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Scientists blast iron with powerful X-rays, then watch its electrons rearrange

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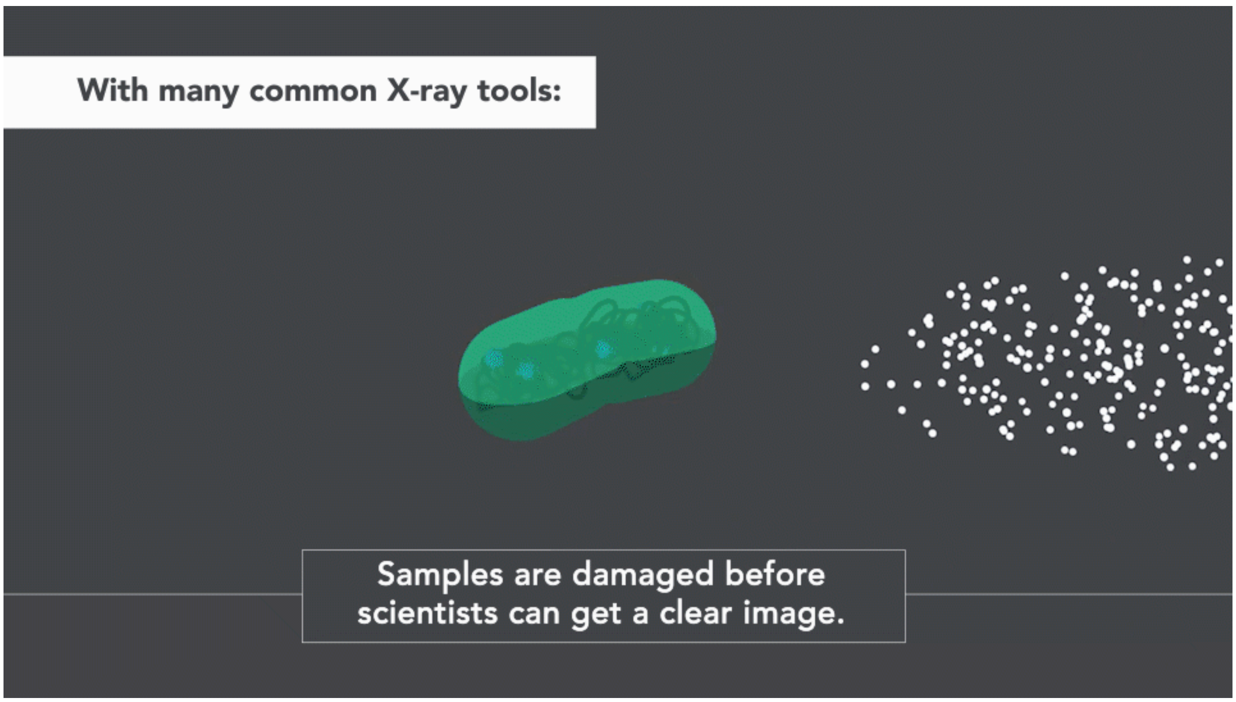


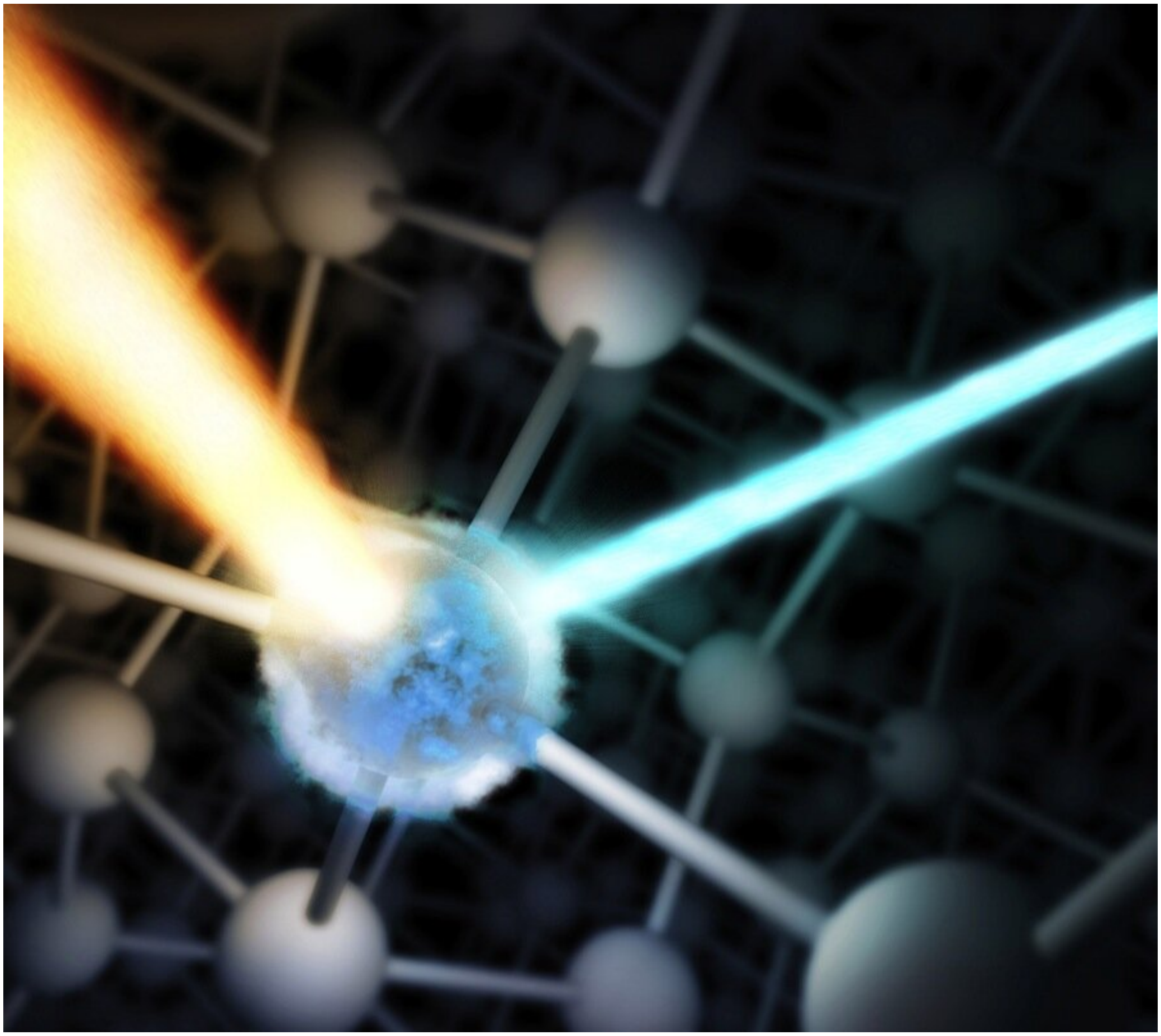
This animation depicts the "probe before destroy" imaging technique made possible by SLAC's Linac Coherent Light Source (LCLS) X-ray laser. On the left, longer-duration X-rays produced by more conventional research facilities can destroy or damage samples as they pass through them, which can make it challenging to capture high-quality images before damage occurs. The ultrabright, ultrashort X-ray pulses at LCLS, right, can collect the data needed to generate images in the instant before the sample is damaged, preserving the intact features of particles such as cells and viruses. Credit: Chris Smith/Olivier Bonin/SLAC National Accelerator Laboratory

