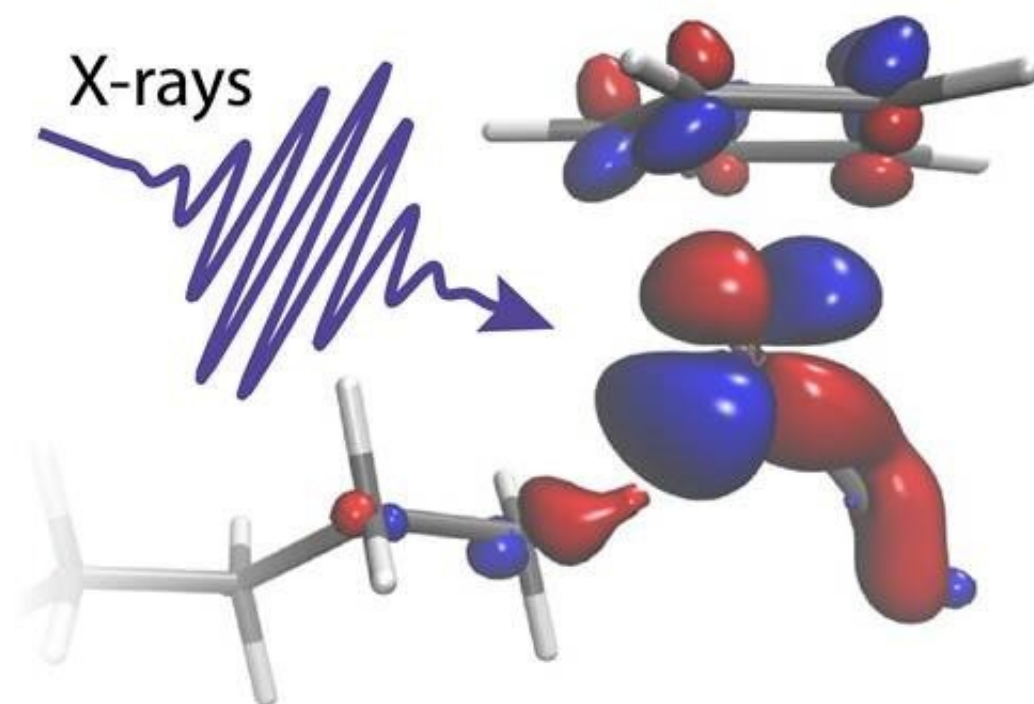


X-rays visualize how one of nature's strongest bonds breaks

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An X-ray flash illuminates a molecule. Credit: Raphael Jay

The use of short flashes of X-ray light brings scientists one big step closer toward developing better catalysts to transform the greenhouse gas methane into a less harmful chemical. The result, published in the

journal *Science*, reveals for the first time how carbon-hydrogen bonds of alkanes break and how the catalyst works in this reaction.

Methane, one of the most potent greenhouse gases, is being released into the atmosphere at an increasing rate by livestock farming as well as the continuing unfreezing of permafrost. Transforming methane and longer-chain alkanes into less harmful and in fact useful chemicals would remove the associated threats, and in turn make a huge feedstock for the [chemical industry](#) available. However, transforming methane necessitates as a first step the breaking of a C-H bond, one of the strongest chemical linkages in nature.

Forty years ago, molecular metal catalysts were discovered that can easily split C-H bonds. The only thing found to be necessary was a short flash of visible light to "switch on" the catalyst and, as by magic, the strong C-H bonds of alkanes passing nearby are easily broken almost without using any energy. Despite the importance of this so-called C-H activation reaction, it remained unknown over the decades how that catalyst performs this function.

The research was led by scientists from Uppsala University in collaboration with the Paul Scherrer Institute in Switzerland, Stockholm University, Hamburg University and the European XFEL in Germany. For the first time, the scientists were able to directly watch the catalyst at work and reveal how it breaks those C-H bonds.

In two experiments conducted at the Paul Scherrer Institute in Switzerland, the researchers were able to follow the delicate exchange of electrons between a rhodium catalyst and an octane C-H group as it gets broken. Using two of the most powerful sources of X-ray flashes in the world, the X-ray laser SwissFEL and the X-ray synchrotron Swiss Light Source, the reaction could be followed all the way from the beginning to the end. The measurements revealed the initial light-induced activation

of the catalyst within 400 femtoseconds (0.0000000000004 seconds) to the final C-H bond breaking after 14 nanoseconds (0.000000014 seconds).

"The time-resolved X-ray absorption experiments we performed are only possible at large-scale facilities like SwissFEL and the Swiss Light Source, which provide extremely bright and short X-ray pulses. The catalyst is immersed in a dense octane solution, but by taking the perspective of the metal, we could specifically pick the one C-H bond out of hundreds of thousands which is made to break," explains Raphael Jay, Researcher at Uppsala University and lead experimentalist of the study.

To interpret the complex [experimental data](#), theoreticians from Uppsala University and Stockholm University teamed up and performed advanced quantum-chemical calculations.

"Our calculations allow us to clearly identify how electronic charge flows between the metal catalyst and the C-H group in just the right proportion. We can see how charge flowing from the metal onto the C-H [bond](#) glues the two chemical groups together. Charge flowing in the opposite direction instead acts as a scissor that eventually breaks the C and the H atom apart," explains Ambar Banerjee, postdoctoral researcher at Uppsala University.

The study solves a 40-year-old mystery about how an activated [catalyst](#) can actually break strong C-H bonds by carefully exchanging fractions of electrons and without the need for huge temperatures or pressures. With their new tool to hand, the researchers next want to learn how to direct the flow of electrons to help develop better catalysts for the chemical industry in order to make something useful out of methane and other alkanes.

More information: Raphael M. Jay et al, Tracking C-H activation with orbital resolution, *Science* (2023). DOI: [10.1126/science.adf8042](https://doi.org/10.1126/science.adf8042).
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Provided by Uppsala University

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