Scientists work on creating molecular-sized microchip elements

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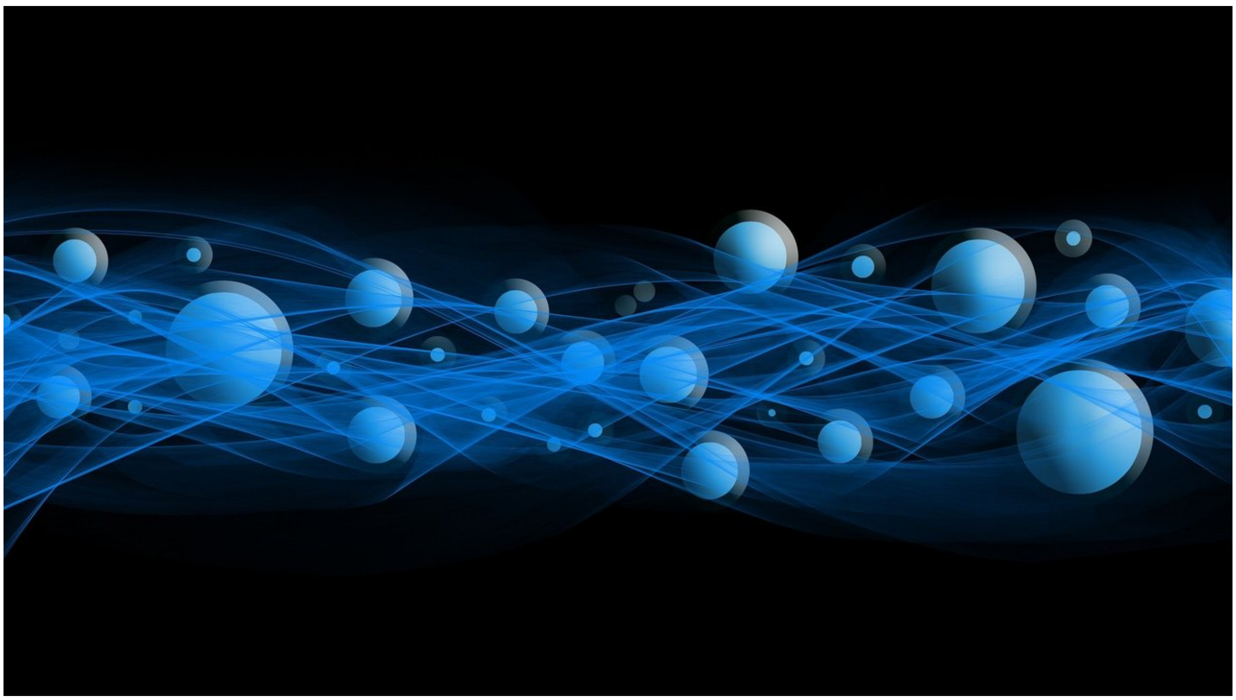

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Modern silicon-based integrated circuits (ICs) have reached the practical limits of miniaturisation, while the use of organics can potentially allow the creation of microchip elements as large as a single molecule. Scientists from the Russian National Research Nuclear University MEPhI (MEPhI) are actively conducting studies in this field. They have recently published the results of their modeling changes in agitated molecules of organic semiconductors in the *Journal of Physical Chemistry*.

There are several reasons why organic electronics are considered to be a promising field. The raw materials for them are easily accessible and the use of organic materials allows molecular-sized IC elements to be made, thus bringing them closer to the internal structures of living organisms.

One such promising possibility is the design of directed organic molecular and functional materials. Right now, Russian researchers are summarising global experience in these spheres and conducting predictive modeling.

"Our group is conducting predictive modeling for organic electronic materials, specifically for organic light-emitting diode (OLED; used in light-weight high-quality displays capable of bending). The OLED emits light, when electrons coming from a cathode meet with (electron) holes coming from anodes and engage in recombination. The state, when an electron and a hole are mutually attached but don't recombine, called an exciton, can last relatively long, and is often localised within a single molecule," said Alexandra Freidzon, assistant at the National Research Nuclear University MEPhI and scientist at the Photochemistry Centre of the Federal Scientific Research Centre.

According to Freidzon, the migration of an exciton's quasiparticle to neighbouring molecules allows the colour and the effectiveness of light emission of OLEDs to be conveniently controlled. For that purpose a light-emissive layer can be placed between n- and p-type layers of organic semiconductors, carrying electrons and holes respectively, with these quasiparticles "meeting" in the middle-layer, engaging in recombination and staying attached to each other.

"We have studied how excitons behaves in a molecule of a typical hole semiconductor, which is also used as a matrix for the emissive layer, and it turned out that excitons localise not on the entire molecule, but on certain parts of it and can migrate between them. Excitons can do it under the influence of small perturbations, such as the ones caused by the presence of another molecule," Freidzon added.

MEPhI's researchers have studied the mechanism and the speed of exciton's migration from one end of the molecule to another and discovered that the migration goes very fast only one way and it can be fostered by certain intramolecular fluctuations.

The authors of the research study believe that it's now possible to study how the presence of neighbouring molecules affect this process and suggest the modification to the exciton-carrying molecule in order to make the process of transferring agitation energy to the emissive molecule more efficient. Such work is a the heart of virtually designing functional materials—scientists single out the material's key functions and then build a model, describing the process of its function. This allows them to determine the main factors affecting the processes' effectiveness and thus to suggest modifications to certain functional materials if needed.

The scientists at MEPhI stress that they are only beginning to understand exciton's migration process within the molecule in organic semiconductors, but will soon be able to present suggestions on modifying the molecules used in OLED display's emissive layers.

More information: Ilya D. Krysko et al. Theoretical Study of the Intramolecular Localization and Migration of a Triplet Exciton in the N,N′-Di(1-naphthyl)-N,N′-diphenyl-(1,1′-biphenyl)-4,4′-diamine (α-NPD) Molecule, *The Journal of Physical Chemistry C* (2019). DOI: 10.1021/acs.jpcc.8b10726

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