X-ray free-electron lasers, such as the Linac Coherent Light Source (LCLS) at the Department of Energy's SLAC National Accelerator Laboratory, produce intense X-ray pulses that allow researchers to image biological objects, such as proteins and other molecular machines, at high resolution. But these powerful beams can destroy delicate samples, triggering changes that can affect the outcome of an experiment and invalidate the results.

To combat this, researchers use a method called probe-before-destroy, which allows them to collect precise information from samples in the instant before they're blown apart, generating images that preserve information on the molecular structure of biological particles such as cells, proteins and viruses. But until recently, it was unclear how much this method could be trusted for measuring the behavior of electrons, since powerful X-rays can affect electrons much faster than atoms. This could limit the technique's applicability to ultrafast chemical processes, such as those involved in catalysis.

Now, a team led by SLAC scientists Roberto Alonso-Mori, Dimosthenis Sokaras and Diling Zhu has found a way to get a precise idea of how to tune the X-ray beam to make sure electronic structure is not damaged before they measure it, providing higher confidence in the results of XFEL experiments. In a first, the team observed how electrons behaved in the first few femtoseconds, or millionths of a billionth of a second, after an an iron sample was blasted with intense laser pulses. Their results, recently published in *Scientific Reports*, demonstrate how specific properties of the X-ray beam, such as pulse length or intensity, can affect an atom's outermost electrons, which are the ones that participate in making and breaking bonds during chemical reactions.

The results will allow scientists to fine-tune pump-probe experiments, in which one laser pulse initiates a reaction in a sample and an X-ray pulse immediately measures the rearrangement of the electrons. By varying the time between the laser and the X-ray pulses, researchers can make a series of images and string them into a stop-motion movie of these tiny, fast motions, offering insights into light-activated chemical reactions.



This illustration shows an optical laser pulse (red) and an X-ray laser pulse (light blue) striking a sample. The use of synchronized laser pulses in the same experiment, known as the "pump-probe" technique, is common for SLAC's Linac Coherent Light Source X-ray laser, and a timing tool developed by an international team allows more precise measurements of the arrival time of laser pulses at LCLS. Credit: Greg Stewart/SLAC National Accelerator Laboratory

"These experiments are a key tool in our team's research program," Sokaras says. "The ability to carefully access the 'acceptable' range of LCLS conditions will allow us to perform pump-probe studies that are both reliable and unprecedented."

The team worked closely with the LCLS accelerator group to deliver even shorter than usual X-ray pulses to study how the electrons rearranged in the first few femtoseconds of the blast. A electron beam streak camera, the XTCAV, was instrumental in precisely measuring the length of the X-ray pulses.

Alonso-Mori says, "The study validates methods that have been used at LCLS in the past few years, settling the debate about whether they are valid or if the data collected is already altered in the first few femtoseconds by the intense X-ray pulses."

To follow up on this research, the team hopes to probe the electronic structure with even higher intensity, taking advantage of recent progress in shaping and controlling the X-ray beam.

"This can be used to further understand the initial stages of warm dense matter formation processes at XFELs," says Zhu, "which offer insight into the formation and evolution of planetary systems."

More information: Roberto Alonso-Mori et al. Femtosecond electronic structure response to high intensity XFEL pulses probed by iron X-ray emission spectroscopy, *Scientific Reports* (2020). DOI: 10.1038/s41598-020-74003-1

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