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Superatoms in quasi – zero – dimensional nanostructures

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ABSTARCT

This review summarizes the results of theoretical studies of superatoms (or artificial atoms) – nanodimensional quasiatomic structures formed from spatially separated electrons and holes (hole moving in the volume of a semiconductor (dielectric) quantum dot and an electron localized on the outer spherical interface between the quantum dot and a dielectric matrix). It is shown that out of these superatoms can construct quasimolecules and quasicrystals that have pre-determined physical and chemical properties. The possibility of experimental study superatoms and their role in a variety of physical and chemical phenomena, as well as in technical applications.

Keywords: superatom, spatially separated electron and hole, quantum dots, quasimolecules, quasicrystals

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INTRODUCTION

For the development of mesoscopic physics and chemistry was essential idea superatoms (or artificial atoms) [1-7]. Superatom are nanosized quasi-atomic structure formed from spatially separated electrons and holes (the hole in the volume of the quantum dot and the electron is localized on the outer spherical quantum dot matrix dielectric interface) [1-7]. This terminology may be correct, given the similarity of the spectra of discrete electronic states of atoms and superatomic and the similarity of their chemical activity [1-7].

In [1, 2] describes quasi-atomic model of nanodimensional heterostructures (superatoms), consisting of a spherical nucleus (quantum dot (QD)) of the radius *a* and a dielectric constant ε_2, in the volume that contains the semiconductor material doped with donors selectively surrounded unalloyed semiconductor matrix with a dielectric constant ε_1 (with a band gap *E*g area smaller than the band gap QD). Donor electrons flow into the matrix , while in QD appears positive charge is determined by the number of donors *N* (heavy hole effective mass is much larger than the effective mass of the electrons remain in the volume QD) . When the radius QD *a* (about 5 nm), depending on the solubility limit of the impurity in the semiconductor material QD, value *N* can be set to the order of several tens and even exceed all known numbers of the table of Mendeleev [1,2]. The

minimum radius of *a* QD scan, which allows to describe superatom with a mesoscopic approach is based on the size (about 1.5 nm) [1,2]. The ionization energy of the superatom does not exceed (10 - 100 meV) , which allows to modify its quantum states with weak electromagnetic fields.
Application of semiconductor nanostructures as the active region nanolasers prevents binding energy of an exciton in the QD [8, 9]. Therefore, research aimed at finding the semiconductor nanostructures, which would be observed a significant increase in the exciton binding energy in QD, are relevant [3 -9]. The effect is a significant increase in the binding energy of an electron in a hydrogen superatom [3-7] allows to detect experimentally the existence of such superatoms at room temperatures and will stimulate experimental studies nanostructures, containing superatoms that can be used as the active region nanolasers working on the excitonic transitions. In effect, the occurrence of superatoms and in the effect of substantially increasing the energy of the ground - state superatom , the pivotal role played by the interface (QD- dielectric (semiconductor) matrix) [3-7].

The review devoted to the study of some aspects of the theory superatoms of spatially separated electrons and holes.

MATERIALS AND METHOD

Superatoms in quasi – zero – dimensional nanostructures

In [3-5] proposed a new model of an superatom, which is quasi – zero – dimensional nanosystem consisting of a neutral spherical QD (nucleus superatom) radius *a* and that includes within its scope semiconductor (dielectric) with a dielectric constant ε_2, surrounded by a dielectric matrix with a dielectric constant ε_1. A hole *h* with the effective mass m_h moves in the QD volume, while an electron *e* with the effective mass $m_e^{(1)}$ lies in the dielectric matrix. In such nanostructure lowest electronic level is situated in the matrix and humble hole level is the volume QD. Large shift of the valence band (about 700 meV) is the localization of holes in the volume QD. Large shift of the conduction band (about 400 meV) is a potential barrier for electrons (electrons move in the matrix and do not penetrate into the volume QD) . Since the dielectric constant ε_2 of QD is far superior to the dielectric constant ε_1 of the surrounding matrix QD, the energy of the polarization of electron interaction with the interface (QD - matrix) is the localization of the electron in the polarization well near the outer surface of the QD [3-5]. Therefore, there is a possibility of electron draining of QD in a matrix and electron localization in polarization hole near the outer surface QD (hole moving volume QD) [3-10].
The energy spectrum of superatom (exciton of spatially separated electrons and holes) from QD radius $a \geq ac$ (about 4 nm) is fully discrete [3-5]. This is called a hydrogen- superatom . The energy spectrum of the superatom consists of a quantumdimension of discrete energy levels in the band gap of the dielectric matrix. Electrons in superatom localized in the vicinity of the nucleus (QD) [3-7]. The electrons moving in well-defined atomic orbitals. Serve as the nucleus of QD containing in its volume semiconductors and insulators [3-7]. Ionization energy superatoms take large values (of the order of 2.5 eV), which is almost three orders of magnitude higher than the binding energy of the excitons in semiconductors [3 –7].
We briefly discuss the possible physical and chemical effects, which are relevant for the results. In our proposed [3 -7] model of a hydrogen superatom localized on the surface of the QD is a valence electron. In a quasi-atomic structures of the outer valence electron can participate in a variety of physical and chemical processes, similar to the atomic valence electrons in atomic structures. When

