Researchers will „pimp out“ the organic dye fluorescein for the needs of toxicology and medicine

Researchers of Siberian Federal University and their colleagues from L.V. Kirensky Institute of Physics of the Siberian Branch of the Russian Academy of Sciences (SB RAS) revealed structural and behaviour features of fluorescein, an organic compound used in medicine and the environmental industry as a highly sensitive probe. The results of their study have been published in Dyes and Pigments.

Fluorescein is a dye, and using it one can hue a wide variety of miniature objects: living cells, drug delivery systems, enzymes, proteins, biopolymers, micelles, carbon nanotubes. This substance appears as orange-red crystals and dissolves in water, but its main advantage is the generosity with which the excited fluorescein molecules emit a bright greenish glow. Having inoculated the particles stained with fluorescein into the human body, it is easy to track their movement – their glow is easily detected by devices, and for example, we will find out whether the drug was delivered to the damaged organ. Or we can understand where a neoplasm has been developing in the patient’s body. Unlike bioluminescent markers, which glow on the principle of living fireflies and are „footloose and fancy-free“, fluorescein needs to be excited from the outside — a beam of light should be directed at it, and its particles will immediately return the light, barely having time to absorb it.

Fluorescein, a representative of an extensive family of xanthene dyes, was synthesized more than a hundred years ago, and it seemed to have been studied well. According to the researchers, however, the thoroughly studied luminous agent still holds some secrets — the structure of fluorescence spectra in a wide pH range has not yet been studied, and the culprit here is the proton transfer that occurs when the molecules of the substance are excited.

„There is very little time between this absorption of a quantum of light and its emission in the form of fluorescence, just a few nanoseconds, but on the scale of a quantum system, an avalanche of events rushes during this period. These events include the molecule itself and its immediate environment — solvent molecules, and this, of course, affects the observed result i.e. fluorescence with its intensity and wavelength (colour). If you get onto the mechanisms of dark processes preceding the glow, then based on this it is possible to create a very sensitive sensor for the state of the environment of the molecule. All optical sensors and fluorescein, in particular, work on this basis. One of the important, competing the emission, processes in fluorescein is the excited state proton transfer. This means that a molecule with very bright green luminescence is a sensor for the presence of proton groups, i. e., for the acidity or pH of the environment. Using all the advantages of optical sensors, fluorescein can be used to determine the local acidity of very specific and inaccessible biological objects, for instance, living cells,“ — said **Evgenia Slyusareva**, professor at the specialized department of Photonics and Laser Technologies, SibFU.

„We analyzed the measurement data obtained by the method of absorption and stationary fluorescence spectroscopy, and the results of calculations based on the time-dependent density functional theory. Thanks to the combination of experiment and theory in solving the

> *problem, we managed to obtain unique information about the behaviour of different ionic forms of fluorescein in the excited state. We believe that these data can be further used to create a highly sensitive sensor working on the principle of "switching on/off" the proton transfer between ionic forms of fluorescein or its derivatives,"* — said **Marina Gerasimova**, senior lecturer at the Department of General Physics, SibFU.

> *„Our work contributes to the understanding of the nature and efficiency of transfer of proton in an excited state. We described this process in the language of quantum chemistry, energy, and the rates of running processes. This will allow us to switch from an empirical language to a language of exact quantitative values. From a fundamental point of view, it is interesting in order to penetrate the secrets of nature, to enhance knowledge of the xanthene family and other luminophores, including green fluorescent protein (GFP) obtained from jellyfish, and from the practical point of view, to achieve the solution of biosensor problems much higher level,"* — summed up **Ms Slyusareva**.

Besides the scientists from Siberian Federal University and the Federal Research Center of the SB RAS, researchers from the University of Nevada (Reno, USA) and the National Institute of Advanced Industrial Science and Technology (Tsukuba, Japan) took part in this research.

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