar winds, gigantic black holes in the center of galaxies, or extremely energetic quasars known as blazars. The researchers are currently exploring the evolution of idealized simulations of these astrophysical phenomena. They recently produced four animations of current-driven instabilities such as those found in the Crab Nebula.

## References

Benoît Cerutti, Dmitri A. Uzdensky, and Mitchell C. Begelman, *The Astrophysical Journal* **746**:148 (2012).

Dmitri Uzdensky, Benoît Cerutti, and Mitchell C. Begelman, *The Astrophysical Journal Letters* **737**:L40 (2011).

# WAY FASTER THAN A SPEEDING BULLET

The interface between a gas and a solid is a remarkable environment for new investigations. Lots of fascinating chemistry takes place there, including catalysis. Catalysis is acceleration of a chemical reaction that is caused by an element like platinum that remains unchanged by a chemical reaction. For instance, platinum catalyzes the transformation of carbon monoxide (CO) into carbon dioxide ($CO_2$) in automobile catalytic converters. A better understanding of catalysis could improve the efficiency of manufacturing important chemicals as well as expanding our fundamental knowledge of chemistry.

The challenge for Fellow David Nesbitt and his group is figuring out how catalysis works at the molecular level. Such an understanding requires a detailed understanding of the interface between a gas and a solid.

Former research associate Joseph Roscioli, former graduate student Dan Bell, graduate student Dan Nelson, and Nesbitt came up with a nifty method for studying one gas/solid interface. They investigated the interface between a gas (hydrochloric acid, or HCl) and a solid gold-nanocrystal surface on mica. They fired a supersonic jet of cold HCl molecules (about 1–2 K) at a hot flat surface (about 500 K). The cold jet of gas traveled way faster than a speeding bullet before crashing into or bouncing off the surface.

For the experiment, the group shined an ultraviolet laser about 100 microns (millionths of a meter) above the gold surface. When the laser tickled the supersonic HCl molecules, the molecules lost an electron and became positively charged. This gentle process didn't affect the molecules' speed. However, it allowed the researchers to use an electric field to coax the ions into going in a particular direction. The electric field also accelerated the charged molecules, or ions, so that when they struck a metal plate, they hit it with sufficient energy to liberate 1–10 million electrons.

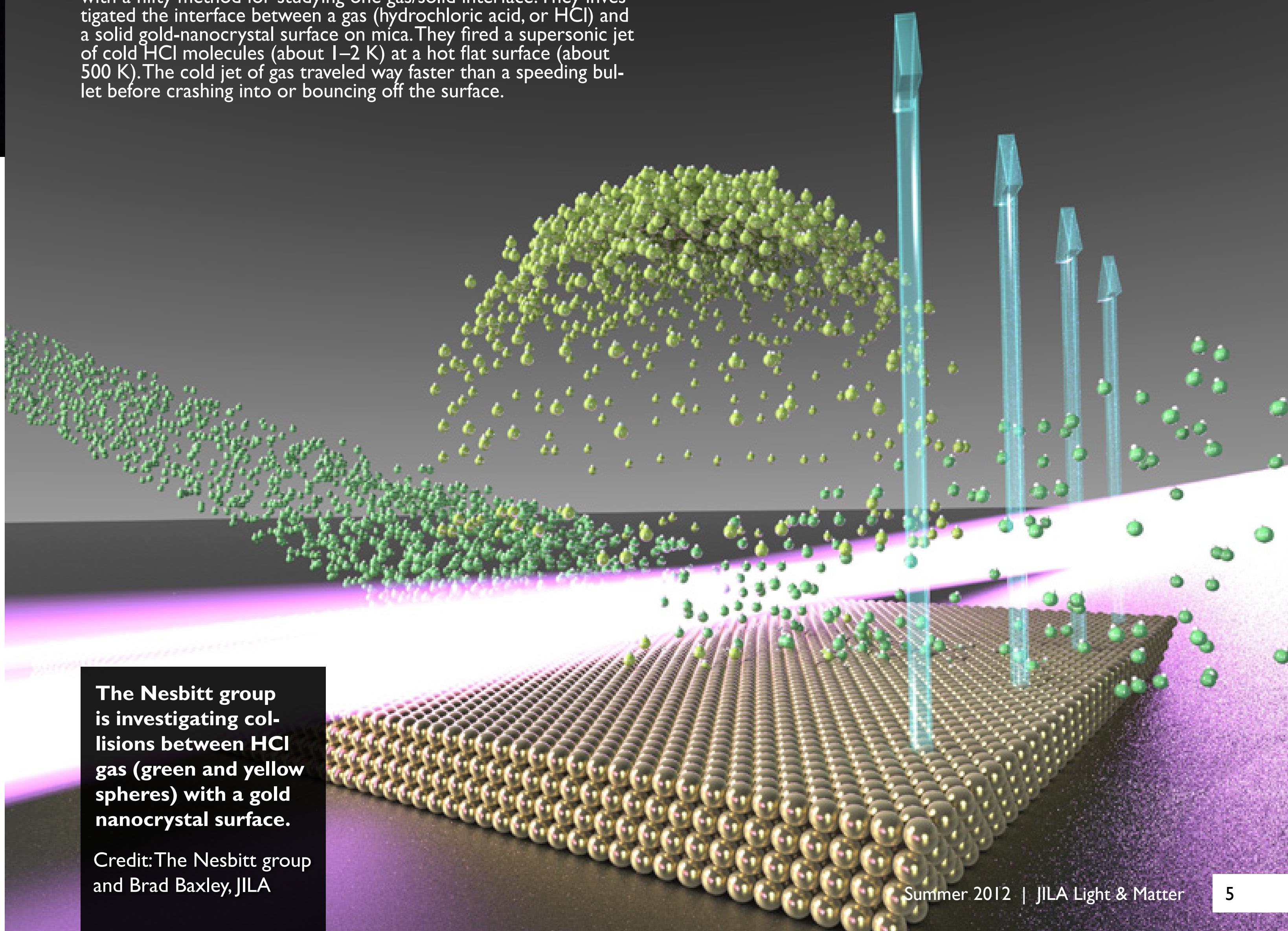
When the electrons hit a phosphor screen, they made sparks of light, which were recorded by a camera. The results of 10,000–20,000 laser pulses were then fed into a computer. The computer created a velocity map of the ions, which allowed the researchers to determine the location, relative speed, and temperature of the ions after they scattered off the gold surface.

The researchers discovered that about 70% of the HCl molecules "swam" around on the gold surface before lifting back off — at the same temperature as the gold surface (500 K). The remaining HCl molecules immediately bounced off the surface rotating furiously at a temperature of 1000 K.

In the future, the Nesbitt group plans to coat its gold surface with sulfur atoms, creating a forest-like surface. Next the group will chemically engineer the tops of the "trees" on this surface and investigate chemical reactions with carbon-containing molecules. The researchers hope to engineer collision experiments with various different molecules.

