

Scientists find a new dopant for organic electronic devices

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The energy levels of the studied systems and a synchrotron X-ray diffractogram measured on a thin film of an organic semiconductor doped with a derivative of [3]-radialene. Credit: The Lomonosov Moscow Stte University

A team of the Lomonosov MSU researchers in collaboration with their German colleagues from the Institute of Polymer Research in Dresden (Leibniz Institute) believe a particular molecule could lead to the development of organic electronics. The results of the work were published in *Advanced Materials*.

The researchers found that a derivative of [3]-radialene, a molecule known for nearly 30 years, can be used to create organic semiconductors. Dmitry Ivanov of Moscow State University believes that the achievement will greatly contribute to the fabrication of <u>organic</u> <u>light-emitting diodes</u> and new classes of organic solar cells.

Organic or "plastic" electronics is a relatively young scientific field that emerged 15 to 20 years ago. Such devices are still inferior to standard silicon-based electronics in terms of performance, and are also less durable. But they also have advantages—lightness, thinness, flexibility, transparency, and most importantly, <u>plastic electronics</u> are much cheaper than silicon. The main applications of <u>organic electronics</u> include solar cells, which could be much cheaper than silicon-based modules and thus cover larger surface areas. Also, organic electronics can be used to design organic light-emitting devices and field-effect transistors.

The molecule [3]-radialene is a so-called dopant, whose addition to a semiconducting polymer substantially increases its electrical conductivity. Existing dopants for inorganic semiconductors have been widely used for decades, but according to one of the article's co-authors,



Dmitry Ivanov, organic semiconductors are a new frontier. Currently, the most commonly used dopants are fluorinated dopants. They can dramatically increase the electrical conductivity of many organic semiconductors, but not all polymers that are used today in "plastic" electronics are suitable.

"Together with our Drezden colleagues, we decided to design a completely new type of low molecular weight dopant for organic semiconductors," says Dmitry Ivanov. "And here, it was important to choose a molecule that was not only suitable in its energy levels, but which would mix well with the polymer—so that in contact with the polymer, it does not segregate into a separate phase, eventually crystallizing and losing contact with the polymer."

The main contribution of Ivanov's laboratory in this work consisted of exploring the physics of the phase transitions, the physics of mixing in such binary systems—in other words, finding a suitable candidate in terms of polymer physics.

And such a candidate was found. It happened to be a derivative of [3]-radialene. This is a small planar molecule in which the carbon atoms are connected to form a triangular structure. Among other potentially interesting compounds, [3]-radialene has the most energetically suitable LUMO level, i.e. the lowest unoccupied molecular orbital. This means that with its help, the electrons are easily extracted from the semiconducting polymer matrix, becoming free charges and thereby increasing the conductivity of the doped material. [3]-radialene thus becomes the strongest dopant for the organic semiconductor among those that are known in the scientific literature.

The experiments with the [3]-radialene, also confirmed by the results of quantum-chemical calculations, show that the substance is well mixed with a semiconducting polymer and allows researchers to increase the



<u>electrical conductivity</u> of the polymer by several tens and even hundreds of times. It has been found that the dopant molecules are included in the polymer crystalline lattice and form the so-called co-crystal. And the formation of co-crystals, according to Ivanov, is one of the main reasons for the high efficiency of the new compound.

The new dopant, as well as its fluorinated analogues, belongs to the category of electron-deficient organic dopants, Dmitry Ivanov says. "Fluorine substituents are known to strongly pull the electrons from the central part of the molecule, which increases the whole conductivity of the doped polymer. In the present work, the chemical structure of the dopant is completely different, and appears to be even better. Perfect mixing of our dopant with the polymer matrix is, I think, the key to its performance. This could pave the way to fabrication of new organic solar cells with improved characteristics. We also think about production of organic field-effect transistors. I think it will give a significant boost to the development of organic electronic devices."

More information: Yevhen Karpov et al, High Conductivity in Molecularly p-Doped Diketopyrrolopyrrole-Based Polymer: The Impact of a High Dopant Strength and Good Structural Order, *Advanced Materials* (2016). DOI: 10.1002/adma.201506295

Provided by Lomonosov Moscow State University

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