Orbital and spin magnetism in semiconductor nano-objects

Contents

半導體奈米元件的軌道與電子自旋磁性

中文摘要

半導體奈米結構超穎物質是一項在大範圍頻率下操縱電磁場極具潛力的人造物質，特別是在應用、元件和基礎研究方面。以下是其在此領域迫切需要被實現的項目：實現大規模的量子運算，在可見光波段的負折射率超穎物質，在非磁性物質下顯現出人造磁性，...等。半導體奈米結構超穎物質(或系統)應在適當的半導體奈米素材下發展。這項三年計劃的主要目的在於解決半導體奈米結構領域中重要的問題:非尋常的磁特性。我們主要聚焦於下列兩個項目:定量的描述可控形狀大小和材料參數的半導體奈米素材的靜態和動態磁性；在外加磁場下, 大量奈米素材之間的量子和電磁交互作用。
在這項計畫中,我們發展出一套設計和控制非磁性半導體奈米素材(量子點,量子環,量子點分子)
及其組合的靜態和動態磁性的方法。
幾個研究的方向將在期末報告中詳細提及。第一個是對於擁有非尋常軌道磁性半導體奈米素材的磁光響應一般性的描述，包括多規模混和離散-
連續模型。第二個是關於磁量子位元在非磁性半導體奈米素材的操控。第三為實際形狀和材料的整體半導體奈米素材磁特性的模擬(此模擬是由我們所發展出的映像法為立基的)。另外，我們也對於半導體奈米素材綜合的磁和光特性的描述制定出一般性的理論方法。
更甚者,我們第一次把模擬的結果解釋如下:
1.由實驗的結果我們可知,半導體量子環的不均勻強烈的影響著其磁化強度和磁化率以及其溫度的穩定性。
2.單一奈米環的形狀不對稱性強烈影響著侷限在環中的單一激子能量不尋常的反磁性位移抑制。
3.由實驗所觀察到的一群三量子環的激子激光頻譜,
其不對稱和寬廣的峰包特性可能是由這群量子環分散的徑向高度(幾何形狀)造成。
根據這些結果我們已有一些發表。

關鍵字：軌道磁性, 半導體奈米素材,量子點分子,奈米環

Orbital and spin magnetism in semiconductor nano-objects

Abstract

Nano-structured semiconductor meta-materials potentially can manipulate electromagnetic fields within a very wide range of frequencies, which is particularly beneficial for many applications and devices, as well as for new basic science. The short list of possible urgent implementations in this field consists of realizations of large scale quantum computation, meta-materials with the negative refracting index in optical range, static and dynamic artificial magnetism in basically non-magnetic materials, etc. Nano-structured semiconductor meta-materials (systems) should be developed and assembled on the base of appropriate semiconductor nano-objects. The major purpose of this three-year theoretical project was to address most important problems in the emergent research field of semiconductor nano-systems with unusual magnetic properties. Two aspects have been obtained our attention: - the proper quantitative description of the static and dynamic magnetism in semiconductor nano-objects with controllable geometry, sizes, and material parameters; - the theory of mutual quantum and electromagnetic interactions between semiconductor nano-objects for systems containing few (or many) nano-objects under external magnetic fields.

In this project we developed theoretical methods for the design and controllability of static and dynamic magnetic properties of non-magnetic semiconductor nano-objects (quantum dots, nano-rings, quantum dot molecules) and ensembles combined from them.

Few directions of the research have been pursued, as described in details in this final report. The first is the general description of the magneto-optical response form systems of semiconductor nano-objects with unusual orbital magnetism, which includes a generalization of the multi-scale hybrid discreet-continuum model. The second is a study on a magnetic qubit implementation in non-magnetic semiconductor nano-objects. The third is the modeling of magnetic properties of ensembles of semiconductor nano-objects with realistic geometries and material content. The modeling was based on the mapping method proposed and developed by us. In addition, we have formulated a general theoretical approach to a comprehensive description of the magnetic and optical properties of dispersive ensembles of semiconductor nano-objects.

In particular our simulation results have explained for the first time:

1. The experimental fact that the dispersion in the semiconductor ring ensembles very strongly affects the magnetization and magnetic susceptibly and stabilize the temperature properties of them.
2. The strong impact of the wobbling asymmetry of a nano-ring on the unusual suppression of the diamagnetic shift of the energy of a single exciton confined in the ring.
3. The appearance and properties of the wide asymmetrical excitonic peaks in the photoluminescence spectra of the triple ring ensembles known from the experiment.

The broadening is preferably caused by dispersion of the radial height profile (geometrical shape) of the rings in the ensembles.

Several publications have been performed based on our results.

Keywords: Orbital magnetism, Semiconductor nano-objects, Quantum dot molecules, Nano-rings

1. Introduction (Purpose and Brief Literature Review)

The demand for modern multiband and multifunctional nano-based semiconductor devices stimulates the development of novel components and subsystems, those are required to be re-configurable and controlled dynamically. In this domain composite materials (meta-materials, artificially structured materials) offer a very promising direction of the future development (see, e.g., [1-6] and references therein). Meta-material properties derive from properties of the constituent material content. For nano-structured metamaterials in particular, incorporating tunable nano-sized components into metamaterials or having nano-components with active and controllable inclusions leads to tunable properties, regardless of the origin of the modulation.

Modern technological progress in semiconductor technology made it possible to fabricate artificial semiconductor nano-structured meta-materials. Those new materials, can be constructed from very small objects, typically a few tens of nanometers in size (se for instance [7-14]). Nano-structured semiconductor meta-materials potentially can manipulate electromagnetic fields in very wide diapason, which is particularly beneficial for potential applications and devices, as well as for new basic science. For instance, it is well known that systems assembled form many nano-sized elements are required to perform large-scale quantum information processing [15-17], for bio and medical imaging [18-20], etc. Obviously, such systems can be developed and assembled only on the base of appropriate nano-structured metamaterials. The short list of possible urgent implementations in this field consists of realization of large scale quantum computation, meta-materials with the negative refracting index in optical range, nano-imaging and drag control for bio-medical applications, static and dynamic artificial magnetism in basically non-magnetic (conventional semiconductor) materials, etc. In recent years the knowledge of the physical properties of semiconductor nano-sized objects, like quantum dots, nano-rings, nano-wires, and quantum dot molecules, with respect to their transport, magnetic and optical behavior has increased considerably [7-14].

In our previous works we have demonstrated theoretically a wide range of opportunities to obtain extraordinary (unusual) dynamic and static magnetic properties of semiconductor nano-objects [21-23]. We also found that for some nano-objects (with and without spin-orbit interaction) we can achieve static and dynamic artificial magnetism using basically non-magnetic materials [24-30].