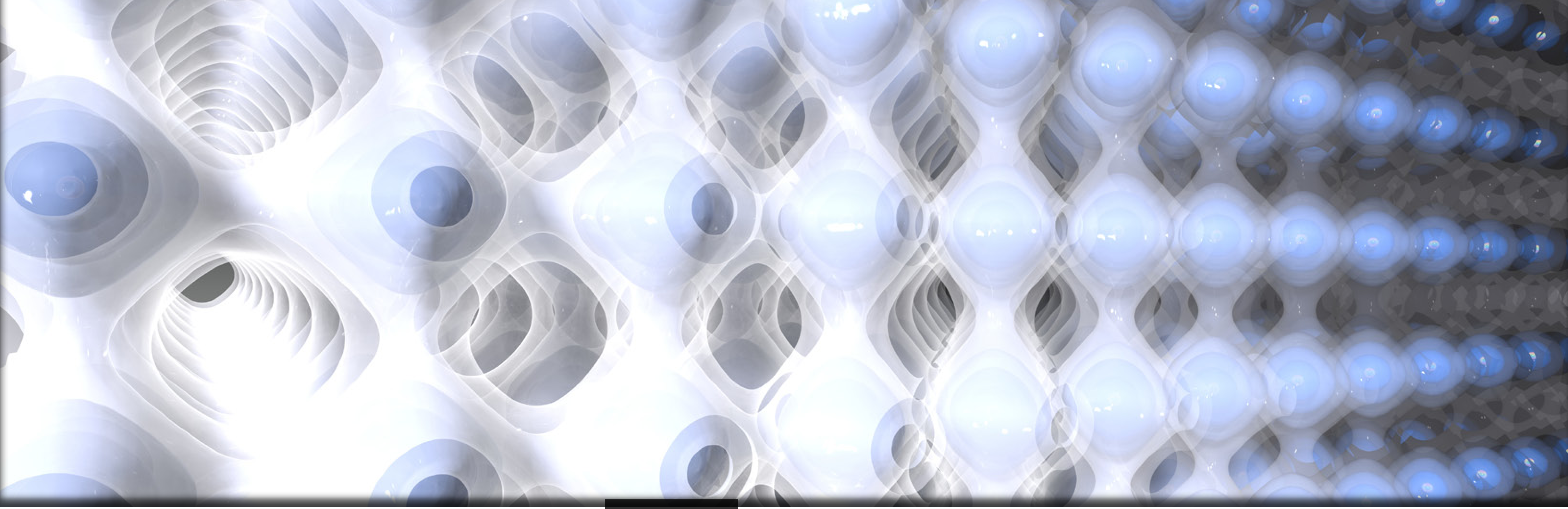
## Reference

J. R. Roscioli, D. J. Bell, D. J. Nelson, and D. J. Nesbitt, *Physical Chemistry Chemical Physics* **14**, 4070–4080 (2012).



**The Nesbitt group is investigating collisions between HCl gas (green and yellow spheres) with a gold nanocrystal surface.**

Credit: The Nesbitt group and Brad Baxley, JILA



Artist's conception of a three-dimensional optical lattice.

Credit: The Rey group and Brad Baxley, JILA

# NEW FLAVORS OF QUANTUM MAGNETISM

News Flash! The Rey group has discovered another good reason for using alkaline-earth atoms, such as strontium (Sr) or Ytterbium (Yb), in experimental quantum simulators. Quantum simulators are systems that mimic interesting materials or mathematical models in a very controlled way. The new reason for using alkaline earth atoms in such systems comes from the fact that their nuclei come in as many as 10 different magnetic flavors, i.e., their spins can be in 10 different quantum states.

When people normally think about magnetism, they often think of the two most common magnetic flavors: spin up and spin down. And, when the spins of billions and billions of iron atoms all line up in one of these two directions, the result is the familiar bar magnet.

But things are never so simple and straightforward in the quantum world. It's as if in addition to spin up and spin down in alkaline earth atoms, there were also eight more unique spin directions such as spin forwards, spin backwards, or spin diagonal. (Of course, in this case, the spin directions are just a convenient analogy for quantum spin states.)

The multi-flavored alkaline earth atoms have some real advantages in quantum simulation. Inside a simulator, a set number of alkaline-earth atoms with ten flavors can actually make the whole system get five times colder than the same number of atoms with only two flavors. This result was entirely unexpected.

Conventional wisdom said that a higher number of magnetic flavors in the atomic nuclei would cause the lowest-possible temperature of the system to be higher than that of a system with a lower number of magnetic flavors!

"I was so shocked when we first saw this, I spent a whole day trying to find the error in my calculation," said Kaden Hazzard, an NRC (National Research Council) postdoc with the Rey group.

But, Hazzard hadn't made a mistake. The Rey group has proved conventional wisdom wrong — and opened the door to some novel experiments with the quantum simulator in the Ye lab.

Since the simulator is already kept at ultracold temperatures, the newly discovered relationship of cooling to an increased number of spin states means that it should theoretically be possible to cool highly controlled atoms down to nano-Kelvin temperatures. Such temperatures are needed to directly observe quantum magnetism in action.

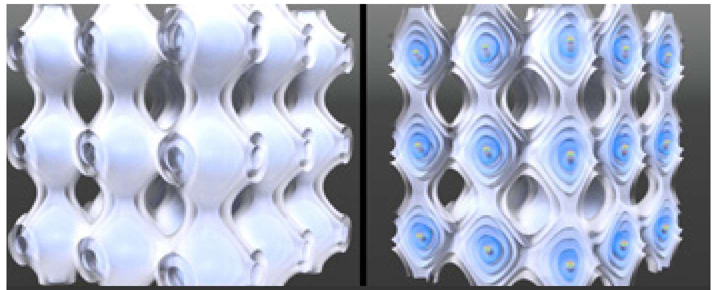
"When you get alkaline earth atoms really cold, that's when you can see the most interesting physics," Hazzard said.

Because of the unique properties of alkaline earth atoms, scientists will soon be able to study what happens when different magnetic flavors interact and produce spin ordering. For instance, as a simulator gets colder, random flavors may take on their preferred spin direction at regular intervals inside a three-dimensional lattice, like the ones shown here.

This behavior will set the stage for the creation of antiferromagnets and spin liquids. In antiferromagnets, random magnetic flavors assume their preferred directions at utralow temperatures of below 1 nK. Spin liquids can occur when interactions or geometrical factors frustrate the antiferromagnetic order, causing it to "melt." In the resulting spin liquid, spins can fluctuate through different states even near a temperature of absolute zero.

Antiferromagnets and spin liquids have not yet been observed in the laboratory. But, the Rey group's predictions give hope that they soon may be seen soon in simulators using alkaline earth atoms.

The work on the new flavors of quantum magnetism was done by Hazzard, Fellow Ana Maria Rey, and their colleagues Victor Gurarie and Michael Hermele from the University of Colorado. Research associates Salvatore Manmana and Gang Chen as well as colleague Adrian Feiguin of the University of Wyoming worked with Hazzard and Rey on foundational work for the new theory. The Rey group is continuing its investigations of quantum magnetism with colleagues in Germany and Austria.



Looking inside a three-dimensional optical lattice. Each lattice site is occupied by one strontium atom. The nucleus of each atom has 10 possible quantum spin states.

Credit: The Rey group and Brad Baxley, JILA

References

Kaden R. A. Hazzard, Victor Gurarie, Michael Hermele, and Ana Maria Rey, *Physical Review A* **85**, 041604 (R) (2012).

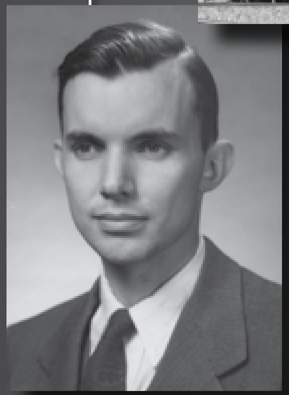
Salvatore R. Manmana, Kaden R. A. Hazzard, Gang Chen, Adrian E. Feiguin, and Ana Maria Rey, *Physical Review A* **84**, 043601 (2011).

# THE FIRST 50 YEARS

**1958**

Lewis Branscomb, Mike Seaton, and Richard N. Thomas attend the annual meeting of the International Astronomical Union in Moscow, where they began to develop ideas for an institute that would bring together atomic physics and astrophysics.

NBS Director, Allen Astin, convinces Lewis Branscomb to keep the joint venture as part of NBS.



**1962**

CU is selcted as the home for the new joint institute.

On April 13, 1962, the Joint Institute of Laboratory Astrophysics (JILA) is officially founded.