two hydrogen superatoms, since some critical distance *D*c between the surfaces of QDs, which is less than the value of the two exciton Bohr radius *aex* in superatom, the atomic orbitals of the two valence electrons overlap and form a covalent bond. The result is a quasi-molecules [6].

Of these superatomic possible to construct quasimolecules , as well as quasicrystals (or supercrystal) [6]. It is very important that in these quasicrystals is possible to control the period and symmetry " supercrystals lattice". As a result of quasicrystals can be synthesized (quasi one-dimensional and quasi-two), which have pre-determined physical (optical, electrical [11-13] etc.) and chemical (types of chemical bonds , and photochemical and oxidation processes, catalysis, adsorption [14,15]) properties. This fact apparently will simulate and investigate physical and chemical effects which are difficult to implement in natural solids (for example: electron gas Wigner crystallization low density; metallic bond between the superatoms which may form quasimolecule; the study of electron- hole (exciton and biexciton) of the liquid , and the ability to form superatoms many new chemical compounds with unique properties).

In the above models [1 - 7] superatoms have the ability to attach its *e*- electron orbitals *N* (where *N* can vary from one to several tens). In this superatoms to be *N* – valence. This new effect causes a high chemical activity and opens new opportunities superatoms related to their strong oxidizing properties, a substantial increase in the intensity of photochemical reactions in catalysis and adsorption as well as their ability to produce many new chemical compounds with unique properties (in particular, quasimolecules and quasicrystals (quasi one-dimensional and quasi-two)). Such many- effects may be related to the localization of charges in many semiconductor (metal or dielectric) of the nanoparticles in the nanostructures [3 - 7]. In particular, the charge of the same sign by the Coulomb repulsion this localization can occur only on the size $a \geq a$c (n) of nanoparticles (where the *n*- charge critical radius *a*c (*n*) which increases monotonically with the number of charge *n*).

Thus, the possible existence of many - electron quasi - two - dimensional spherical nanostructures (ie giant superatomic) from singly at $a > ac$ to many-electron over a flat surface [10]. These many-body effects may occur on nanoparticles synthesized in the semiconductor matrix , where such processes may be involved carriers of different characters [10]. In the case when the charge carrier of one sign are conditions for penetration of the nanoparticles , and no other, may form macroscopic multielectronic superatoms (such cluster atoms [10]) , capable of holding a large number on the orbits of the electrons.

CONCLUSION

The review devoted to the study of some aspects of the theory superatoms of spatially separated electrons and holes. It is shown that the effect of substantially increasing the energy of the electron in superatom containing QD ZnSe, allows experiments to detect the existence of hydrogen-superatomic at room temperatures and will stimulate experimental research of the nanostructures, which can be used as the active region nanolasers working on the excitonic transitions. Found that out of superatomic possible to construct quasimolecules and quasicrystals that have pre-determined physical and chemical properties. This circumstance allows to simulate and investigate physical and chemical effects which are difficult to implement in natural solids. We also discuss the possibility of an experimental study of superatoms and their role in various phenomena of physics and chemistry, as well as in technical applications. Thus, superatoms, have a number of properties, apparently inherent quasi – zero – dimensional nanostructures caused mainly influenced by surface effects, in particular, the presence of the interface (QD - dielectric (semiconductor) matrix).

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