Quantum achievement unlocked: Scientists capture motion of molecules in action

By making the fastest beams ever produced by a compact X-ray instrument, ASU researchers create 'molecular movies,' with implications for the biomedical, semiconductor and renewable energy fields

By Joe Caspermeyer, ASU News
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Advancing X-ray science to ever greater heights in the 21st century is why a dedicated group of Arizona State University scientists continue to push and make a series of new firsts at their one-of-a-kind, compact X-ray science facility, called ASU X-Beams Labs.

Having solved their first protein structure, the ASU scientific team have been working to produce ever faster X-ray pulses — an achievement needed to successfully capture the motion of molecules of great biomedical, semiconductor, renewable energy or quantum material science importance in action.

Now, they have successfully completed the latest in a series of commissioning experiments, making the fastest X-rays beams and first time-resolved studies of quantum dynamics ever produced in a compact X-ray instrument.

With the latest results, and the continued development of the X-ray facility made possible by the National Science Foundation and private philanthropic support, the full capabilities of ASU's compact X-ray facility will officially begin as a national user facility for the worldwide scientific community.

"Our goal is to make a world class, compact X-ray facility which will transform the way we study proteins, perform imaging and control quantum processes," said Arvinder Sandhu, the director of ASU X-Beams Labs and professor of physics. "This result proves to the scientific community that we are officially open to conduct research experiments to advance our knowledge and understanding."

Making movies of atoms in motion

Any quantum material experiment places a premium on timing. Like using a high-speed camera to take a snapshot of a hummingbird’s wings, the compact light source parameters can be set by the scientists to control the precise timing of the X-ray pulses. Such precision and timing are needed to capture the dynamics of atoms at quantum scales.

How fast? In the X-ray research community, these so-called time resolved studies can capture movements so fast, they happen at the femtosecond level (15 millionths of a second). One second is to a single femtosecond as one second is to 32 million years, to better grasp the scale.

The latest ASU X-Beams demonstration was a critical test of the first of two instruments planned, a compact X-ray light source’s, or CXLS', ability to help ASU scientists see — using ultrafast X-ray pulses — the molecular dynamics of the quantum realm.

To make the experiment work, the researchers had to control the timing of both the X-ray beam and infrared laser to reach the sample at almost exactly same time, within one nanosecond of each other.

Their experimental target was 1T-tantalum disulfide (TaS2), a quantum material whose properties are not fully understood and ripe for the scientists to further explore. The 1T phase of TaS2 exhibits an electron rearrangement, that ripples like a stone thrown into a pond into charge density waves, making it an ideal candidate for next-generation electronics, including memory storage, sensors and topological quantum computing.

In the experiment, they heated the material with an 800 nanometer beyond the red light part of the visible spectrum, or near infrared laser pulse.

Once heated, the TaS2 atoms become instantly excited, and the heat changes the arrangement of atoms and electrons into the charge density wave. As this happens, the motion can all be captured by an X-ray pulse diffraction from the sample on to a downstream detector, creating “molecular movies” that are recorded much faster than the blink of an eye to understand these changes — well before heat or damage from the experiment alters the sample.

Quick draw gunslingers

Timing is everything and must be ultraprecise. If the X-ray beam hits the sample too early or too late for the IR laser — even nanoseconds off — the atoms of the sample would become excited and then go back down to their steady state before they could detect a change in the arrangement of the atoms.

It’s a little bit like the days of an Old West gunfight, only instead of trying to be the quickest draw, the gunslinger’s bullets would need to hit and deflect off each other in midair.

TaS2 was also chosen because it exhibits dynamic properties across different temperatures. The ultrafast laser pulse instantaneously melts the complex, shifting the TaS2 crystal pattern of atoms and electrons into a highly fluctuating state. At room temperature, TaS2 is in what is called a nearly commensurate charge density wave form, or a highly regular pattern of electron positions inside a

crystal lattice. This form can transition to a more irregular, or incommensurate phase, a more dissolved, higher energy state structure of the electron cloud under laser excitation.

“The X-ray measurements tracked the birth and growth of the new incommensurate phase, watching smaller microscopic domains merge into larger, coherent regions over a timeframe ranging from a few picoseconds to several nanoseconds,” said Samuel Teitelbaum, an ASU assistant professor of physics who is an expert on such measurements.

Capturing these transitions is critical to understand how a material would behave under heat stress, where it may ultimately fail, as anyone who has ever fried a circuit board knows. More importantly, this experiment is broadly representative of a whole class of experiments that can now be studied at ASU CXFEL facility.

A team of about 80 researchers have been working in tandem to make the CXFEL research facility a reality. Among them are laser experts, computer scientists, engineers and biologists.