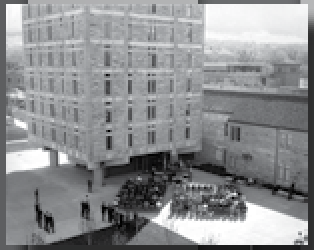
**1964**

JILA By-laws are drawn up, discussed and adopted.

**1966**

JILA B-Wing is completed.

**1967**



JILA tower construction is completed.

**1969**

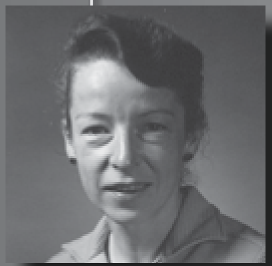
James Faller's idea for a lunar laser-ranging experiment is realized when astronauts Neil Armstrong and Edwin Aldrin place a retro-reflector on the Moon on July 21, 1969.

**1972**

Jan Hall and Dick Barger make a hundredfold more accurate measurement of the wavelength of light.

**1974**

Katharine Gebbie becomes JILA's first woman fellow.



**1975**

Douglas Gough and Juri Toomre found the field of helioseismology.

**1976**

Addendum to the original 1962 MOU expands the scope of JILA activities.

**1977**

NBS changes the name of its JILA division from the Laboratory Astrophysics Division to the Quantum Physics Division (QPD).

**1979**

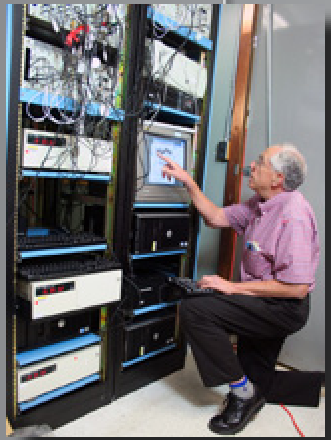
JILA has 2000+ scientific publications.

**1982**

Jan Hall and NBS colleagues measure the speed of light, paving the way for the official adoption in 1983 of a revised definition of the standard meter.

**1983**

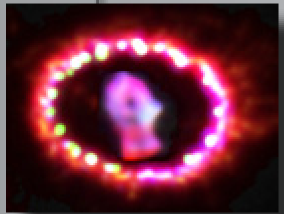
Judah Levine and colleagues at NBS begin tackling the modernization of time transfer.



**1987**

JILA turns 25.

Supernova 1987A appears in the sky. Dick McCray will study it for the next 25 years.



**1988**

S-Wing is completed.

NBS becomes the National Institute of Standards and Technology (NIST).

**1991**

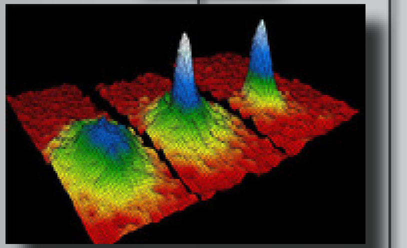
JILA astrophysicists gain observing time on the new Hubble Space Telescope.

**1992**

Self-study raises issue of giving priority to hiring women and minorities.

**1995**

Carl Wieman, Eric Cornell and their collaborators observe the world's first Bose Einstein Condensate (BEC).

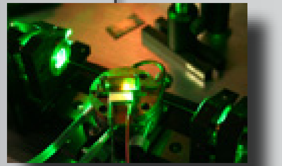


**1996**

Fellows celebrate their 500th Fellows meeting.

**1999**

Jan Hall, Steve Cundiff, Jun Ye create an optical frequency comb from a femtosecond mode-locked laser.



**2001**

Carl Wieman and Eric Cornell receive Nobel Prize in Physics.

**2003**

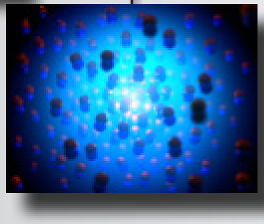
Deborah Jin and her team create the world's first fermionic condensate.

**2005**

Jan Hall receives the Nobel Prize in Physics for his contributions to the development of the laser.

**2008**

Jun Ye and Deborah Jin create world's first ultracold molecules, opeing the door to an entire new field of ultracold chemistry.



**2011**

Three Fellows are selected by President Obama to fill key leadership positions in science and technology. Carl Wieman becomes Associate Director for Science in the White House Office of Science and Tecnology Policy, Margaret Murnane is appointed as a member of the President's Committee on the National Medal of Science, and Carl Lineberger becomes a member of the National Science Board.

**2012**

50th anniversary of founding of JILA.

X-Wing construction is completed.

# THE SECRET LIFE OF MAGNETS

The Kapteyn/Murnane group and scientists from NIST Boulder and Germany have figured out how the interaction of an ultrafast laser with a metal alloy of iron and nickel destroys the metal's magnetism. In a recent experiment, the researchers were able to observe how individual bits of quantum mechanical magnetization known as "spin" behaved after the metal was heated with the laser. The researchers included newly minted Ph. D. Chan La-O-Vorakiat, former research associates Stefan Mathias and Mark Siemens, graduate student Emrah Turgut, Fellows Henry Kapteyn and Margaret Murnane, NIST Boulder's Tom Silva, and colleagues from the University of Kaiserslautern, Peter Grünberg Institute, and University of Denver.

Metals like iron and nickel get magnetized because the spins of all their individual atoms get lined up and point in the same direction. Since every spin is like a tiny bar magnet (with a north and south pole), when trillions and trillions of spins get lined up, the resulting magnet is large enough for people to see — which is why it's possible to explore how magnetism works in the everyday world. Many scientists, including those who did this experiment, investigated magnets when they were children. That's one reason they were interested in figuring out exactly what was going on with the individual atoms inside a magnetized metal.

In the magnetized alloy of iron and nickel, both kinds of atoms act like members of a marching band moving in unison across a football field. Imagine that the spins of the iron atoms are the brass section, and the spins of the nickel atoms are the woodwinds.

When a laser strikes this "marching band," at first something very strange happens: The brass players (iron spins) start walking off in random directions, but the woodwinds (nickel spins) keep marching in unison. Soon, however, the nickel spins also start walking off in random directions, and the entire magnetic band is in disarray. The whole process takes about 240 quadrillionths of a second.

