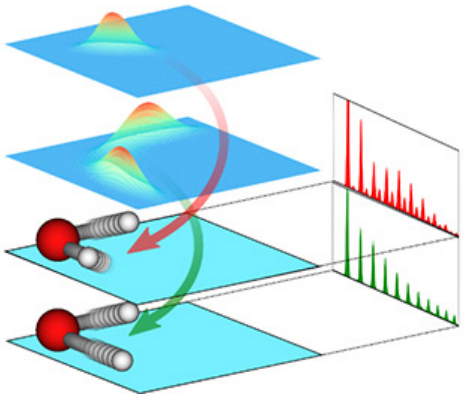
The scientists have found a way to open spatial gates

An international research team, with the participation of the scientists from Siberian Federal University, has found a way to ensure high-accuracy molecular motion control.



The capabilities of theoretical physics are connected with changes in the concept of the nature of things, and this is what holds great potential in control of the processes, which traditionally were considered to be beyond control. In the paper published in the British journal Nature Communications (8:14165, 2017), by using the discovered effect of spatial quantum gates, X-ray serves as an instrument for penetration into the spatial structure of quantum states. In experiments with water molecules under X-rays the scientists examined the vibrational modes of atoms in a series of excited states. This experiment has become a starting point for research and theoretical generalizations. The choice of H_2O molecule is determined by its huge significance for physical chemistry, biology and for life on Earth in general. Also, this molecule is a very convenient object for the study of **the principle of spatial selectivity that allows breaking a complex vibrational mode into particular elementary modes**. Resonant X-ray scattering through short-living highly excited states of a water molecule in the gaseous phase (lifetime is less than a trillionth of a second) has been studied in the work. Different spatial localisation of these excited states plays a key role in spatial filtering.

In prospect, this result can bring a lot of applied effects. First of all, the fundamental research is important for studying material properties, in particular, for manipulating chemical reactions. The developed mechanism of filtering vibrational modes with the use of resonant X-ray scattering may potentially be applied to more complex systems in photochemistry and biophysics.

The results of the work have become possible due to modern experimental techniques, namely to the special X-ray source (synchrotron) in Switzerland. This machine, which has the ultra-high resolution, conforms to the requirements of modern science that allowed observing the principle of vibrational modes breaking.

> According to **the authors of the paper**, *"The experimental technique has made an incredible step forward in increasing the resolution: this accuracy is equivalent to measuring the weight of the 10 tonnes of cargo with an accuracy of 1 gram."*

Due to ultra-high spectral resolution, modern resonant inelastic X-ray scattering data provides a unique opportunity for filtering the ground-state vibrations and thus a detailed study of their properties.

The Russian team of the scientists is represented by Dr Victor Kimberg and Professor Faris Gel'mukhanov from Laboratory for Nonlinear Optics and Spectroscopy, Siberian Federal University, who developed a theoretical model and performed a high-level computer-assisted mathematical modeling.

> As **Victor Kimberg** considers, *"Even fairly simple molecules, such as the H2O molecule, have various types of a vibrational motion of atoms, called 'vibrational modes'. The interaction of these modes leads to a very complex 'molecular dance'. And the capability to control such*

motions, in particular, analysing one particular type of it, serves as a key to understanding and controlling of the molecular reactions."

Faris Gel'mukhanov says, *"The spatial gates are the effect of a spatial selection of vibrational states, where filtering becomes a result of resonant X-ray scattering through highly excited states with different spatial localisation."*

The work is the result of the international cooperation of scientists from Germany, Sweden, Russia, Switzerland and Brazil. The studies were initiated by the co-authors of the paper, the German scientists who had sent the results of their experiment to the Krasnoyarsk scientists. The unexpected results raised questions that eventually changed the views of theorists. This work has a classical synergistic effect when the result of the joint work of theorists and experimenters far exceeds the sum of their independent studies. Thanks to new technological capabilities, the most accurate experimental data were obtained and the most accurate calculations were made, which made it possible to develop the existing theory.

The scientists have already begun to work on the next research task: using the same methods study the water molecules in their "liquid" state. The topic of "liquid water" is actively discussed in the modern scientific community, and the demand for its development is getting higher.

Maya Smolina, Press Service of the SibFU, 15 february 2017