“This achievement establishes CXLS as a unique femtosecond X-ray source for investigating ultrafast structural changes in quantum systems,” Sandhu said. “Our next objective is to study the time-resolved dynamics in protein crystals.”

“The proteins chosen for their next experiments will be of vital importance for their roles in human diseases or renewable energy applications," said Petra Fromme, who is the scientific director of this project.

Compact X-ray science heats up for broader applications

The ASU X-Beams Labs facility will ultimately house two instruments dedicated to new discoveries and become a beacon for the scientific community.

The construction of a second, more tunable and faster instrument, the CXFEL femtosecond laser, is well underway, and expected to be completed in 2028. The scientific team will continue to build upon the lessons learned from the CXLS and conduct more experiments to optimize the CXFEL.

“We are trying to make a unique facility that we are building in two phases,” Sandhu said. “It's a first-in-the-world kind of facility, to produce ultra-fast X-ray pulses that have applications in scientific, industrial or in medical settings. We are trying to make an X-ray laser at a university, in a very compact footprint. And this has not been done before.”

The ASU Core Research Facilities’ Machine Shop, part of the Instrument Design and Fabrication Core, supported the development of the CXFEL by custom fabricating thousands of components that went into CXFEL’s construction.

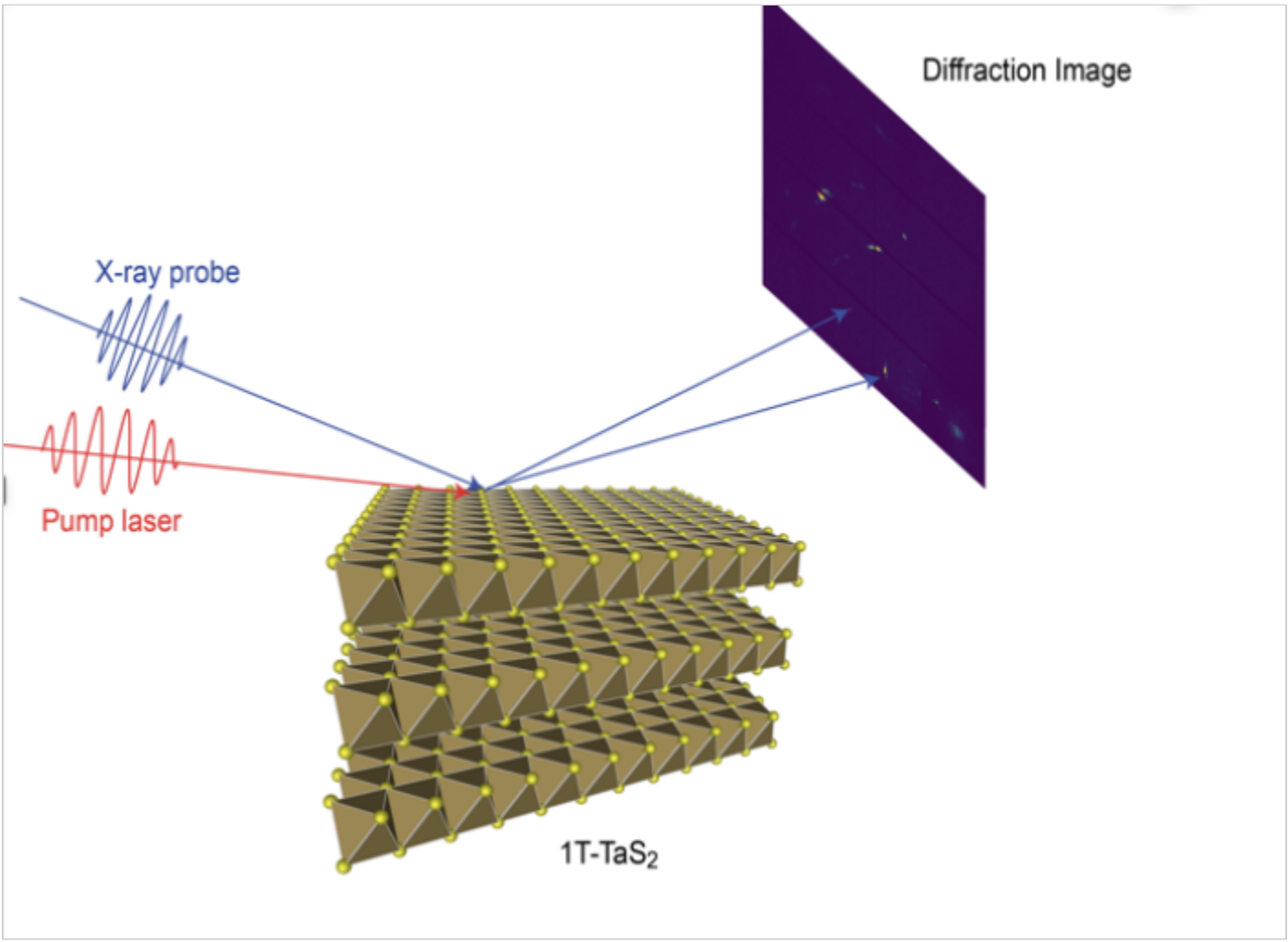
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Main image