It was the main inference of our works referred above (and it is clear now after some preliminary experimental confirmations [14]: to build a robust theoretical basement to the existing knowledge about magnetically-controlled behavior of semiconductor nano-objects and metamaterials made from them. These aspects should be clarified, in order to ensure a proper interpretation of any magnetic and magneto-optical phenomenon for semiconductor nano-objects. Most of the investigations in this domain still focus upon the photo-luminescent, optical, and transport properties. The corresponding knowledge about the dynamic and static orbital and spin magnetism of the semiconductor nano-objects and ensembles of them is particularly not complete.

The purpose of this three-year theoretical project was to address most important problems in this emergent research field. Two aspects have been obtained our attention: - the proper quantitative description of the static and dynamic magnetism in semiconductor nano-objects with controllable geometry, sizes, and material parameters; - the theory of mutual quantum and electromagnetic interactions between semiconductor nano-objects for systems containing few (or many) nano-objects under external magnetic fields.

In this project we developed theoretical methods for the design and controllability of static and dynamic magnetic properties of non-magnetic semiconductor nano-objects (quantum dots, nano-rings, quantum dot molecules) and ensembles combined made from them.

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2. General description of the magneto-optical response form systems of semiconductor nano-objects with unusual orbital magnetism

2.1 Generalized multi-scale hybrid discreet-continuum model

We present fist a general computational hybrid multi-scale (hierarchical) model which allows us to simulate the coherent manipulation of the quantum mechanical states of electrons and holes confined in semiconductor nano-objects and monitor the manipulation by means of traditional magneto-ellipsometry. In our hybrid discrete-continuum model each embedded nano-object gets represented by a single discrete dipole, characterized by a bare excess polarizability. This polarizability includes the screening by the surrounding continues dielectric medium. The embedded bare polarizability tensor of a single nano-object is approximated at the near resonance conditions to be a sum of static and dynamic parts. The dynamic part is described by means of Kramers/Heisenberg type of polarizabilities. Ignoring quantum nonlocal effects the dynamic part of the tensor of the bare embedded polarizability (which has been derived by us) can be written in

terms of the electro-hole overlap integrals and transition energies. To find the static part of the polarizability tensor we implemented an appropriate boundary-value problem for a local electrostatic potential in a complex three-dimensional cubic domain of the host material including one nano-object. For the dynamic part of the polarizability we computed the transition energies and wave functions of electrons and holes confined in the semiconductor nano-object.

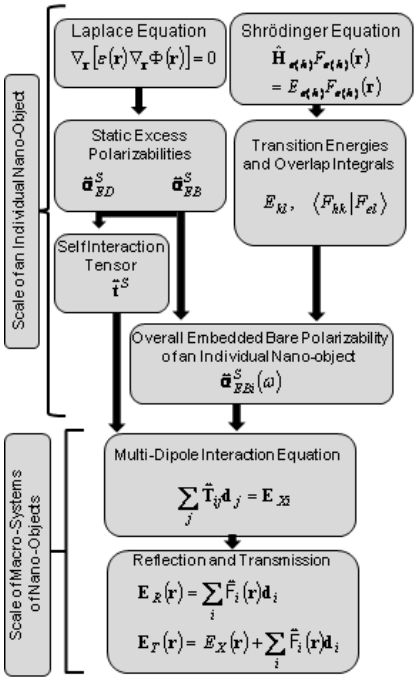

Figure 1. Flow diagram of the model implementation

To obtain the collective optical response one should solve the system of equations similar to known from the discrete-dipole approximation. Our general method (see Figure 1) allows us to simulate the nano-objects of arbitrary shapes. The electron states are described by means of the effective one-band Hamiltonian with the energy and position dependent effective mass and *g*-factor. The valence-band hole states in semiconductor nano-objects (preferably III-V semiconductor compounds) we describe with multiband (4x4) **k·p** Hamiltonian that allowed for valence subband mixing. The electrostatic characteristics, energy states and wave functions of electrons and holes confined in the quantum dot molecules are obtained numerically form solutions of the Schrödinger equation with the appropriate effective Hamiltonians (we use realistic semiconductor material parameters for strained semiconductor heterostructures, with corrected to the strain condition band parameters, etc.) by the nonlinear iterative method using COMSOL multiphysics package. Using our approach we have shown that parameters of the electron and hole quantum states localized in the nano-objects can be retrieved from the collective magneto-optical response of systems of such nano-objects.

As an example of the method implementation we consider impact of the coherent manipulation of electronic states in the double vertical lens-shaped circular quantum dot molecule on the collective magneto-optical response from a layer of those nano-objects (see Figure 2). The manipulation is performed by an external magnetic field applied upon InAs/GaAs quantum dot molecules assembled from the dots with substantially different lateral radii. We treat the semiconductor quantum dot molecules within complete three-dimensional description which allows us to simulate arbitrary directions of the external magnetic field (Figure 2) in contrast to most of the calculations done before. It brings up much wider opportunities to dynamically manipulate electron and hole states in quantum dot molecules. Recently it was demonstrated that in the asymmetrical quantum dots molecules the non-uniform diamagnetic shifts of the lowest electron energy levels lead to their anticrossing (at a certain B_C magnetic field) which yields in a positive peak of the differential magnetic susceptibility of the system (O. Voskoboynikov, PRB 78, 113310, 2008).

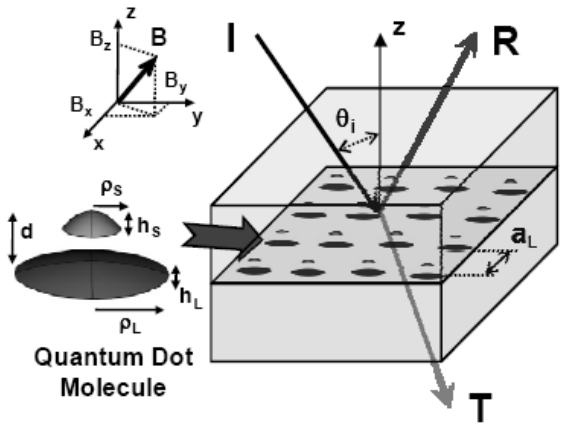

Figure 2. Schematic of the magneto-optics of a layer of embedded semiconductor quantum dot molecules.

