Thesis Title:

Multi-million Atomistic Electronic Structure Calculations in Quantum Dots

Abstract:

Quantum dots grown by self-assembly are typically constructed by 50,000 to 5,000,000 structural atoms which confine a small, countable number of extra electrons or holes in a space that is comparable in size to the electron wavelength. Under such conditions quantum dots can be interpreted as artificial atoms with the potential to be custom tailored to new functionality. In past decade these structures have attracted significant experimental and theoretical attention in the field of nanoscience. The new and tunable optical and electrical properties of these artificial atoms have been proposed in a variety of different fields, for example in communication and computing systems, medical and quantum computing applications. Predictive and quantitative modeling and simulation of these structures can help to narrow down the vast design space to a range that is experimentally affordable and move this part of nanoscience to nanotechnology. The Objectives of this thesis are: (1) to model and simulate the experimental quantum dot topologies at the atomistic scale (2) to theoretically explore the essential physics (i.e. strain, piezoelectricity, optical transitions, stark shift) (3) to assess the potential use of the quantum dots in the real device implementation and to provide the physical insight to the experimentalists. Full three dimensional strain and electronic structure simulations of the quantum dot structures containing multi-million atoms are done using NEMO 3-D to study the impact of the strain and the piezoelectricity. Both single and vertically coupled quantum dot structures are analyzed in detail. The results show that the strain and the piezoelectricity significantly impact the electronic structure of such systems. InAs quantum dots when placed in the InGaAs quantum well red shifts the emission wavelength. Such InAs/GaAs-based optical devices can be used for optical-fiber based communication systems at longer wavelengths (1.3um – 1.5um). Our atomistic simulations of InAs/InGaAs/GaAs quantum dots quantitatively match with the experiment and give the critical insight of the physics involved in these structures. The impact of quantum dot size and shape on the optical matrix element and the optical transitions is studied. Finally, the stark shift in the single and the vertically coupled quantum dots is studied for vertical and in-plane electric field applied.