

## Maths, Physics and Chemistry

# An eye-opening molecular explosion

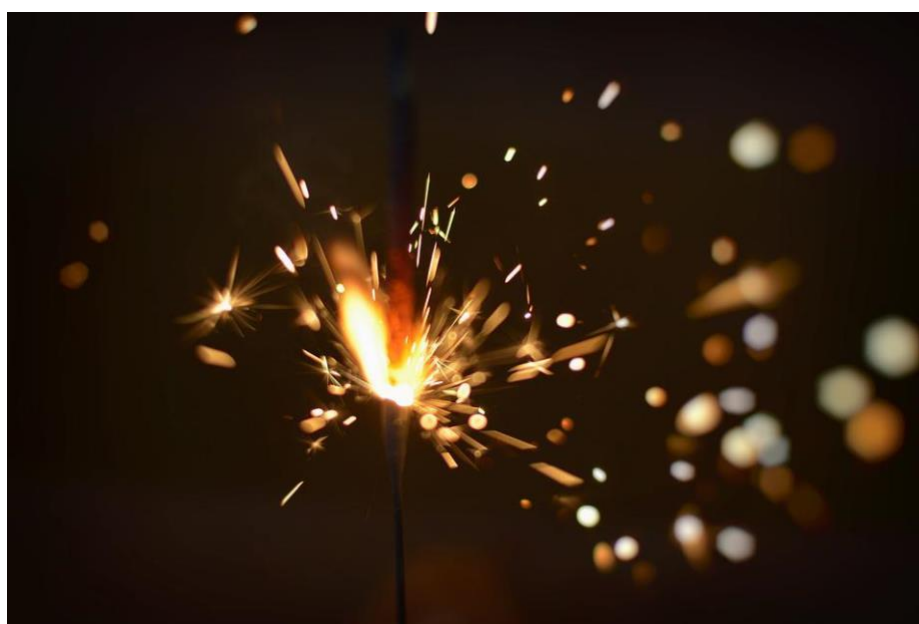
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### ABSTRACT

*Have you ever wondered how plants make use of sunlight to do photosynthesis? What happens inside your eye such that your brain can perceive your smartphone screen or your coffee cup? It turns out this is eventually triggered by tiny rearrangements of individual atoms. Our aim is to develop an imaging method sensitive enough to watch such processes in single molecules on the atomic level.*



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Many macroscopic processes that are part of our everyday lives have their origins in the tiniest motions: a molecule absorbs light, causing atoms to move by fractions of the distance between them, individual bonds to form or break. This determines whether a plant can transform carbon dioxide into oxygen, whether a solar cell can produce energy, whether a drug works against an illness, or your eye sees the world around you. Seeing and understanding the atomic world can thus allow us to get to the very bottom of things, and ultimately help us to understand, for example, how to make solar cells more efficient. However, this is not at all straightforward and there's a long way from seeing, to understanding, to developing applications! So let's start at the very beginning.

To look at something, one uses scattered light - such as that from your kitchen lamp for seeing your coffee cup at breakfast. If the wavelength of the light is sufficiently small - smaller than the object of interest - one can deduce its shape from it. For the microscopic world of molecules, the typical distances between atoms are in the range of about 1 Ångström (a tenth of a nanometer). This means one needs X-ray photons to inspect its details, i.e., to have sufficiently short wavelengths. Such photons can be generated by synchrotrons, accelerator-based light sources which generate X-ray light, and scientists routinely use them to image crystals of molecules with atomic resolution.

If we want to watch dynamic processes such as photosynthesis or eye vision though, there are three main challenges to overcome. First, atoms move

extremely fast. Typical movements happen within 10 to 100 femtoseconds (meaning a millionth of a billionth of a second). In order to watch atomic motion, we therefore need photon pulses (comparable to exposure times in photography) which are at least as short, otherwise the motion is just a blur. Then, the so-called photoexcitations (*i.e.*, the response to the absorbed light) happen in individual molecules. In a crystal, this means that not all of its many molecules behave in the same way at the same time. To observe molecular processes, we therefore want to look at individual molecules one-by-one. Lastly, the probability that an X-ray photon is actually scattered from an atom, such that one can look at it, is very low: at most, about 1 in 10 photons is scattered. The other 9 photons are absorbed by the molecule and induce radiation damage, which usually means blowing the molecule to pieces. The latter is very bad news if one wants to study the intact structures. But it turns out that this (usually unwanted) explosion of the molecule can be a real eye-opener!

In our work, we deliberately blow up our molecules with super-intense and super-short X-ray pulses. Such light pulses are extremely difficult to produce. They require usage of a less widely available, X-ray free-electron laser facility, for example the European XFEL. After triggering a very rapid and “clean” explosion of the molecule, we measure the speed, direction and mass of all fragments which splat on our detector. The forces between the ions during the explosion are dominated by Coulomb repulsion,

giving a direct link back to the molecular structure just before the explosion. The conditions in our experiment are chosen such that only one molecule interacts with each X-ray pulse – an important prerequisite to examine single molecules at a time.

So far, we’ve demonstrated that this tool can take a high-resolution snapshot of a molecule – but this is only the beginning, and there are still many avenues to explore in the future! These first images show a planar, two-dimensional molecule, but our data contain all the information about the third dimension as well. Moreover, we can look at correlations: if one atom moves in a certain direction, we can deduce what the other ones do. And, last but not least, the exposure time with our X-ray pulses is so short that we can use them to not only take photographs, but also to record movies of molecular motion in the future.

As a next step, we want to challenge the method further, for example by testing how large the molecules can be, and whether we can image more complex structures. We also need to better understand how to look at and interpret all of the recorded multidimensional data. We expect these results to be a stepping stone for using Coulomb explosion imaging at existing and upcoming free-electron lasers around the world. Our results are eye-opening with respect to the inspected molecule, but as well to the remaining challenges for our experimental method.