In this study we have shown unusual consequences of the electronic non-uniform diamagnetic shifts for the magneto-optical transitions (as an example in Figure 3 and the following figures we present simulations those were performed for InAs/GaAs quantum dot molecule which is non-uniform in *z* direction with the following geometry parameters: ρ_L = 25 nm, ρ_S = 9.5 nm, h_L = 3 nm, h_S = 4 nm, and a few interdot base-tobase distances *d*). We have found that when the strength of the magnetic field is approaching $B_C \approx 10.7$ T the anticrossing manifests redistribution of the electronic wave function inside the quantum dot molecule: the electronic wave function of the state $e1_s$ relocates

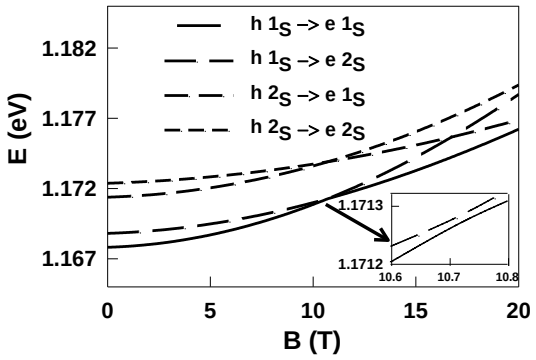

Figure 3. Lowest transition energies in the double dot molecule as functions of magnetic field B||z. Inset: the anticrossing region.

from the large dot to the small one. On the contrary, the second state $e2_S$ relocates from the small dot to the large one. At the same time, the probability density of the hole state $h1_S$ remains to localize in the large dot and the probability density of the hole state $h2_S$ - in the small dot. So the magnetic field acts as a dynamic coupling factor for energy states localized in different dots on the analogy of the interdot distance in the static approach. Consequently corresponding overlap integrals are changed drastically by the magnetic field change (see Figure 4). The described above effects very clearly result in the ellipsometric angles Ψ and Δ for the light reflected from the layers on the semiconductor quantum dot molecules (Figure 5). As it was already mentioned changes in magneto-optical response of a layer of quantum dot molecules emerge from the changes in the quantum mechanical configuration of the molecules. The direct accessibility of the quantum information from the QDMs such as individual dipole strengths, transition energies, and overlap integrals by means of the measurement of the ellipsometric parameters is one of the attractive aspects of our approach.

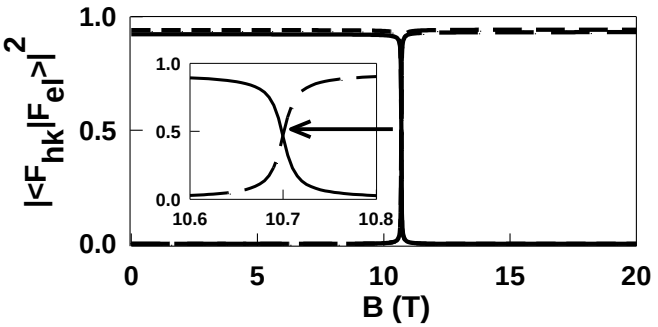

Figure 4. Overlap integrals for the lowest transition energies
in the double dot molecule as functions
of magnetic field B||z. Inset: the anticrossing region.

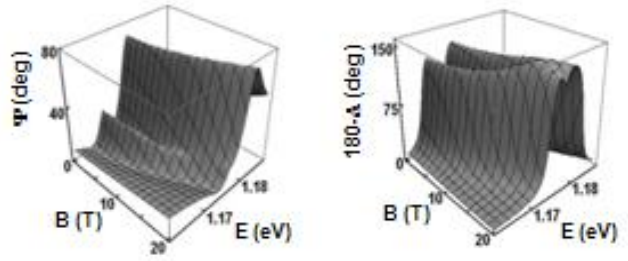

Figure 5. Ellipsometric angles of a layer of quantum dot molecules

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2.2 Magneto-optics of three dimensional arrays of semiconductor nano-objects including magneto-exitonic effects

The hybrid discrete-continuum model (see above) makes it possible to simulate complex optical properties of three dimensional arrays (ensembles) of semiconductor nano-objects embedded in a dielectric matrix. Each embedded nano-object gets represented by a single discrete dipole, characterized by a bare excess polarizability. This polarizability includes the screening by the surrounding continues dielectric medium. To obtain the collective optical response one should solve the system of equations similar to known from the discrete-dipole approximation. The method allows us to simulate the collective magneto-optical response the nano-objects of arbitrary random shapes and positions within the arrays. Using the method we theoretically studied the optical

response of three-dimensional InAs/GaAs quantum dot multilayered structures (see Figure 6). First we defined the optical response of an isolated layer of embedded quantum like it was describe in Section 2.1. Then using the propagation-matrix approach we express the amplitudes of incident, reflected and transmitted electromagnetic waves in a multilayered structure by the reflection and transmission coefficients of the isolated layers. We studied the overall reflectance and transmittance dependencies on the number of layers and distance between consecutive layers.

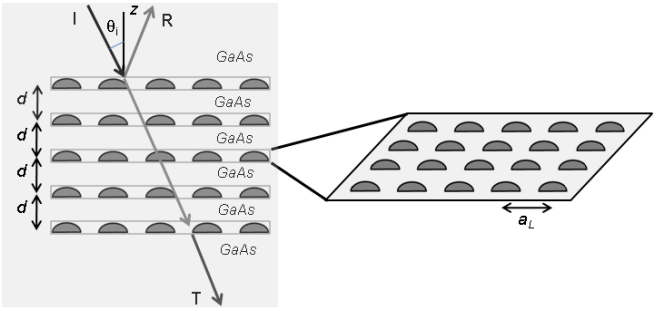

Figure 6. Scheme of the quantum dot multilayer structure.

The reflectance of the structures including several layers InAs/GaAs lens-shaped quantum dots (2 nm in height and 15 nm in radius) for s-polarized light is shown in Figure 7. The peaks in the reflectance relate to the allowed optical transitions in the quantum dots. Clearly, for a single layer the reflectance is weak. However the reflectance still reproduces important information on quantum mechanics of individual quantum dots.

