Physicists' algorithm predicts the optical properties of molecules

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Credit: Tomsk State University

Scientists of the Tomsk State University (Russia), with colleagues from Sweden and Finland, have created an algorithm for calculating the photophysical and luminescent characteristics of molecules. This

algorithm makes it possible to calculate optical and luminescent properties (luminosity and quantum yield of fluorescence) of molecules and substances with high-precision methods of quantum chemistry. The results are published in *Physical Chemistry Chemical Physics*.

"With this algorithm, we can predict the properties of molecules and substances with a computer, and it's much cheaper than buying equipment to synthesize them and measure their properties," says Rashid Valiyev, one of the authors of the study, an associate professor of the TSU Faculty of Physics. "This provides an accessible tool for analysis and prediction. And based on our prediction, we can synthesize more specific queries with the desired properties in various areas. Now, for example, in another project, we are planning research on predicting the properties of traditional medicines."

The researchers who created the algorithm also include Victor Cherepanov (TSU), Gleb Baryshnikov (TSU and KTH Royal Institute of Technology in Stockholm, Sweden), and Dage Sundholm (University of Helsinki, Finland). For calculations, they used the photophysical theory and model of Bixon and Jortner; as a tool for calculating the required quantities they used modern non-empirical methods of quantum chemistry without fitting experimental coefficients. Thus, it was possible to predict the properties of organic and organometallic molecules without synthesizing them in advance.

The algorithm will enable the design of molecules and substances for future optical devices such as organic LEDs and lasers. The research was conducted in the project New Electroluminescent Materials for Highly Efficient Organic Light-Emitting Diodes (OLEDs), whose head is Rashid Valiyev.

Organic light-emitting diodes (OLEDs) are a cheaper and more environmentally friendly alternative to traditional inorganic light sources.

The process of manufacturing OLEDs is also relatively simpler. Organic LEDs have an advantage over conventional incandescent lamps, because they operate at low power and exhibit high efficiency. They emit light but almost no heat; moreover, they illuminate a much larger surface in comparison with incandescent lamps, thanks to their controlled direction of radiation.

The scientists calculated the optical characteristics of the known molecules used in OLED technology (Alq3, Ir (ppy) 3, hetero[8]circulenes), photodynamic therapy (psoralen), laser technology (PM567) and in applications of nanotechnology (polyacenes and porphyrins). At present, using this algorithm, the team is investigating the luminescent properties of carbazole derivatives, hetero[8]circulenes, in order to obtain a recipe for creating highly efficient OLEDs devices based on these compounds.

"We all consist of molecules, and physics lies at the heart of everything, even chemistry and biology. Basically, my work takes place at the intersection of three sciences—physics, chemistry, and biology. Astronomy, and specifically, astrochemistry is another science that is even closer to it. Discoveries and achievements are now being made at the intersection of sciences, rather than in a narrow specialized area; any science develops in the collaboration," says Rashid Valiyev of his research.

Provided by Tomsk State University