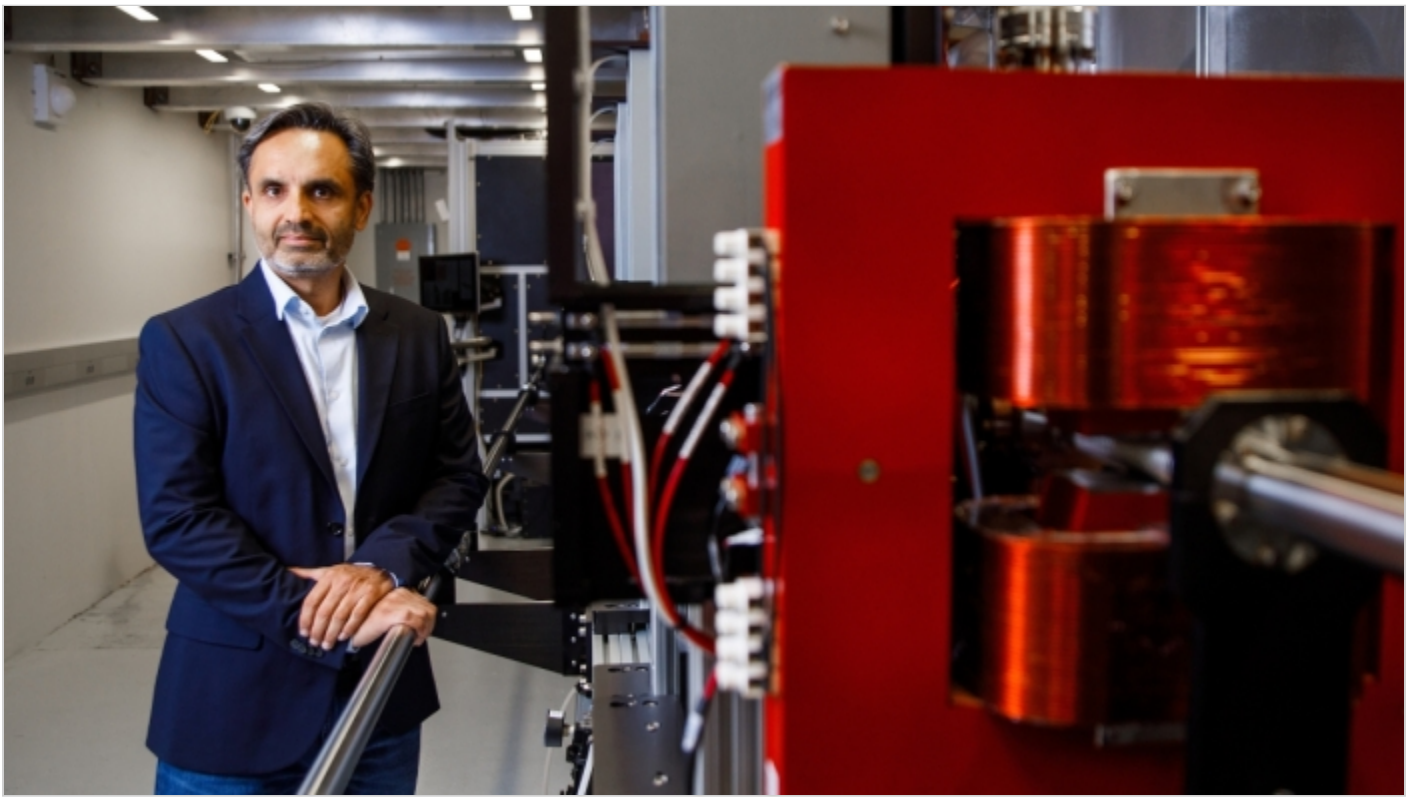
ASU electrical engineering graduate student Shreya Tripathi (left) and research scientist Aaron LaForge work in the hutch of the CXFEL Lab in Tempe. Photo by Samantha Chow/Arizona State University

Text image(s)