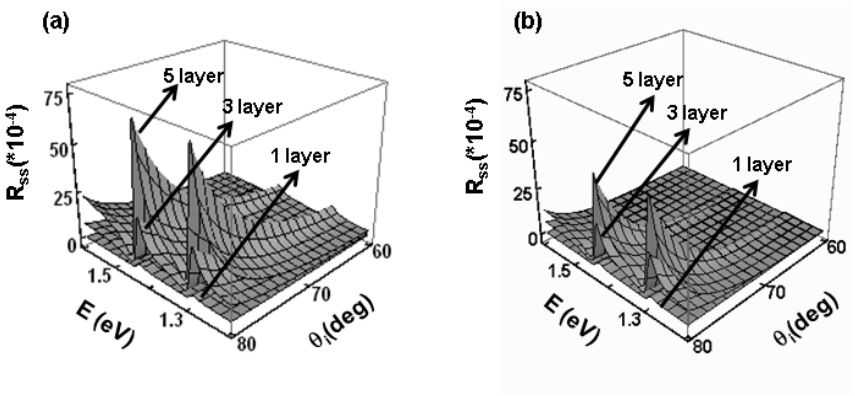

Figure 7. Reflectance of the quantum dot multilayered structures as a function on the transition energy and angle of incidence: (a) d = 10nm and (b) d = 50nm.

When the number of the layers in the structure increases the overall reflectance of the structure considerably enhances (Figure 6). For large enough distance between the layers d the interference becomes significant and this leads to the appearance of the periodical peaks in the reflectance. The dependence of the overall reflectance on the transition energy and distance d for the structure consisting of five layers is presented in Figure 8. The figure shows that the interference effects become significant for certain distances between layers in the structures.

In addition, we have considered impact of the coherent manipulation of electronic states in double vertical lens-shaped circular quantum dot molecules on the effective permittivity of three-dimensional arrays made from these nano-objects. The manipulation is performed for asymmetrical InAs/GaAs quantum dot molecules assembled from the dots with substantially different diameters and when an arbitrary directed external magnetic field **B** is applied to the system (as it was described in Section 2.1). The magnetic field dependencies of the lowest optical transition energies are shown in Figure 3. The optical response of a single molecule is described by means of Kramers/Heisenberg type of polarizabilities. Then we have calculated components of the effective

permittivity tensor for three-dimensional arrays of the quantum dot molecules Clausius – Mossotti relation.

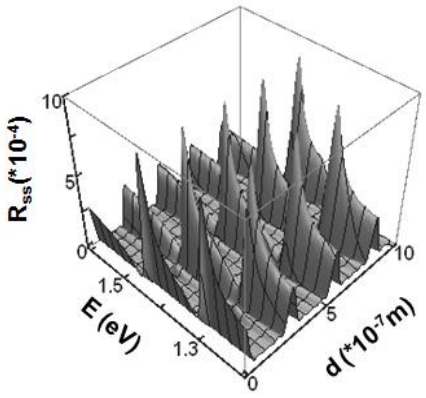

Figure 8. Reflectance of the quantum dot multilayered structure consisting of five layers as a function on the transition energy and distance between the consecutive layers.

To illustrate impact of the quantum mechanical properties of individual InAs/GaAs quantum dot molecules on the overall optical characteristics of the arrays we show in Figures 9-11 the real and

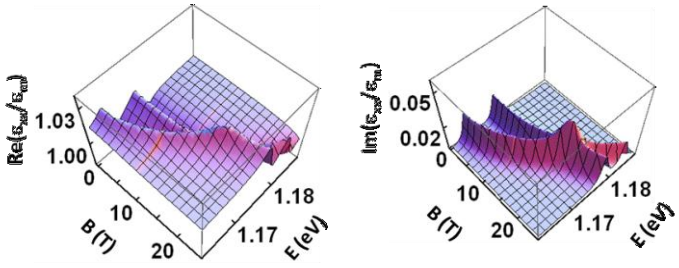

Figure 9. Effective permittivity of an array of embedded quantum dot molecules (distance between the dots in the quantum dot molecule is 20 nm, B||z): (a) real part and (b) imaginary part.

imaginary parts of the diagonal components of the effective permittivity tensor as functions on the optical transition energy and magnetic field for different direction of the magnetic field and inter-dot distance with a molecule (the density of the molecules is $N = 1.6\text{x}10^{16}$ cm^{-3}). The calculation results clearly suggest measurable values for changes of the effective permittivity. The direct accessibility of the quantum information from the quantum dot molecules such as individual dipole strengths, transition energies, and overlap integrals by means of the measurement of the effective permittivity of arrays of quantum dot molecules is one of the attractive aspects of our approach.

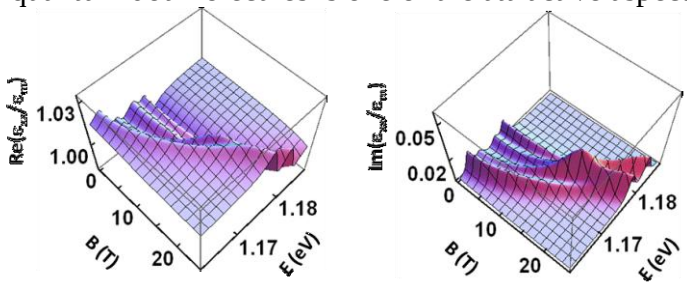

Figure 10. Effective permittivity of an array of embedded quantum dot molecules (distance between the dots in the quantum dot molecule is 10 nm, B||z): (a) real part and (b) imaginary part.

We emphasize that according to our results the magneto-optical data on the effective permittivity can reproduce important information on the quantum mechanics of the molecules. The approach can be potentially useful for the design of new nano-structured metamaterials.

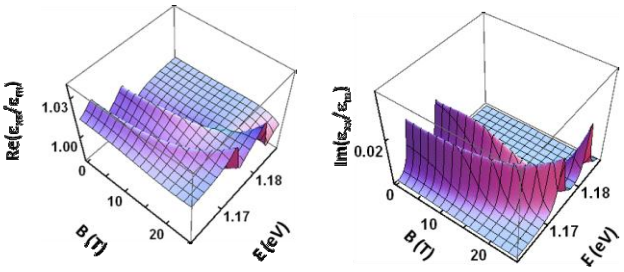

Figure 11. Effective permittivity of an array of embedded quantum dot molecules (distance between the dot s in the quantum dot molecule is 20 nm, B⊥z): (a) real part and (b) imaginary part.

Published in:

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3. Magnetic qubit implementation in non-magnetic semiconductor nano-objects

The possibility of manipulation and reconfiguration of electron wave functions in three-dimensional space is related to the iso-spin (a mark of the actual position of an electron in quantum dot molecules) in complete analogy to the electron's spin orientation. So, coherent dynamical

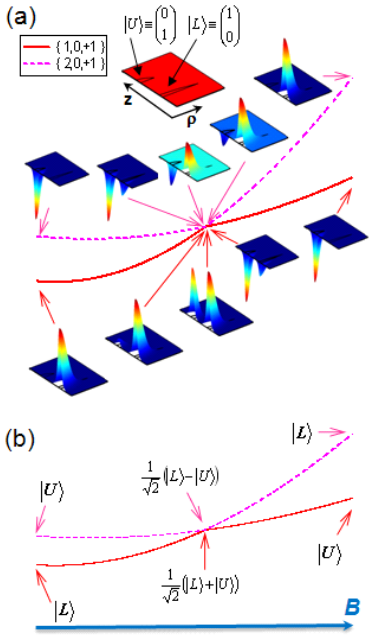

Figure 12. Schematic of the dynamic coherent manipulation of (a) the electronic wave functions and (b) magnetic qubit in the asymmetrical quantum dot molecule.

manipulation of the electronic configuration in quantum dot moleculess is a key target for application of semiconductor nano-devices in quantum information technology.