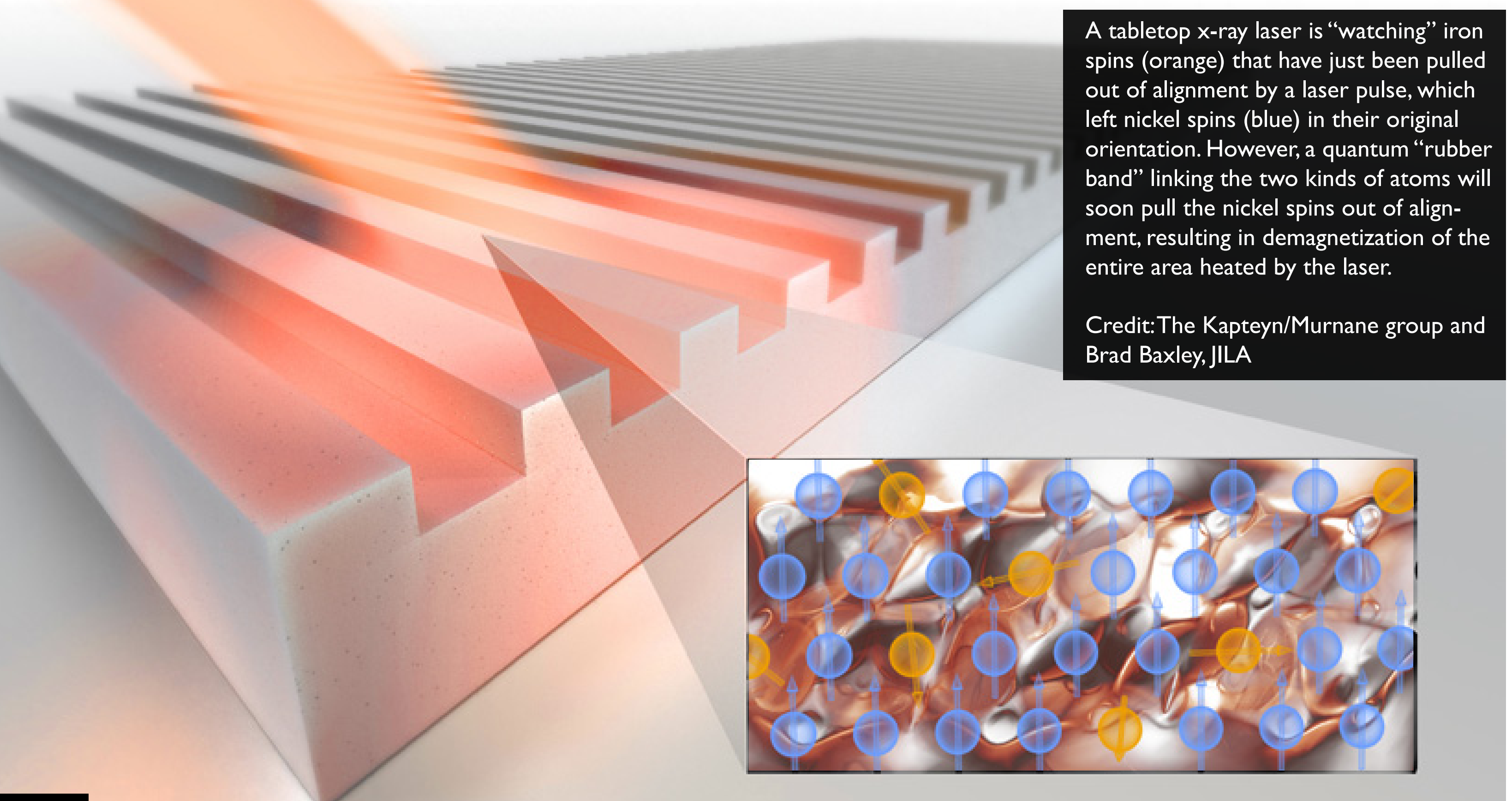
Here's what happens in detail. The iron spins likely "see" the ultrafast light more readily than the nickel spins (for reasons that are not yet completely understood). The light quickly heats up and randomizes the iron spins, which is why the brass players are the first ones to start wandering around aimlessly. However, the iron spins and the nickel spins are strongly linked by a special kind of rubber band called a quantum exchange interaction. Soon after the brass players head off in different directions, the exchange interactions kick in. Individual nickel spins get pulled out of alignment by the strong rubber bands connecting them to the iron spins that are already wandering aimlessly. And, once the brass players (iron spins) start wandering around, it takes only a few quadrillionths of a second for them to literally drag the nickel spins out of alignment.

The researchers discovered they could enhance the delay between the demagnetization of iron and nickel by adding copper atoms to their metal alloy. The dilution of the alloy with copper made the quantum exchange interactions (rubber bands) weaker. Because the rubber bands were weaker, it took longer for the iron spins to pull the nickel spins out of formation.

The researchers were able to figure out the details of the physics of demagnetization by watching what happened in response to the ultrafast laser pulse with a tabletop x-ray laser invented at JILA. The in-depth understanding of demagnetization gained through this investigation will be invaluable in the development of a new generation of magnetic data-storage devices.

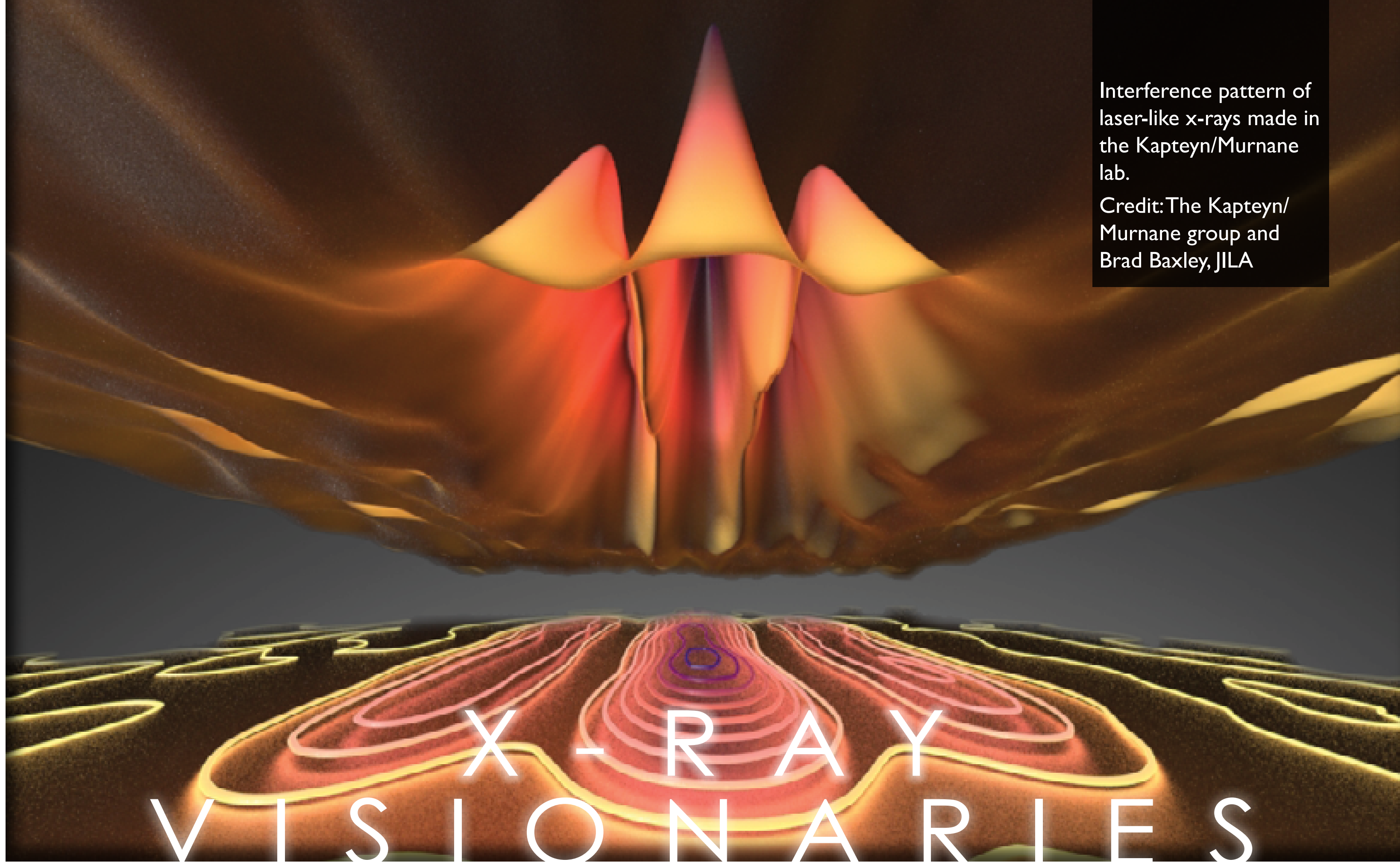
Reference

Stefan Mathias, Chan La-O-Vorakiat, Patrik Grychtol, Patrick Granitzka, Emrah Turgut, Justin M. Shaw, Roman Adam, Hans T. Nembach, Mark E. Siemens, Steffen Eich, Claus M. Schneider, Thomas J. Silva, Martin Aeschlimann, Margaret M. Murnane, and Henry C. Kapteyn, *Proceedings of the National Academy of Sciences* **109**, 4792–4797 (2012).



