SibFU Researchers come up with X-ray scissors to cut molecules selectively

A research team from Siberian Federal University and Institute of Physics (Federal Research Center, Krasnoyarsk Scientific Center SB RAS predicted a new physical phenomenon — recoil-induced molecular dissociation in hard-x-ray photoionization. The recoil effect is caused by electronic and photon intermolecular momentum transfer. In particular, the researchers forecasted that recoil experienced by a hydrogen molecule during the absorption of an X-ray photon and the emission of a photoelectron leads to a break in the chemical bond of the hydrogen molecule at photon energies greater than 5 keV. The research article is published in the peer-reviewed journal Physical Review A.

> *‘The recoil effect can be observed on the example of the recoil of a canon when it shoots a missile (fig. 1A). This effect is a consequence of the fundamental law of conservation of momentum (or in other words, the quantity of motion) and is fundamentally manifested by the Compton effect (the Nobel Prize in Physics awarded in 1927), the Mössbauer effect (the Nobel Prize in Physics awarded in 1961), and laser cooling methods for atoms and molecules (several Nobel Prizes).*
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> *We studied the recoil effect during the photoelectron emission within the photoionization of a molecule by X-ray radiation. At moderate photon energies, the recoil effect is caused by momentum exchange between the atom and the electron emitted from it. Depending on the direction in which the electron flies out (fig. 1B and 1C), the transfer of the electron momentum to an atom leads to excitation of vibrations and rotations in the molecule. We have already observed both of these effects within the experiment using synchrotron radiation,’* said **Dr Faris Gelmukhanov**, one of the authors of the study, chief researcher at the Laboratory of Nonlinear Optics and Spectroscopy (Department of Science and Innovation).

To study the recoil effect, the researchers conducted rigorous quantum calculations, which resulted in vibrational and rotational states near the dissociation threshold ED caused by an increase in the energy of the X-ray photon, and, consequently, the recoil energy Eot. With a further increase in the recoil energy (Eot> ED) the chemical bond breaks and the molecule breaks down. Continuing the previous analogy with the canon and the missile, we can say that in this case, the canon loses, for example, wheels. The chemical bond of the hydrogen molecule H2 breaks in the area of hard X-ray radiation at photon energies above 5 keV.

Besides, it turned out that in the area of hard X-ray radiation emission, the photon momentum becomes comparable with the photoelectron momentum. This means that to describe the physics of the studying phenomenon, we need to take into account even the photon momentum and tool up with the Relativistic Theory (also known as Einstein's Theory of General Relativity). Moreover, the rotational and translational degrees of freedom become entangled necessitating the description of nuclear wave packet dynamics beyond the framework of standard perturbation theory considering strong coupling between rotational and translational motion.

Photon energies higher than 5 keV are available at all modern synchrotrons, i. e. at SOLEIL, SPring-8, MAX-IV, and PETRA synchrotrons. Experimental verification of the new effect discovered by the Siberian researchers is planned to be performed in France with GALAXIES beam of SOLEIL synchrotron. The most accessible for the first experimental observation of the effect is the registration of fragments of the dissociation of a hydrogen molecule using the so-called time-of-flight spectroscopy, where the effect will be confirmed by an increase in the kinetic energy of the fragment with increasing photon energy. According to the analysis results already achieved within the research, the investigated effect can be experimentally verified for a number of molecules in clusters of inert gases and molecules adsorbed on the surface.

‘The research performed is the basis for studying the substance, its structure, its interaction with synchrotron X-ray radiation, and also for taking into account the effect under study when developing new materials and technologies. In particular, our developments may be in demand in future experiments using the 4th generation Specialized Synchrotron Radiation Source SSRS-4 which will be assembled in Novosibirsk. We believe that there our results will be in demand when planning new experiments, which means that they will contribute to the emergence of breakthrough technologies in domestic X-ray spectral studies. In nature, the predicted effect can be observed in the upper atmosphere where the intensity of hard x-ray radiation is quite high,’ noted **Dr Sergey Polyutov**, co-author of the article, leading researcher at the Laboratory of Nonlinear Optics and Spectroscopy (Department of Science and Innovation, SibFU).

Fig. 1A. Before the shot, the full impulse of the cannon-missile system equals zero since the system is at rest. After the shot, the canon momentum P = Mv (the product of the canon mass M and the canon velocity v) should equal the missile momentum mV with the sign reversed. This way we can calculate the speed of the velocity of the cannon (or recoil energy): Eot=E m/M. This means that the recoil energy (Eot) is less than the missile energy (E) by m/M times.

Fig. 1B illustrates that with a sufficiently large recoil momentum (blue arrow), the chemical bond can break and the molecule dissociates. The same can happen during a rotation induced by recoil (**fig. 1C**). The cause for the bond breaking in the latter case is the centrifugal force (**fig. 1D**).

24 march 2020

Web page address: https://news.sfu-kras.ru/node/22992