The coupling and entangling control in quantum dot molecules can be performed by variation of the distance between dots (static tuning) or external fields (dynamic tuning). In this work we theoretically studied coherent manipulation of electronic states in an asymmetrical quantum dot molecule performed by changing external magnetic field.

A magnetic qubit manifests itself by turning the magnetic susceptibility of the quantum dot molecule into the paramagnetic domain. This result is particularly interesting because the system is built from diamagnetic semiconductor materials. We consider a system of two vertical lens-shaped circular InAs/GaAs quantum dots (Figures 2 and 12). The calculations are done for the full three-dimensional model of an InAs/GaAs quantum dot molecule with the hard-wall confinement potential (see Section 2.1). This allows us to simulate the magnetic dependence of the electron energy states in a system of very asymmetrical shape: the quantum dots have substantially different diameters (19 and 50 nm) and different heights in contrast to most of the known simulations. In our approach we use realistic semiconductor material parameters (for instance the band offset of the InAs/GaAs strained heterostructure, corrected to the strain conditions band parameters, etc.).

For our system (with a relatively large inter-dot distance) we can consider two iso-spin states, in which the electron occupies the lower or upper dot. The non-uniform diamagnetic shift of the lowest energy levels in different dots leads to their anti-crossing and the relocation electronic wave ground state functions from lower L dot to upper U dot (L and U stand for the “Lower” and “Upper” dots in Figure 12). For our system (with a relatively large inter-dot distance) now we can consider two iso-spin states, in which the electron occupies the lower or upper dot

$$|L\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |U\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

with energies E_L and E_U correspondingly. When the two states are energetically close, the temperature is low we can omit other states in the quantum dot molecule and the system can be approximated by a two-level model (qubit). The effective iso-spin Hamiltonian for states $|L\rangle$ and $|U\rangle$ can be written as $\hat{H} = \overline{E} + E\hat{\sigma}_z - T\hat{\sigma}_x$, where $\hat{\sigma}_z$ and $\hat{\sigma}_x$ are the Pauli operators, $\overline{E} = (E_L + E_U)/2$, $E = (E_L - E_U)/2$, and $T = \langle L|\hat{H}|U\rangle$ is the inter-dot tunnelling matrix element.

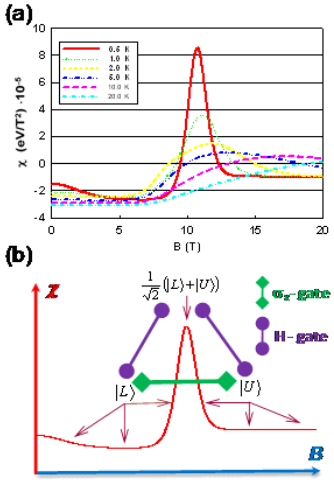

Figure 13. Schematic of the quantum gate’s realization in the asymmetrical quantum dot molecule:
(a) magnetic susceptibility of the single electron
(b) asymmetrical double dot molecule
(c) at different temperatures; (b) quantum gate's control.

In this interpretation switching the magnetic field from $B_1 < B_C$ to $B_2 > B_C$ (and visa versa) rotates the iso-spin eigen-states $|L\rangle \Leftrightarrow |U\rangle$ and forms few single qubit gates. Near the anti-crossing point, when $E_L \approx E_U$ the Hamiltonian $\hat{H}$ forms the Hadamard gate [15]. In addition, rapid (periodical) switching of the magnetic field can cause very general unitary transformations for the qubit. We note that results of those transformations can be controlled by monitoring of the magnetic response of the system (see Figure 13) (for instance – the differential magnetization

$$M = -\frac{\partial F}{\partial B}$$

or magnetic susceptibility of the system

$$\chi = \frac{\partial M}{\partial B},$$

where F stands for the system's free energy).
It follows from this theoretical study that experimental investigation of the magnetic properties of asymmetrical quantum dot molecules will yield interesting results for further development of the quantum informatics.

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4. Modeling of magnetic properties of ensembles of semiconductor nano-objects with realistic geometry and material content

4.1 Realistic geometry and material content mapping onto smooth three dimensional potentials of semiconductor nano-objects. Examples

A number of methods for simulation of the egienstates and wave functions of electrons in semiconductor nano-objects have been proposed and developed. Most of them require very large scale computation including complex chemical, mechanical, and structural modeling. But, if we want to study physical properties of the nano-objects it is very important to go far beyond the solu-

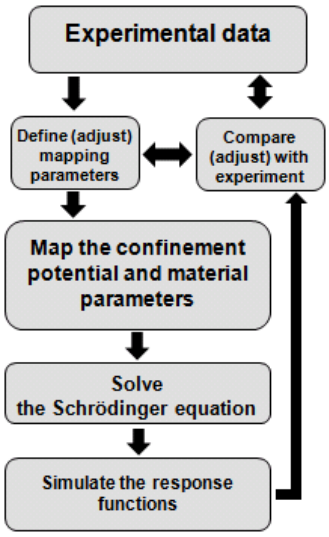

Figure 14. Flow diagram of the mapping procedure.

tions of the basic egienvalue problems. Therefore, there is a need on a method which efficiently generates physical properties of the nano-objects on the base of cumulative experimental knowledge of their geometrical, structural, and material composition.

In our work we have proposed a computational method which allows us to map realistic geometry, strain and material composition of semiconductor nano-objects (known from experiments) on smooth three dimensional potential's and parameter's profiles for electrons confined in the objects. The method allows us very efficiently and economically to simulate and study physical properties of semiconductor nano-objects within a wide range of the parameter's change (Figure 14).

