Faculty Search Committee
Department of Physics
Indiana University
Bloomington, IN 47405-7105

October 1, 2003

**Letter of Transmittal**

Dear Sir/Madam:

I wish to apply for the tenure track assistant professor position in the area of Theoretical Condensed Matter Physics as advertised on the web-site of the Department of Physics. Enclosed is a copy of my curriculum vitae, along with a list of references.

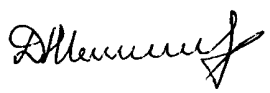
I have recently been working as a postdoctoral associate on first principles simulation of semiconductor nanocrystalls, under the guidance of Professor Jim Chelikowsky at the University of Minnesota. I have a broad background in theoretical and computational science; my research interests are mainly in the areas of computational solid state physics with emphasis on nanoscale simulations. I have also had considerable experience teaching undergraduates in physics.

I am currently working on simulations of double quantum dots with Professor Jean-Pierre Leburton at the University of Illinois at Urbana-Champaign. These systems play an essential role in recent proposals for quantum computation. Further details are given in my curriculum vitae.

I am very committed to pursuing a career in academia, and look forward to hearing from you regarding my application. If you wish to discuss my educational and research background in further detail, please call me at (217) 244-6913.

Thank you for your time and consideration.

Sincerely yours,



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**Research Statement**

Dmitriy Melnikov

Because of potential applications in optoelectronics and biophysics, the study of semiconductor nanocrystals (quantum dots) is a very active field of research. Optical and electrical properties of these confined systems are known to be quite different from their bulk counterparts. In particular, quantum confinement can change the optical properties of nanocrystals, resulting in superior properties for various device applications when compared to those of bulk materials. The characteristics of such devices are strongly affected both by materials in which the nanostructures are embedded (other semiconductors or insulators, colloidal or organic suspensions) and by the ubiquitous impurities always present in modern day materials.

To this end, many theoretical methods (effective mass theory, density-functional theory, Green function method, quantum Monte Carlo, and configuration interaction) have been utilized to understand and predict characteristics of these systems. Quantum dots can be regarded as a sort of "testing ground" for novel computational methods: the regime of nanosizes can be explored by very sophisticated approaches, applicability of which to large many-atom systems is not always transparent, and comparison with available reproducible experimental data can help to separate winners, i.e., methods capable of both describing already observed phenomena and predicting new ones, from losers.

Recently, shallow impurities in group IV nanocrystals have attracted considerable attention due to their potential for quantum computation. Making use of the real space *ab initio* pseudopotential density-functional theory (DFT), we have performed calculations for silicon nanocrystals with their surface passivated by hydrogen in which one of silicon atoms is replaced by phosphorus. The system showed properties remarkably different from those of pure silicon nanocrystals such as a notable absence of the quantum confinement effect on the ionization energy and strong localization of the dopant electron around the impurity site, manifesting itself in an increase of the hyperfine splitting. It is important to continue the study of various shallow defects (both donors and acceptors) and to consider, in particular, the interaction between the dopant states and dangling bonds arising due to the incomplete surface passivation, changes in the absorption threshold, and so on.

To date, the problem with surface passivation of nanocrystals essentially precluded an intensive theoretical study of quantum dots made of other than group IV materials. As an attempt to move in the direction towards the understanding of properties of realistic quantum dot systems, this presents an opportunity to investigate silicon (or germanium) nanocrystals in other preferably wide-band gap materials. The resulting atomic relaxation pattern on the dot/matrix interface and penetration of the wave functions into the surrounding matrix will affect the optical properties of interim quantum dots; in particular, one would expect a much less pronounced size dependence of the higher energy excitations in absorption spectra, in agreement with experimental observations.

Another project is to study III-V and II-VI quantum dots. In a way, these dots are more interesting that those made of group IV materials as there is a wealth of experimental data accumulated on them. As noted, surface passivation is a problem as these dots are usually covered with organics.

However, it has been found that even the simplest, brute force approach on projecting out the states localized on the surface (dangling bonds) gives rise to good agreement with experiments for both band-gap values and absorption spectra. More sophisticated ideas of treating the surface have also been proposed and need to be explored. As soon as the problem with surface passivation is solved, it will be possible to perform calculations for such properties as the Lande *g*-factor (magneto-optics), Auger recombination times (Auger recombination is essential for quantum dots lasers), and so on.

The largest limitation of the present day *ab initio* methods is the size of the quantum dots which is accessible for simulations: to date, the limit is about 1,000 atoms. However, the majority of experimentally fabricated quantum dots are of a much larger size (of the order of 100 nm). This dictates utilization of other approaches for the description of such systems that are based on the effective mass approximation. Among them, effective mass density-functional theory with a local spin density approximation for electron exchange and correlation potential is one of the most popular. The multi-scale calculations based on this method have given a very good understanding of the electronic properties of single quantum dot systems.

However, most practical applications, such as quantum computation, require two or more interacting quantum dots (quantum dot molecules) for which the local density approximation exhibits an exemplary failure: the triplet state of a two electron double dot system becomes the ground state (the singlet-triplet problem is also known as the Holy Grail of quantum computation). This is attributed to the wrong asymptotic dependence in the exchange-correlation functional. This situation can be remedied by utilizing other functionals available from quantum chemistry which ensure proper asymptotic dependence. While the same result could be also achieved by means of quantum Monte Carlo or configuration interaction calculations, the density-functional approach is still beneficial as (1) it is much faster than either of those two methods, and (2) it will allow us to examine time-dependent properties of these systems.

The time-dependent characteristics become of special interest when an idea of quantum computation is taken into account: at its basis, quantum computation involves the change of spins of two electrons in a two dot system (a swap operation). It has been proposed that this could be achieved by applying a time-dependent magnetic field. The spin decoherence time is also a very important characteristic for any working quantum computation system. This means the problem of two interacting spins in two quantum dots in a magnetic field becomes essentially time-dependent and could be tackled by means of a time-dependent density-functional theory which has already been extensively applied for molecular simulations.

During my work at the University of Minnesota and UIUC, I have been dealing with both atomistic calculations of smaller systems and multi-scale calculations of large quantum dots. I would like to continue working in both of these directions as those two approaches become more and more inter-twined. In order to simulate time-dependent characteristics of large quantum dots, it will be necessary to adapt an existing *ab initio* code for high-scale numerical simulations on parallel platforms to the time-dependent effective mass DFT. Then, in collaboration with both Minnesota and UIUC groups, it will be possible to apply this unified code to the projects outlined above and to other new and already existing problems and systems such as the electron-phonon interaction, quantum wires and so on.