A tabletop x-ray laser is "watching" iron spins (orange) that have just been pulled out of alignment by a laser pulse, which left nickel spins (blue) in their original orientation. However, a quantum "rubber band" linking the two kinds of atoms will soon pull the nickel spins out of alignment, resulting in demagnetization of the entire area heated by the laser.

Credit: The Kapteyn/Murnane group and Brad Baxley, JILA



Interference pattern of laser-like x-rays made in the Kapteyn/Murnane lab.

Credit: The Kapteyn/Murnane group and Brad Baxley, JILA

# X-RAY VISIONARIES

The Kapteyn/Murnane group had the idea that it might be possible to produce bright, laser-like beams of x-rays using an ultrafast laser that fits on a small optics table. It was one of those "it probably can't be done, but we have to try" moments that motivated them to put together a team that includes the Becker theory group, and 16 collaborators in New York, Austria, and Spain. The lead scientist on this effort, Dr. Tenio Popmintchev, was most concerned about the possibility of an explosion, because to generate x-rays at high photon energies, the laser needed to be focused into a fiber containing high-density helium gas at pressures as high as 80 atmospheres. Eighty atmospheres is 80 times the normal air pressure at sea level.

The process the team used to convert laser light into x-rays is called high harmonic generation, or HHG. It produces x-rays when electrons are first plucked from atoms by the laser and then smashed back into their parent ions when the oscillating field of the laser reverses, like the motion of a boomerang. The atoms emit any excess energy gained by the electrons as higher-energy photons that are high harmonics of the original laser light. Harmonics of light are like the higher-frequency overtones heard when a piano key or guitar string is struck violently.

In a recent experiment reported in *Science*, the researchers showed that by using a laser with relatively long wavelengths (~4 microns), they could produce x-rays with short wavelengths (corresponding to high photon energies) that span from the ultraviolet into the soft x-ray region.

This is a surprising result. Scientists previously used visible laser wavelengths to produce laser-like beams of x-rays using HHG. However, this method limited the bright x-ray emission to lower energies in the x-ray spectrum. However, these x-ray waves could not add constructively and keep in step with the laser wave above a certain limit. In the new study, the x-rays emerged with a range of energies and wavelengths (or colors if our eyes could see x-rays). In theory, when the different x-ray wavelengths are added together, they could produce the fastest strobe light in existence — as short as 2.5 attoseconds. One attosecond is one quintillionth of a second, or $10^{-18}$ s.

Such short bursts of light will make it possible to capture the fast dance of electrons and atoms inside molecules or materials with nanometer resolution in thick samples in three dimensions. This capability should allow scientists to understand the limiting speeds of electronics, energy harvesting, catalysis, or data storage. Until now, such questions could only be explored by large and expensive x-ray facilities.

In the future, it may be possible to generate higher energy x-rays from lasers, which would improve the crispness of medical x-rays, making it possible to use a pencil-thin x-ray beam instead of a broad beam (like those from light-bulbs). The technology may even allow scientists to produce even faster x-ray bursts — measured in zeptoseconds. A zeptosecond is one sextillionth of a second, or $10^{-21}$ s. This is the time scale of things that happen inside the nucleus of an atom! For an idea how fast this is, it takes light 350 zs to travel the width of a hydrogen atom. Zeptosecond x-ray laser pulses will allow researchers to take an almost leisurely stroll through the quantum states of matter.

The 20 researchers involved in this complex project included senior research associates Tenio Popmintchev and Agnieszka Jaron-Becker, graduate students Ming-Chang Chen, Dimitar Popmintchev, and Susannah Brown, former research associate Paul Arpin, Fellows Andreas Becker, Margaret Murnane, and Henry Kapteyn as well as their colleagues from the Vienna University of Technology, Cornell University, and Universidad de Salamanca.

Reference

Tenio Popmintchev, Ming-Chang Chen, Dimitar Popmintchev, Paul Arpin, Susannah Brown, Skirmantas Alisauskas, Giedrius Andriukaitis, Tadas Balciunas, Oliver Mücke, Audrius Pugzlys, Andrius Baltuska, Bonggu Shim, Samuel E. Schrauth, Alexander Gaeta, Carlos Hernàndez-Garcia, Luis Plaja, Andreas Becker, Agnieszka Jaron-Becker, Margaret Murnane, and Henry Kapteyn, *Science* **336**, 1287–1291 (2012).

# New Beginnings

In Roman mythology, Janus is the god of beginnings and transitions, of doors and bridges, as well as endings and time. The aptly named Janus supercomputer at CU is bringing new opportunities in high-performance research computing to JILA. Since the fall of 2010, JILA groups directed by Andreas Becker, Mitch Begelman, Chris Greene, Ana Maria Rey, and Juri Toomre have used more than 25 million CPU hours on Janus for research in astrophysics and AMO physics.

Janus was assembled in October of 2010 at a site near 38th and Arapahoe in Boulder. Testing of the new supercomputer began in 2011 during the month of January, which was also the origin of Janus' name. CU's first supercomputer was specifically designed for massive parallel processing. It contains 16,415 total cores (CPUs) and can perform 814 trillion floating-point operations per second. The entire operation uses 500 kW of electricity; about 10% of that amount is used for air conditioning.

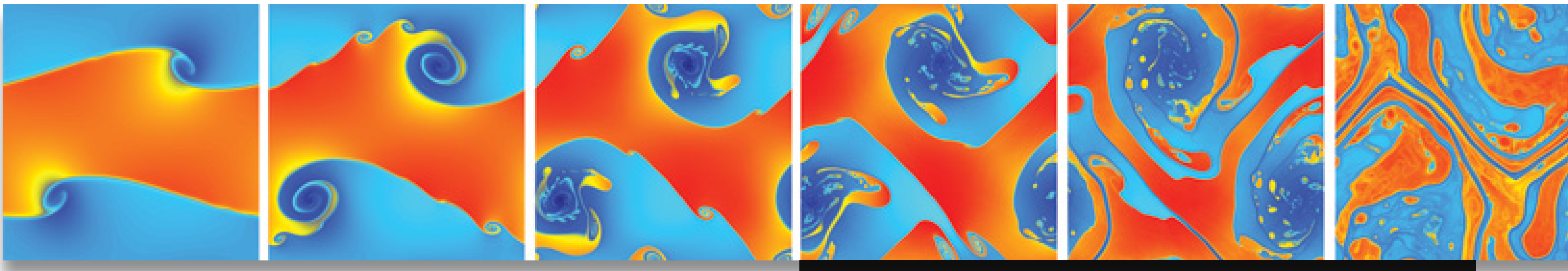
"It's astonishing how CU's research computing infrastructure has gone from nearly zero two years ago to this," said Peter Ruprecht, who recently left JILA to join the Research Computing Group. "Janus is like having 100 JILIAC clusters with a petabyte of storage along with a high-speed research network across campus that connects to these resources."

The Janus Supercomputer

Credit: Joel Frahm and Zebula Sampedro, University of Colorado

It's no wonder JILA's astrophysicists and AMO theorists are united in singing Janus' praises. During the summer of 2011, Graduate student Greg Salvesen (Begelman group) used 5 million CPU hours on Janus to complete a fluid instability analysis for his Master's thesis project. Using the ATHENA code, he explored Kelvin-Helmholtz (K–H) instabilities in jets emitted by black holes and other astrophysical objects. This kind of instability is the reason flags wave. It occurs when two fluids flow past each other and something "tickles" the interface, causing waves to form. Both fluids can become very turbulent. Salvesen was interested in instabilities that form at the boundary between a jet and the material around it.