In our method we assume (this is a very standard condition) that the object was grown at a flat substrate parallel to (x,y) plane. The height of the object in z-direction (the system growth direction) is presented by a function $h(x,y)$. Using analysis of the experimental structural and composition information obtained from AFM (atomic force microscopy) and X-STM (cross-sectional scanning tunneling microscopy) measurement the function $h(x,y)$ can be readily discovered and even analytically approximated for most of the objects. Three-dimensional confinement potential $V(x,y,z)$ for electrons can be found from the composition dependent band offset. The mapped confinement potentials we use to define the mapping functions

$$M(x,y,z) = \frac{\left[V_{\max} - V(x,y,z)\right]}{\Delta E_C},$$

where $\Delta E_C = V_{max} - V_{min}$ is the electronic band offset in the system, and V_{min} is the minimum value of the potential (inside the object). This function accumulates experimental information about geometrical shapes and compositions of the rings and it allows us to present the position-dependent effective band parameters of electrons (holes) (effective masses, band gaps, etc.) and dielectric constant of the system as well. The energy eigenstates and corresponding envelop wave functions of electrons and holes (with and without interaction between them) now can be found like it was described in Section 2. Our method allows us efficiently and economically to simulate and study physical properties of semiconductor nano-objects and adjust important parameters of them.

Examples. We simulated diamagnetic response in the asymmetrical (wobbled) nano-rings and asymmetrical quantum dot molecules with realistic semiconductor parameters for InAs/GaAs nano-structures with complex strained composition according to the experimental data (as it was described in Section 2). To demonstrate the method efficiency we first consider the application of the mapping procedure to the simulation of the magnetization of a single electron asymmetrical (wobbled) InAs/GaAs nano-ring (Figure 15).

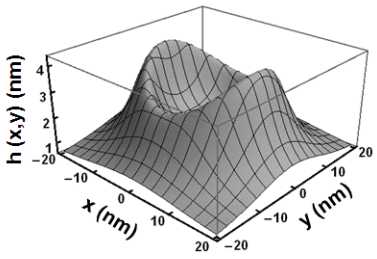

Figure 15. Geometry of an asymmetrical nano-ring.

The resulting mapped confinement potential for electrons in the nano-ring is shown in Figure 16. It carefully reproduces all known three-dimensional experimental geometry and composition data available in the literature. In the same time, the potential projection on (x,y,0)-plane is completely equivalent to the approximate two-dimensional “adiabatic” potentials used by other authors.

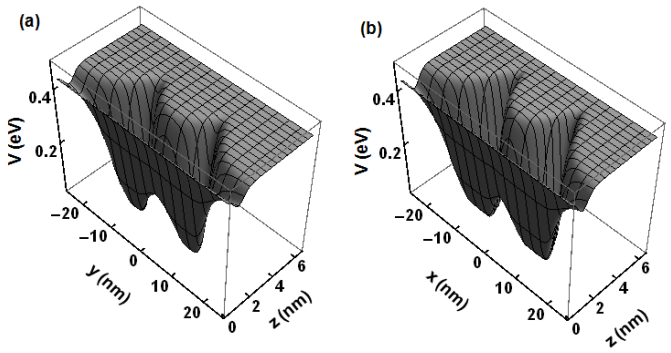

Figure 16. Two projections of the electronic confinement potential (InAs/GaAs nano-ring) on (a) (0,y,z) and (b) (x,0,z) planes.

In addition in Figure 17 we demonstrate our method application for asymmetrical quantum dot molecules, objects with very different from rings geometry.

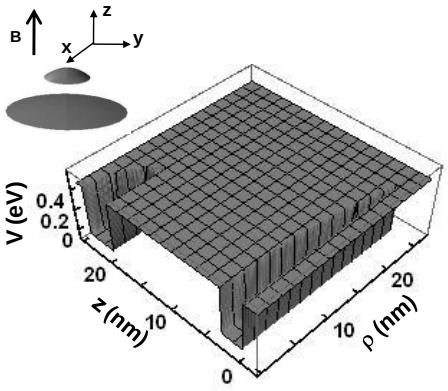

Figure 17. Mapped confinement potential of a double dot molecule

We have found that for both systems occupied by a single electron at zero temperature the differential magnetic susceptibility χ has a positive peak near 12T. With temperature increasing the peaks remain Lorentz-like shaped and gradually disappear. For both systems considered the peaks are results of the convergence of two lowest energy levels when the magnetic field increases.

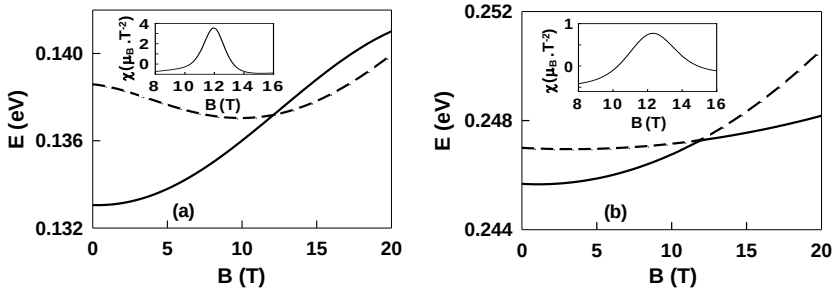

Figure 18. Magnetization of single electron of (a) ring and (b) quantum dot molecule at temperature T =1.2K

But for the rings the wave functions of those levels have different symmetry and levels cross. At the same time, for the quantum dot molecule the wave functions have the same symmetry and the levels anticross (as it was discussed in Section 2 and shown in Figure 18). Although topologies of the systems are different the electronic energy levels' convergence leads to a very similar and unusual diamagnetic response for both systems. Based on our results we can assume that this unusual diamagnetic response can be observed in nano-objects where the lowest energy states are close enough and they converge when magnetic field is applied to the system and the diamagnetic shift is performed to be non-uniform for different energy levels.

In addition we simulated the magneto-exciton-biexciton systems confined in the asymmetrical wobbled InAs/GaAs nano-rings, using a smooth three dimensional confinement potential which realistically describes electronic properties of the rings. Recently it was found experimentally that in the single InAs/GaAs nano-ring's magnetoexitonic emission demonstrates an interesting discrepancy with the conventional theory: the diamagnetic shift of a single exciton's peak is considerably smaller than that predicted by the traditional theory. It was also found that a perfect in geometry wobbled nano-ring is particularly hard to achieve. Normally, the wobbling of a ring is asymmetrically unbalanced (see Figure 19, where the wobbling asymmetry is quantified by the following asymmetry parameter: $\delta_h = \left[(h_+ - h_-)\backslash h_+\right]\cdot 100\%$). To make a link to realistic three-dimensional shapes of the rings we use our mapping method, which makes it possible to project the ring's actual geometry onto the position dependent effective masses, energy gap, band offsets of electrons and holes confined in the ring.