Graphic illustrating the first quantum experiment. Courtesy of Samuel Teitelbaum/ASU Department of Physics

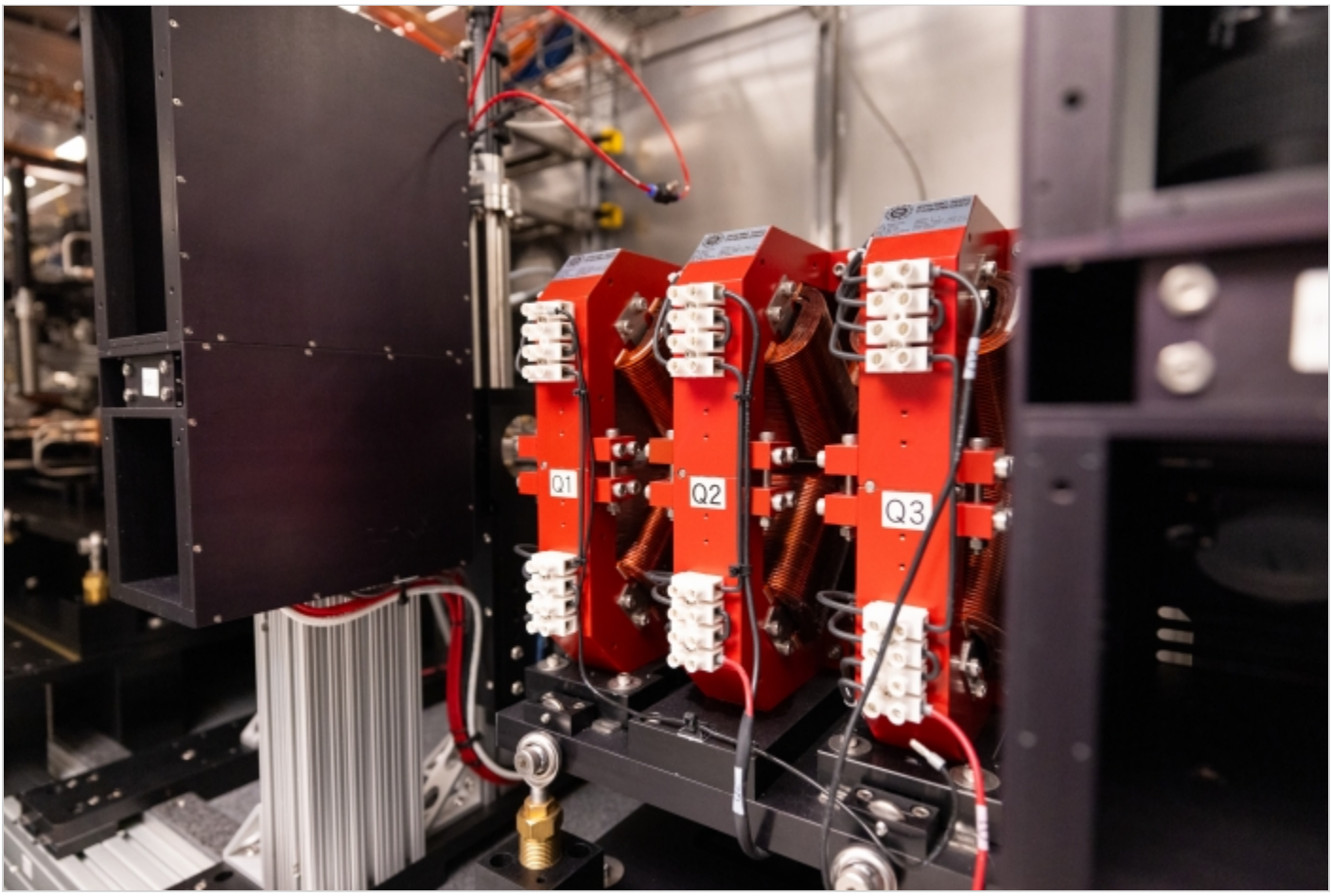
Gallery



“Our goal is to make a world class, compact X-ray facility which will transform the way we study proteins, perform imaging and control quantum processes,” said Arvinder Sandhu, the director of ASU’s CXFEL lab and professor of physics, posing next to the compact light source instrument at ASU's X-Beams facility. “This result proves to the scientific community that we are officially open to conduct research experiments to advance our knowledge and understanding.”



Research lab assistant Antonella Semaan observing the laser at the CXFEL Lab in Biodesign C.



A series of quadropole magnets (labeled Q1, Q2 and Q3) helps focus an electron beam used to generate ultrafast X-rays to perform the experiments.



ASU's CXFEL research team.