"Jets are propelled incredible distances through space," Salvesen explained. "We expect them to be subject to K-H instability, but we don't see them break up." For his project, he studied energy transfer due to the K–H instability and attempted to pin down the instability's fundamental nature. The progression of instabilities between a jet (orange) and its surrounding space (blue) is shown in the figure. Salvesen's project is the highest-resolution two-dimensional simulation ever done with ATHENA.

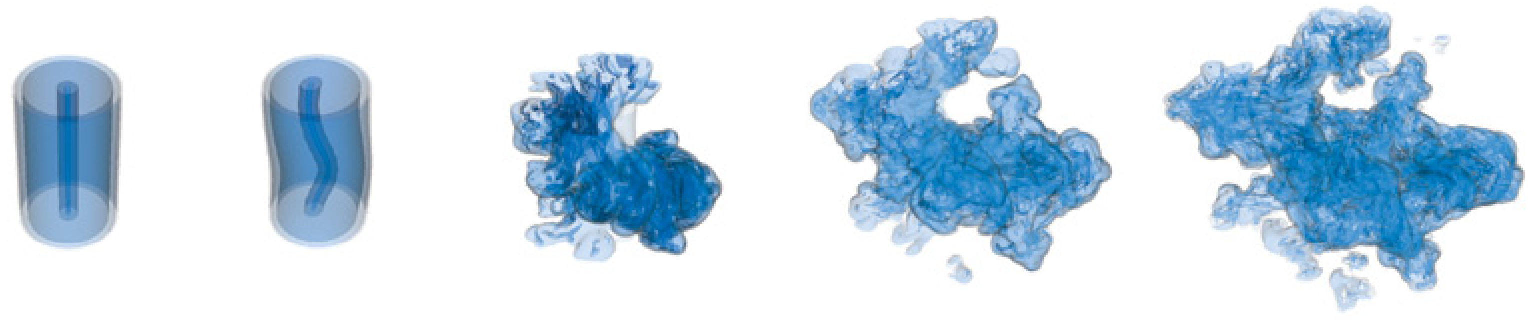


Kelvin-Helmholtz instability modeled by graduate student Greg Salvesen using the Janus supercomputer.

Credit: Greg Salvesen, JILA

Salvesen puts the research that Janus made possible in perspective. "This work would have taken roughly 150 years to complete on a MacBook," he said.

Postdoc Sean O'Neill (Begelman group) also used Janus to explore current-driven fluid instabilities. Current-driven instabilities are like K-H instabilities, but driven by flows of electrons that produce magnetic fields. They can travel at nearly the speed of light. Janus made it possible for O'Neill to study current-driven instabilities in the context of astrophysical flows, including relativistic jets and pulsar-powered systems such as the Crab Nebula. The figure shows the evolution of a current-driven instability that can occur inside a jet traveling close to the speed of light.



Current-driven instability modeled by postdoc Sean O'Neill using the Janus supercomputer.

Credit: Sean O'Neill, JILA

Because of O'Neill's work and Salvesen's K–H study, the Begelman group was the single largest user of Janus during the fall of 2011. The group has already secured another 4.9 million CPU hours on Janus for 2012.

After some initial difficulties in porting existing codes over to CU's new supercomputer, Toomre group members are now exploiting the capabilities of Janus as well. Graduate student Kyle Augustson is running detailed simulations of fluid dynamics in the interior of F-type stars, which are a little bigger and hotter than the Sun and have an unusual near-surface shear layer. Graduate student Ben Greer is looking at helioseismic data from the Sun obtained by the Solar Dynamics Observatory to analyze real subsurface flows and compare them with simulations. Graduate student Chris Chronopoulos is investigating magneto-rotational instabilities of the Sun. And, graduate student Nick Nelson is exploring the relationship of buoyant loops in the Sun's magnetic field to the boundary between the Sun's convection zone and its radiative interior.

In the AMO world, theorists are using Janus to explore the quantum world. Since early 2011, for example, postdoc Yujun Wang (Greene group) has relied on Janus for research on Efimov physics.

With Janus, he and his colleagues were able to show that the Efimov effect persists with dipolar atoms in an electric field. The atoms first studied were bosons capable of occupying the same quantum state. In the Efimov effect, three such atoms can stick together in an infinite number of quantum states, even though any two cannot form a molecule.

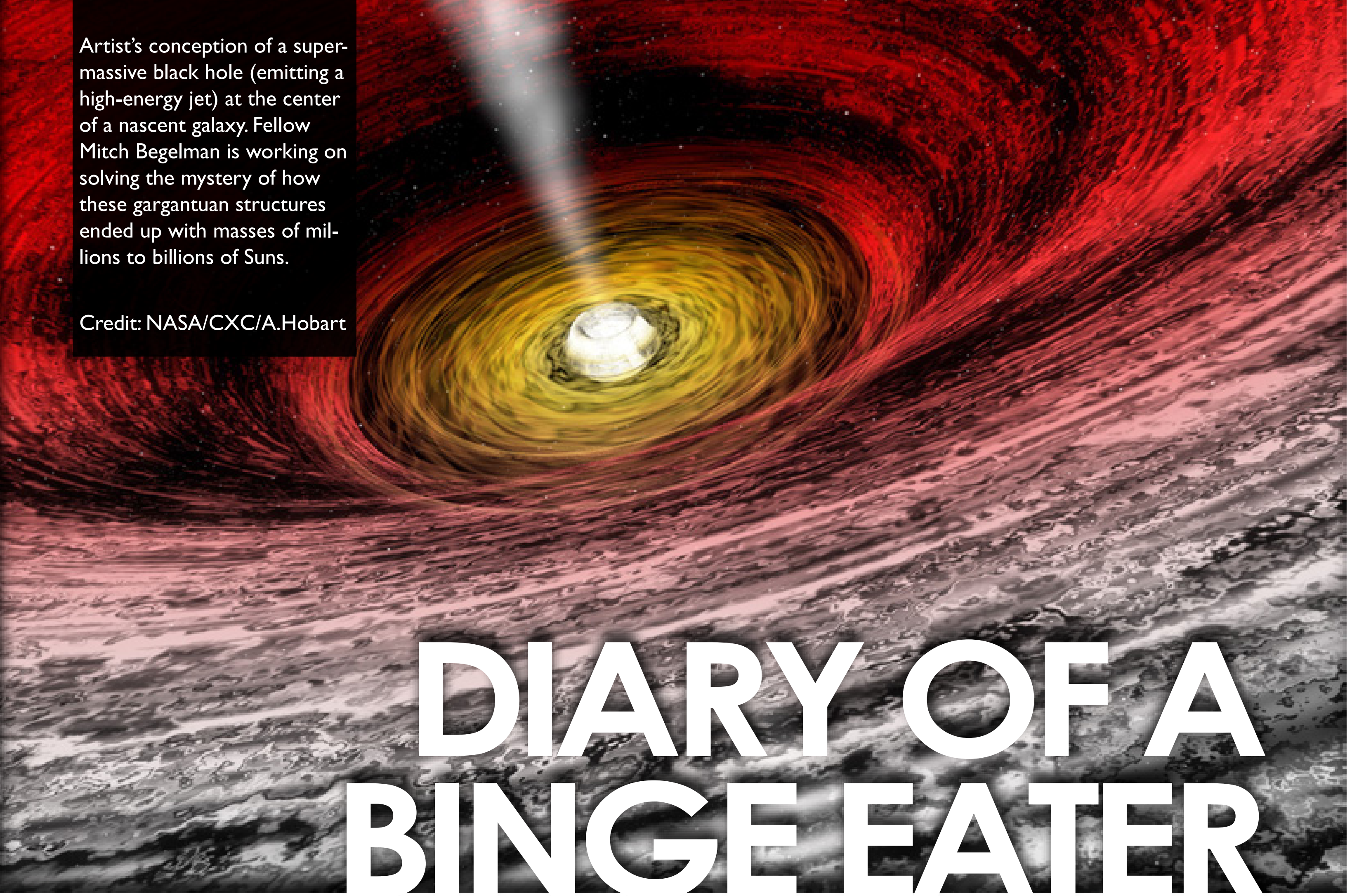
More recently, Wang has been exploring the strange behavior of fermions, which cannot occupy the same quantum state, under the same conditions inside a Bose-Einstein condensate where Efimov trimers form. Janus is a critical part of this research, which is revealing unexpected new physics.