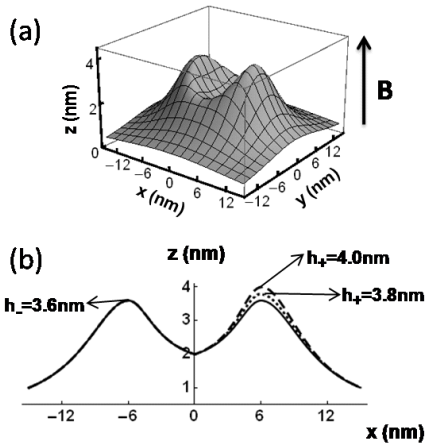

Figure 19. (a) Geometry of the asymmetrically wobbled InAs/GaAs nano-ring for $\delta_h \approx 5.5\%$. (b) Projection of the ring height onto the *x*-*z* plane for: $\delta_h = 0\%$ (solid curve); $\delta_h \approx 5.5\%$ (dotted curve); $\delta_h \approx 11\%$ (dashed curve).

Using the methods described in Section 2 incorporated with the Hartree and exact diagonalization methods as well we simulated ecxitonic and biexcitonic recombination energies, binding energies and their diamagnetic shifts and compare those results with experimental data obtained from the magneto-photoluminescence measurement.

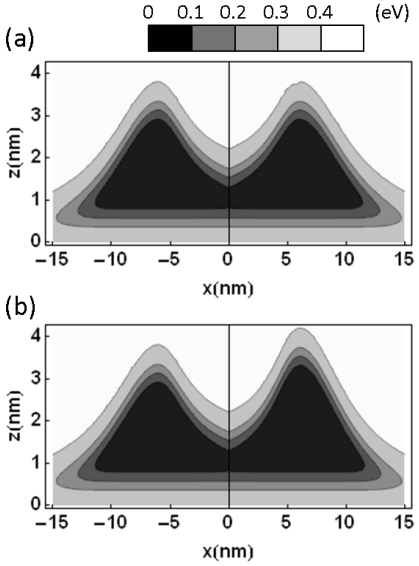

Figure 20. The electronic confinement potential projected onto *x*-*z* plane for (a) $\delta_h = 0\%$ and (b) $\delta_h \approx 11\%$.

We have found that using the realistic geometry and composition of the asymmetric nano-ring in our simulations (Figure 20) we are able to reproduce experimental data with good accuracy and explain the experimentally obtained difference in diamagnetic shifts of excitons and biexcitons.
We theoretically demonstrated the impact of the wobbling asymmetry of nano-rings on the diamagnetic shift of the single exciton's peak. The excitonic wave function is equally distributed in both side of the ring along *x*-direction when δ_h = 0%. At the same time if δ_h exceeds 10% the wave function is already localized in the potential valley at the positive *x*-side (Figures 21). This is a clear reason for the suppression of the diamagnetic shift $\Delta E_X = E_X(B) - E_X(0) \approx d_X \cdot B^2$ (where $E_X(B)$ is the magnetic field dependent exciton's ground state energy and d_X is the diamagnetic shift coefficient) since the diamagnetic shift coefficient is defined by the wave function distributions. In our simulation we have achieved a very good agreement with experimental data (see Figure 22). We argue that the diamagnetic shift's suppression reproduces actual asymmetry in the ring geometry.

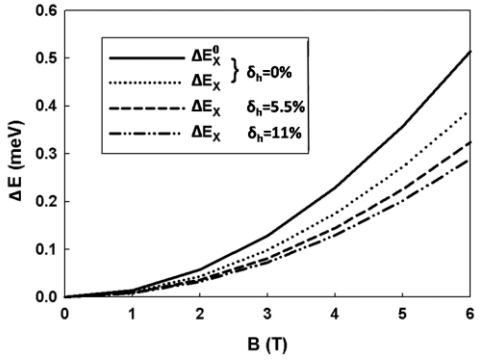

Figure 21. Diamagnetic shift of the ground state energy of the exciton confined in the ring for different wobbling asymmenries (ΔE_X^0 presents the optical transition energy diamagnetic shift for non-interacting electrons and holes).

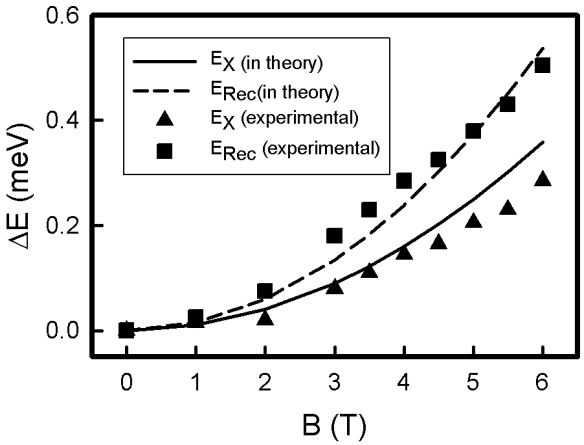

Figure 22. Diamagnetic shift for excitons confined in a nano-ring.

Published in:

1. L. M. Thu, W. T. Chiu, Ta-Chun Lin and O. Voskoboynikov, " Effect of the geometry on the excitonic diamagnetic shift of nano-rings", Physica Status Solidi C vol. 8, no. 2, pp. 375–377, March 2011.

2. Thu Le Minh and O. Voskoboynikov," Simulation of an Asymmetrical Nano Ring by Mapping of the Realistic Electronic Confinement Potential", AIP Conference Proceedings, vol. 1233, pp. 952-957, May. 2010.

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4.2 Magnetic and electromagnetic responses of ensembles of semiconductor nano-objects

The nano-objects demonstrate very promising properties for practical applications, but the inherent dispersion of their material and geometrical parameters (shape and size) leads to the almost uncontrollable inhomogeneous broadening of the collective physical characteristics (for instance peaks in magnetic and magneto-optical response's dependencies on the magnetic field or excitation energies). The physical characteristics of dispersive ensembles of semiconductor nano-objects of complex geometries and material compositions should be simulated using the multidimensional (multiparametric) distribution function, which cumulatively reproduces variations of the object parameters. To analyze dispersive ensembles of nano-objects of complex geometrical shapes, we have defined a multidimensional (multiparametric) distribution function $P(\{x_i\})$ that describes dispersions of all appropriate parameters $\{x_i\}$ (such as size, anisotropy in geometry, composition, etc.). Using the mapping method (recently derived by us) we are able to very efficiently compute energy states and wave functions of electrons and holes confined in the nano-objects within a wide range of sizes, shapes, and compositions. Thus, we can simulate ensembles with multiparametric distributions.
To demonstrate our method, we theoretically studied the magnetic response of asymmetrical wobbled nano-rings, which possess much more sophisticated shape than quantum dots (Figure 15). It was predicted by us (see Section 3 and Section 4.1) that the differential magnetic susceptibility of a single electron ring should demonstrate the positive peak in the differential magnetic susceptibility at low temperatures which has to be addressed to the Aharonov-Bohm crossing between two lowest energy states of the electron confined in the ring (see Figure 23). Then the peak position and amplitude strongly depend on the actual geometrical and material parameters of the rings

