

Atomistic calculations of electronic and optical properties of semiconductor quantum dots and nanocrystals

**Tuesday, January 8, 2013 10:00AM
Burton Morgan Building, Room 129**

Dr. Marek Korkusinski

National Research Council of Canada, Ottawa, Canada

The significant interest in self-assembled quantum dots, dot molecules, and colloidal nanocrystals is due to their potential utilization in a new class of photonic devices, including lasers, detectors, optical media for photovoltaics. These systems are also important for coherent devices, such as quantum computing elements, optical memories, sources of single photons and entangled photon pairs. At present, optical spectra of individual dots, without the inhomogeneous broadening, can be measured with the accuracy of tens of μeV . This creates the need for theoretical tools allowing to understand the properties of existing devices and to make accurate predictions in the design phase. To accomplish this, ab-initio computational tools with atomistic precision are needed. The multiscale computational platform QNANO has been developed at the National Research Council of Canada to meet this challenge. The first steps of the procedure are similar to Purdue's NEMO application and involve atomistic definition of the sample, optimization of structure geometry, and calculation of the single-quasiparticle states within the tight-binding model. The electronic properties obtained thus far are then used in computation of dipole and Coulomb matrix elements and calculation of energies and wave functions of interacting N electrons and M holes. This allows to compute emission and absorption spectra, and thus make contact with the experiment. Two specific cases will be discussed: (i) the emission spectra of multiexciton systems confined in a self-assembled quantum dot and (ii) multiexciton generation via Auger coupling in highly excited colloidal nanocrystals. However, the described approach has limitations, which can be traced to an incomplete knowledge of the single-particle wave function obtained in the semiempirical tight-binding model. Overcoming these limitations would allow allowing to compute the particle self-energies and vertex corrections, which are crucial in predictive modelling of optics of semiconductor nanostructures. Steps aimed at improving the discussed approach will be suggested.

About the Speaker: Marek Korkusinski received his PhD in 2004 at the National Research Council of Canada. His doctoral research focused on electronic correlations in semiconductor quantum dots. In 2004 he joined Professor Gerhard Klimeck's group at Purdue University, where he contributed to the NEMO3D project by porting it to large scale cluster systems and by using the platform to investigate the electronic and optical properties of quantum dots and dot molecules. Next, he joined the National Research Council, where he is currently a staff researcher.

Dr. Korkusinski's research interests include the theory of electronic, optical, and transport properties of semiconductor nanostructures computed ab initio or using semiempirical atomistic approaches. Dr. Korkusinski has also an extensive experience in modelling and design of quantum computing elements composed of lateral gated quantum dot devices. In such devices complexity arises from the need to control coherently a large number of electrons in an environment created by a nontrivial sample design, and subject to various sources of decoherence. Dr. Korkusinski is the author or co-author of 80 publications and holds a US Patent for a coded quantum computing element.

