Tytuł projektu

Kwazi-molekuły z kropek kwantowych definiowanych fazą krystaliczną: uczenie maszynowe

Project title

Artificial molecules from crystal phase quantum dots: machine learning approach

Dyscyplina /Area of science

Nauki fizyczne

PROJECT DESCRIPTION

Project goals

- To utilize machine learning techniques to solve the inverse computational problem of matching spectra to nanostructure's morphological properties
- To develop theory and run high-performance atomistic calculations of excitons (electron-hole pairs) in artificial molecular systems formed by coupled crystal phase quantum dots embedded in semiconductor nanowires
- To understand properties of multiple crystal-phase quantum dots formed by zinc-blende sections in wurtzite nanowires, with a particular emphasis on GaAlAs systems
- To understand how quantum dot dimensions and distances between individual quantum dots, affect spectra of excitons confined in these nanowire artificial molecules

Outline

Crystal phase quantum dots [AKOPIAN] are new type of nanostructures that can be grown with monolayer precision and have atomistically sharp interfaces [ASSALI,HARMAND]. Since recently it is also possible to grow and measure photoluminescence spectra of nanowire-embedded double quantum dots [KHOSH]. While single quantum dots could be called as 'artificial atoms', coupled quantum dots can be denoted as solid state analogues of molecular systems.

Regarding potential applications of nanowire quantum dots, the bright exciton recombination is considered as a tool for generation of entangled photons through the biexciton-exciton cascade [JONS] whereas the dark exciton recently gained a significant attention as a candidate for long-lived, though optically addressable quantum bit [SCHWARTZ, ZIEL1]. Double, or multiple quantum dots in nanowires are far less studied, and quantum dot molecules should have several advantages over single quantum dot systems in various entanglement generation schemes [KOSH].

The goal of the project is to develop theory and run highly demanding atomistic calculations for a family of nanowire-embedded artificial molecules. These will be

constituted by multiple GaAlAs crystal-phase quantum dots formed by zinc-blende sections in wurtzite nanowires [MBB2]. We aim to understand how quantum dot dimensions and distances (and therefore couplings) between individual quantum dots, affect spectra of excitons confined in these nanowire artificial molecules.

To achieve this goal we aim for several major theoretical and computational developments. In particular, we aim to utilize machine learning techniques to solve the inverse computational problem of matching spectra to nanostructure's morphological properties. Machine learning should be of a tremendous help in determining properties, such as dimensions or composition profiles corresponding to demanded spectral properties. In a traditional approach, one is forced to study a very large number of nanostructures in function of height, diameter, shape etc. The multidimensional search over numerous nanostructures is, however, often impractical due to large computational complexity. A machine learning approach should help to solve this inverse problem in a far more efficient way. The results and the knowledge gained during this process would further be important not only from the basic science point of view, but will also act as a guideline for experimentalists.

We have an ongoing and well-established collaboration with two excellent experimental European groups conducting research in the spectroscopy of nanostructures. Owing to these close collaborations, we will have the unique ability to correlate the measured and calculated data.

The project will be conducted in a strong collaboration with NCN OPUS project "Artificial molecules in nanowires: atomistic calculations of excitonic spectra and machine learning", which is focused mainly on InP systems. Therefore, apart from the doctoral school regular salary, the PhD candidate will be able to apply for an additional three year scholarship (additionally up to 4500 PLN monthly, no tax!) in the OPUS project (opening soon; please contact: mzielin@fizyka.umk.pl).

Work plan

1. Initial studies of single crystal phase quantum dots as a prerequisite for quantum dot molecule studies

2. Development of theoretical approaches aiming for computationally efficient description of electron-hole interaction in crystal phase quantum dots

3. Development of a theory using machine learning approach; tests and building of an initial library of results for single crystal phase quantum dots

4. Atomistic, machine-learning supported, calculations of quantum dot molecules in different spatial configurations

5. Writing scientific papers and PhD thesis; auxiliary calculations

Literature

[AKOPIAN] Nano Lett. 10, 1198 (2010)

[ASSALI] Nano Letters 17, 6062 (2017)
[CIRLIN] J. Phys. D Appl. Phys. 50, 484003 (2017)
[HARMAND] Phys. Rev. Lett. 121, 166101 (2018)
[JONS] Scientific Reports 7, 1700 (2017)
[KHOSH] Nature Communications 8, 15716, (2017)
[MBB1] Nano Lett. 12, 6 6206 (2012)
[MBB2] Nano Lett. 2016, 16, 1081 (2016)
[ROZANSKI] Phys Rev B 94, 045440 (2016)
[SCHWARTZ] Phys. Rev. X 5, 011009 (2015)
[ZIEL1] Phys Rev B 91, 085403 (2015)
[ZIEL2] Phys. Rev. B 81, 085301 (2010)

Required initial knowledge and skills of the PhD candidate

- ➔ Enthusiasm for science and commitment to hard work
- ➔ Analytical thinking
- ➔ Good knowledge of English
- ➔ Good computer programming skills (or strong will to learn such)
- ➔ Basics knowledge of solid states physics (optional)

Zgłaszający projekt/ Author of the project	
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Proponowani promotorzy i mentorzy/prospective supervisors	
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