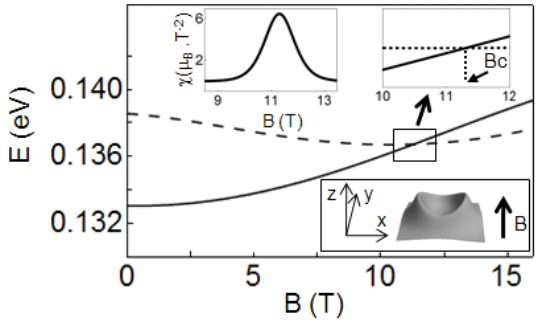

Figure 23. Energy states and differential magnetic susceptibility
(upper left inset, μ_B stands for the Bohr magneton)
of a wobbled nano ring.

such as effective radii, heights, material content, etc. First in this study we have shown, that among many parameters, the radius R_r dispersion in the ring ensemble very strongly affects the magnetization and susceptibly and stabilize the temperature properties of them (Figure 24). This is in a very good agreement with experiments and can be useful for developing of new semiconductor meta-materials with usual magnetic properties.
In addition, using our approach, we have performed a detailed simulation of the photoluminescence spectra of dispersive ensembles of the triple concentric nano-rings (Figure 25) and have addressed the issue of the asym-metrical inhomogeneous broadening of the emission peaks of these nano-objects. To reproduce actual geometrical and material parameters of the rings, we used our mapping method.

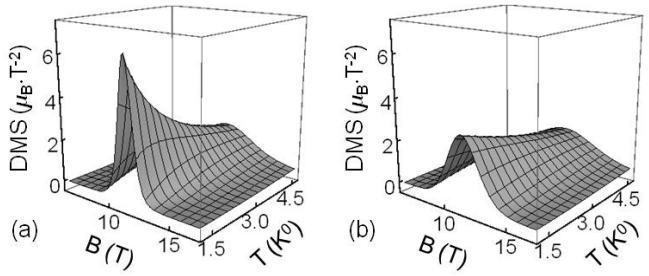

Figure 24. Dependence of the differential magnetic susceptibility (DMS) on magnetic field and temperature: (a) a single ring; (b) differential magnetic susceptibility averaged within an ensemble of the rings.

We have obtained the averaged actual optical emission spectra in good agreement with the experiment by the averaging the excitonic optical characteristics of the rings within their dispersive

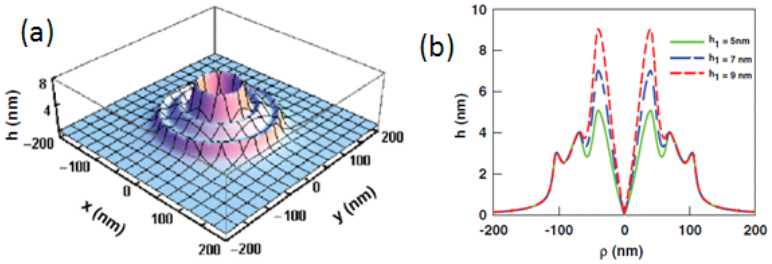

Figure 25. (a) Three-dimensional geometrical shape of a triple concentric nano-ring. (b) Two-dimensional geometry of triple concentric nano-rings with variation of the inner height.

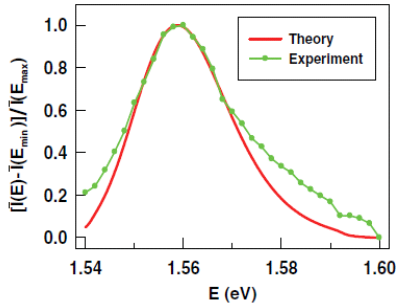

Figure. 26. Normalized averaged intensity of the optical transitions of the ring ensemble as a function of the energy at low temperatures. E_{min} and E_{max} are the positions of the intensities' minimum and maximum.

ensembles (Figure 26). Our simulation results have explained the appearance and properties of the wide asymmetrical excitonic peaks in the photoluminescence spectra of the ring ensembles known from the experiment. The broadening is preferably caused by dispersion of the radial height profile (geometrical shape) of the rings in the ensembles (more specifically, the inner height).
We stress that, using our approach, we are able to clarify the important question of which geometrical and material parameter dispersions are crucial for the broadening of physical characteristics of ensembles of semiconductor nano-objects.

Published in:

1. L. M. Thu, W. T. Chiu, and O. Voskoboynikov, "Negative"-diamagnetism of three dimensional arrays of semiconductor nano-rings", accepted to physica status solidi (b), May, 2011.

2. Yu L. Hsueh, Le M. Thu, O. Voskoboynikov, "Simulation of Spectral Characteristics of Dispersive Ensembles of Semiconductor Quantum Dots", accepted to AES Technical Reviews International Journal, Aug. 2011.
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1. L. M. Thu and O. Voskoboynikov, “Electromagnetic Response of Three-Dimensional Arrays of Quantum Dot Molecules”, accepted to publication in AIP proceedings, Aug, 2011.
2. Yu L. Hsueh, Le M. Thu, O. Voskoboynikov, “Simulation of Spectral Characteristics of Dispersive Ensembles of Semiconductor Quantum Dots”, accepted to AES Technical Reviews International Journal, Aug. 2011.
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6. L. M. Thu, W. T. Chiu, Ta-Chun Lin and O. Voskoboynikov, " Effect of the geometry on the excitonic diamagnetic shift of nano-rings", Physica Status Solidi C vol. 8, no. 2, pp. 375–377, March 2011.
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14. L. M. Thu, W. T. Chiu, Shao-Fu Xue, and O. Voskoboynikov, "Binding energy of magneto-biexcitons in semiconductor nano-rings", Physics Procedia vol. 3, no. 2, pp. 1149-1153, Jan. 2010 (SCI).
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2. L. M. Thu and O. Voskoboynikov, "Electromagnetic Response of Three-Dimensional Arrays of Quantum Dot Molecules", The Advances in Applied Physics and Material Science Congress, Antalya, Turkey, May 2011.
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