"Janus is so powerful," Wang said. "Janus takes just a few hours to do the same calculations that used to take a few months at JILA."

Postdoc Salvatore Manmana (Rey group) is reaping similar advantages from using Janus in his studies of quantum simulation, quantum magnetism, and superconductivity. He is working to predict the behavior of atoms in an experimental quantum simulation underway in the Ye and Jin groups. "Janus is helping me stay one step ahead of them," remarks theorist Manmana.

Janus is helping graduate student Hongcheng Ni do something no one else in the Becker group has ever done: model a weakly bound helium dimer ($He_2$) in four dimensions. Ni is studying the time it takes for information about the charge interactions between two electrons to be transferred from one to the other. So far, he has used 150,000 CPU hours on this problem.

Despite its recent contributions to JILA research, Janus isn't competing with JILA's cluster computers. "Janus was designed to fly through CPU-intensive parallel calculations, but it can't handle the large-memory or disk-intensive jobs needed for such applications as quantum chemistry calculations," Ruprecht said.



Artist's conception of a supermassive black hole (emitting a high-energy jet) at the center of a nascent galaxy. Fellow Mitch Begelman is working on solving the mystery of how these gargantuan structures ended up with masses of millions to billions of Suns.

Credit: NASA/CXC/A.Hobart

# DIARY OF A BINGE EATER

Fellow Mitch Begelman and his colleagues came up with the idea of quasistars to explain the origin of the supermassive black holes found at the center of most galaxies. According to Begelman, quasistars formed when massive amounts of gas were funneled into the center of protogalaxies. This prodigious amount of gas collapsed directly into black holes without forming stars. The resulting black holes grew rapidly by sucking in matter from the great envelopes of gas still surrounding them. This process released enough energy to puff up quasistars, which then radiated light (like stars). The quasistars evaporated after about a million years. However, in that amount of time, the "seed" black holes inside of them could only have acquired masses of about a hundred thousand Suns.

However, the black holes at the center of most galaxies today have masses of millions to billions of Suns. Something must have happened after the quasistars disappeared to cause the seed black holes to grow 10 to 100,000 times bigger.

Begelman recently explored a couple of intriguing ideas about what could have caused the black holes to rapidly increase in size. First, he wondered if conditions in nascent galaxies could recreate quasistars, which efficiently grew black holes while they lasted. However, his analysis showed that it would be impossible to come up with the huge reservoir of gas needed to recreate a quasistar.

Begelman next explored brief episodes of "binge eating" by the seed black holes left behind by the quasistars. He discovered that if the seed black holes were not too massive, it would be possible to force-feed them from a relatively small envelope of gas that was regularly replenished when more gas fell into the galactic center. During a period of force-feeding, the black hole could grow very rapidly as the gravity of the entire galaxy forced matter into it.

Before long, however, energy (in the form of jets) would spew out of the black hole and blow away the envelope. With smaller black holes, most of this gas would be trapped by the gravity of the galaxy. The trapped gas would eventually fall back into towards the black hole and cause the envelope to reform. This process would initiate another period of binge eating.

As the black hole got larger, however, it would fling more and more gas away fast enough to escape the galaxy. Even so, as long as some of the far-flung gas fell back in, episodes of force-feeding/binge eating continued. However, once the black hole grew large enough to fling the entire envelope out of the galaxy, it stopped growing.

The day came when the supermassive black hole literally threw away its next meal. Around the same time, any gas remaining inside the galaxy was forming millions, perhaps even billions of stars. As more stars appeared, it became even less likely that sufficient gas would ever reach the center of the galaxy to feed the now truly monstrous black hole.

What's intriguing about the force-feeding model is that it may help explain an observed correlation between the size of a central supermassive black hole and the size of the galaxy surrounding it. The mass of a central black hole is equal to 0.1% of the mass of the core galaxy. It is also proportional to the fourth power of the speed of the core stars in the central bulge. The feedback mechanism implicit in the force-feeding model may provide an explanation why the appearance of billions of stars in the galactic core correlates with the cessation of black hole growth.

Reference: Mitchell C. Begelman, *The Astrophysical Journal* **749**:L3 (2012).

# MOLDING A STAR SYSTEM OVER 50 MILLION YEARS

Giant planets form inside a disk of gas and dust orbiting a new star. At first, gravitational interactions between the disk and the planets will keep planetary orbits circular, according to Fellow Phil Armitage. But, once the disk begins to disperse, things get very interesting.

Over millions of years, x-rays emitted by the central star evaporate the protoplanetary disk until it eventually disappears. Just before it disappears, the disk becomes thin enough that its gravitational interactions can no longer keep unstable planetary systems in check.

Once they're freed from the grip of the disk, giant planets can turn violently unstable because they have formed rapidly and often very close together. Interactions and collisions among them can send gas and ice giants rocketing into their star, change the shape and inclination of their orbits, or knock them out of the star system. The most energetic interactions also affect the stability of rocky planets nearer to the star as well as the planetoids and debris found out beyond the planet-forming regions. In short, the violent interactions set off by disk clearing appear to be chiefly responsible for the final blueprint of a star system.

Recently Armitage and Nickolas Moeckel of Cambridge University's Institute of Astronomy modeled planet-disk and planet-planet interactions during disk clearing and through 50 million years of planetary system evolution. They discovered that the evolution of planetary systems is complex. Sometimes, there are phases in which massive planets orbit within peculiar gaps, such as the one shown in an artist's conception (below) of exoplanet candidate LkCa 15 b, the youngest planet ever found. LkCa 15 b was discovered with two 10-meter Keck telescopes on the Big Island of Hawaii.

Other times, giant planets will form inside the disk without gaps. And, nearly a third of systems with multiple giant planets will form stable resonant chains as the disk evaporates. These resonant chains protect the system against the most violent interactions. With fewer, if any, violent interactions, it likely that (1) most of the giant planets will survive (in orbits that remain close to circular), (2) three or four terrestrial planets (also in near circular orbits) will survive, and (3) the system will retain a large disk of dust and other debris in orbits beyond those of the giant planets.

