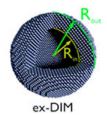
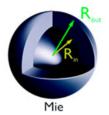
Plasmonic nanoshells for drugs packing and targeted delivery

A research team from Russia, Sweden, and the USA has studied optical properties of atomic size metal nanoshells and simulated their resonance properties based on the original model of atomic interaction. They assume that the results will allow to use nanoshells of a few atoms thickness for single molecules detecting or for targeted drug delivery.





The phenomenon of optical resonance of metal nanoparticles is well studied. Notionally, the simulation of solid nanoparticles is labour saving, so they are widely used in modern medicine, chemistry, biology, solar energy, and photonics. However, about fifteen years ago, researchers predicted the existence of high-Q resonance modes in hollow nanoparticles. Essentially, these nanoparticles can be used as safe containers to "pack" drugs. After entering the human body, the shells of nanoparticles are destroyed, for example, by laser radiation and the drug is released. This approach doesn't give a systemic load on the body, since the drug packed in the shall of a nanoparticle hits its target, the affected organ, without affecting healthy tissue.



'Until now, it has been hard to simulate such objects. Speaking from the perspective of classical optics, scientists can describe the resonance properties of a spherical nanoparticle with a spherical cavity inside. However, the classical models "skid" when trying to simulate the optical response of a nonspherical nanoparticle with a cavity, or a nanoparticle with a non-spherical shaped cavity, or even a nanoparticle with an off-center cavity. Another

challenge to solve is to make such nanoshells less than ten nanometers in size for clinical applications,' said **Vadim Zakomirny**, junior researcher of SibFU Research Department.

In search of a solution, the research team of SibFU with their American and Sweden counterparts applied their recently developed Extended Discrete Interaction Method (ex-DIM). This method allows not only to simulate the optical response of nanoparticles of arbitrary shape, including those with a cavity inside, but also takes into account the position of each atom in a metal nanoparticle.

'A detailed study of the resonance properties of hollow nanoparticles can be applicable for modern biomedicine,' noted **Ilya Rasskazov**, postdoc from the Institute of Optics, the University of Rochester. 'Our systematic studies of hollow nanoparticles explain the positions of optical resonances depending on the total size of the nanoparticle and the thickness of its shell. The huge advantage of the study is the accuracy of calculations. We have applied the



atomic model for finding out the optical properties of hollow nanoshells for the first time. The curious fact is that each atom in a nanoparticle matters and affects the calculation result.'

The study of the international research group is a part of a large complex research on non-standard optical nanoparticles too large for quantum-chemical calculations and too small for classical methods of modern optics. The researchers claim that hollow nanoparticles are a promising object of interest to modern photonics, biomedicine, and chemistry.

The research team includes the research fellows from Siberian Federal University, Royal Institute of Technology (Stockholm, Sweden), Federal Siberian Research Clinical Center under FMBA of Russia (Krasnoyarsk), the Institute of Computational Modelling of the Siberian Branch of the Russian Academy of Sciences, and the University of Rochester (New York, USA).

By the way, the scientific community has already noted this study by including it in 2020 PCCP HOT Articles published in Physical Chemistry Chemical Physics journal of Royal Society of Chemistry.

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