Quantum Bridge: scientists predict new plasmons

A research group of SibFU and Federal Research Centre "Krasnoyarsk Research Centre" of the SB RAS has predicted the existence of a new type of plasmons associated with charge transfer. According to the experts, the obtained result is very bright and promising in terms of creating the basis for producing ultra-sensitive biosensors of the new generation. Their work has been published in Journal of Chemical Physics, a highly-rated international journal.

Nanoplasmonics is considered presently as one of the fastest-growing areas of nanophotonics. It is the discoveries in nanoplasmonics that can make the difference to the development of biomedicine, solar energy and telecommunication technologies. The researchers from SibFU managed to offer a completely new type of plasmon particles which have a significant potential.

> *'In contrast to the well-known classical plasmons that are generated, for example, in silver and gold nanoparticles under the impact of an external electromagnetic field, we checked the plasmons that appear in metal (gold) nanoparticles bound by bridges (linkers) conducting organic molecules (fig. 1).*

> *The behaviour of classical plasmons is well described by classical Maxwell's equations. But in our case, a significant role is played rather by quantum effects, therefore standard programs for solving Maxwell's equations are inapplicable. Besides, there is that problem of describing the properties of nanoparticles, which can be described completely by quantum methods for a reasonable time with a limitation of several hundred atoms in the nanoparticle. To overcome this limitation and calculate plasmon vibrations in the system under consideration, we have developed an original hybrid quantum-classical model that takes into account quantum effects, with the main parameters obtained from quantum-chemical modelling,*' said **Alexander Fyodorov**, one of the authors of the study and professor at SibFU.

The scientists considered a system consisting of two gold nanoparticles bound by a polyacetylene molecule. The nanoparticles in this system manifest metallic properties due to the thermal expansion of energy levels near the Fermi energy, which are important for the implementation of the proposed model of the appearance of plasmons during charge transfer between the two nanoparticles. At the same time, the conducting bridge-molecule is actually a one-dimensional conductor where electrons or holes move ballistically because the mean free path of the carriers significantly exceeds the length of the bridge.

> *'The key point of our model is the consideration of the dynamics of electrons in the system, which is described in the language of the wave function. Under the electric field, conduction electrons are accelerated, which leads to a change in their quasimomentum and kinetic energy. The change of these values can be calculated easily, knowing only the structure of the corresponding zone and the effective mass of the electron. In the theory we've developed, we have constituted a link between quantum and classical values — a quasimomentum, momentum, and an external force impacting the free carriers. The calculations showed that the system under consideration really has metallic properties and can conduct direct or alternating current, which can lead to the appearance of plasmons. At the same time, the plasmon frequency, which is interesting for applications, shifts to the infrared range,'* explained **Pavel Krasnov**, a senior researcher at Siberian Federal University.

The authors of the work carried out a number of necessary quantum-chemical calculations and found that the proposed new type of plasmons and the plasmon frequency associated with them stand out as being highly sensitive to the external environment.

‘We believe that the proposed type of plasmons can be widely used as chemical probes and bioprobes. This is because the conductivity of this bridge-particle will change very sharply during the adsorption of external molecules on the molecule of the bridge, and this, in its turn, will affect the plasmon frequency which is easy to measure. Technically, the hybrid quantum-chemical model we've developed is interesting per se. It lays the foundation for a fairly simple quantum-classical modelling of plasmon systems and can be used in a wide range of unresolved plasmonics problems,’ concluded **Sergey Polyutov**, the research co-author, a leading researcher of Siberian Federal University.

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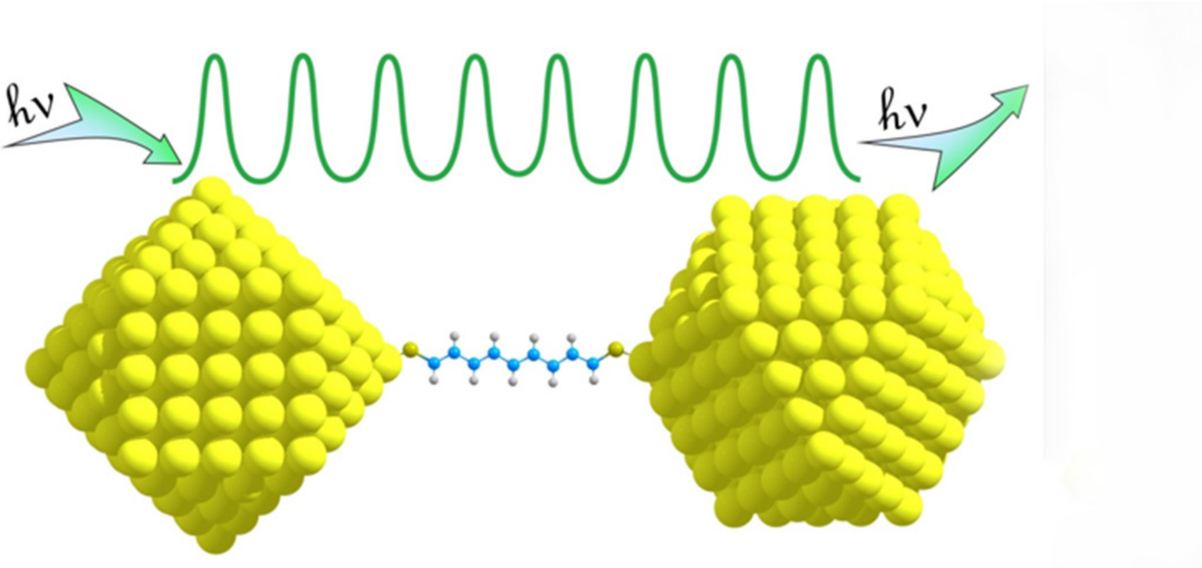

Fig. 1

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