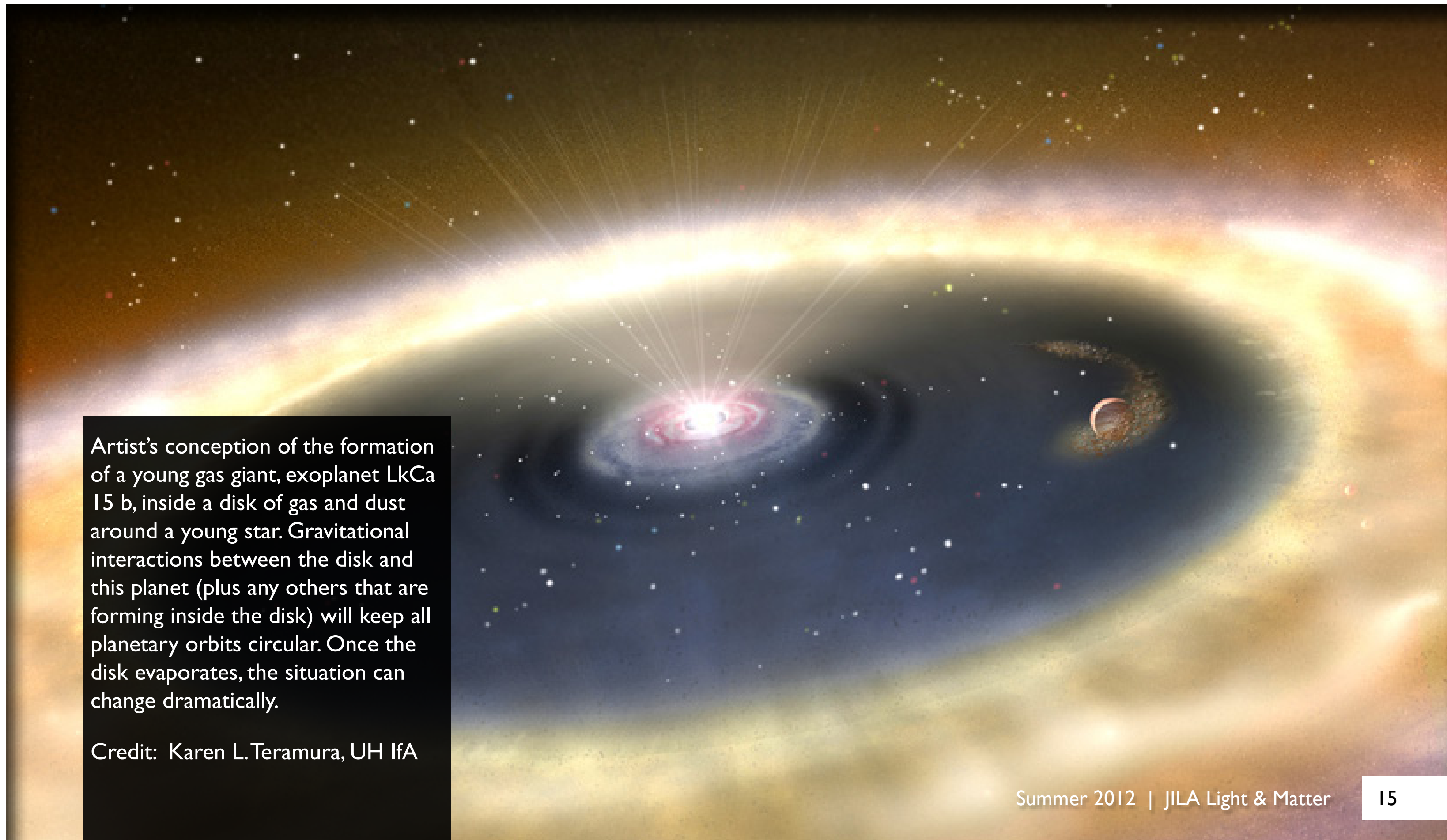
Moeckel's and Armitage's new simulation sheds some light on the layout of the Solar System, with its four gas and ice giants and four terrestrial planets, all in near circular orbits. But, the new simulation doesn't tell the whole story of the evolution of the place we call home. Fifty million years of Solar System evolution can't account for the relatively puny debris disk (known as the Kuiper Belt) orbiting the Sun out beyond the planet Neptune.

Armitage says that the event responsible for putting the Kuiper Belt on a crash diet occurred after 700 million years of Solar System evolution. That's when Uranus and Neptune moved out into their present orbits and interacted with the then much-larger Kuiper belt. The outward movement of the two planets hurled comets and asteroids every which way. Some flew out into space and others bombarded the Moon, Earth, Mars, and the moons of the giant planets.

This kind of late bombardment, which resulted in the Kuiper Belt becoming a mere shadow of its former self, actually appears to be quite rare. In earlier work, Armitage showed that the presence of a large outer disk of dust and debris in a star system is predictive of the presence of inner rocky planets like our Earth.

Reference

Nickolas Moeckel and Philip J. Armitage, *Monthly Notices of the Royal Astronomical Society* **419**, 366–376 (2012).



Artist's conception of the formation of a young gas giant, exoplanet LkCa 15 b, inside a disk of gas and dust around a young star. Gravitational interactions between the disk and this planet (plus any others that are forming inside the disk) will keep all planetary orbits circular. Once the disk evaporates, the situation can change dramatically.

Credit: Karen L. Teramura, UH IfA

# Alumni Profile:

# CHRIS MYATT

Chris Myatt is a successful entrepreneur who founded Precision Photonics Corporation in 2000, just three years after obtaining a Ph.D. in physics in 1997 under Carl Wieman. In 2009, Myatt became chief executive of a Precision Photonics spin-off company, MBio Diagnostics, Inc. In April of 2012, he sold Precision Photonics for $20 million — the same week he was a featured speaker at the dedication of JILA's new building known as the X-Wing.

Myatt is remembered in JILA as the senior graduate student who helped create the first Bose-Einstein condensate (BEC) in Carl Wieman's lab. "Eric's (Cornell) lab made the first BEC about a year earlier," Myatt says, "but we produced a much bigger condensate." Myatt has been thinking big ever since.

After completing postdoctoral work in quantum computing with Dave Wineland at NIST Boulder, Myatt spent a year at Research Electro-Optics, Inc. in Boulder working on thin-film coatings for mirrors, lenses, and other optical devices. He discovered he "loved making new instruments."

That passion provided the impetus for the founding of Precision Photonics in 2000. There the goal was to make devices that enabled lasers to perform better, e.g., to run hotter, but last longer in applications such as welding. He started the company with Kurt Vogel, who'd been a graduate student with Jan Hall and a postdoc at NIST Boulder.

"Kurt was the only guy I found in JILA on a Saturday evening to tell about making the first BEC in Wieman's lab," Myatt recalls. "Three years later, we decided to work together."

"After we started the company, we traveled all over, making presentations and securing our first orders. Then, we'd run back to the lab to get everything working," remembers Myatt with a smile.

Over time, Precision Photonics hired another six people who had been graduate students or postdocs at JILA or NIST. Then about seven years ago (in 2005), after the telecommunications fiber optics market had "tanked," and about 95% of Precision Photonics' customers went out of business. Myatt's solution was to try his hand at developing medical diagnostics equipment and sensors.

"We tried a few things, and they worked," he recalls, adding that the company quickly involved medical doctors in their development process. Their goal soon became the development of an instrument to diagnose HIV and test the efficacies of HIV therapies. By 2007, medical diagnostics became a separate division of Precision Photonics. Two years later, the company spun out MBio Diagnostics as a separate company. For three years, Myatt ran both companies.

Then in 2012, Myatt decided to sell Precision Photonics and invest in MBio Diagnostics. By then, MBio was making flu tests and hard at work developing a suite of tests for food safety. The company's first test in this area identifies shellfish toxins caused by algal or bacterial blooms in the waters where they breed.

In May of this year, Myatt headed off to Africa to check out a clinical study in Kenya of an MBio Diagnostics test for HIV and syphilis in pregnant women. "We'd like to bundle these tests together to make them more affordable," Myatt said, adding that MBio's goal is to make this suite of tests accessible even in small clinics all over the world.

"The whole process is totally exciting," Myatt says. "I'm also going to Europe to attend medical conferences and to let people know where we're going with medical testing and treatment."


Photo courtesy of Chris Myatt

Myatt's companies have come a long way in just twelve years, thanks in part to his wife Sally Hatcher, a lawyer trained at CU, who has helped him start and run both businesses. Myatt's own ties to CU also remain strong. He was especially pleased when JILA Chair Eric Cornell called early this year and asked him to speak at the dedication of the X-Wing. "I got to tell the story of a former JILA grad student who's done well," Myatt said.

Indeed, he has.

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