

Comparison of Molecular Dynamics simulations of CdS Nanocrystals with Experiment

Chad E. Junkermeier* and James P. Lewis

Dept. of Physics, West Virginia University, Morgantown, West Virginia 26506

Garnett W. Bryant

NIST, 100 Bureau Drive, Stop 8423, Gaithersburg, MD 20899-8423

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Semiconductor nanocrystals are small crystallites or clusters, typically with a lattice structure close to the bulk lattice structure, that are intermediate between bulk semiconductors and molecules with regard to the electronic structure. As the number of atoms in the nanocrystal increases, the discrete energies of the molecular orbitals merge toward a discrete pseudo continuum of energy levels that converges to the solid state band-structure of the bulk material. The energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) decreases with an increasing number of atoms. This change in the ‘band gap’ as the size of the crystal changes is known as the quantum size effect [1]. The use of nanocrystals is being intensely explored for a wide range of optical, electronic and quantum technologies that require systems with discrete spectra [2]. Differences are found when comparing the structural properties of nanocrystals with the bulk properties of the same material. We will need to understand these differences in order to realize novel technologies.

We are studying the properties of unpassivated CdS nanocrystals in the 2 nm size range. Starting with nanocrystals in both the zinc-blende and wurtzite structures. Each nanocrystal was allowed to relax via a molecular dynamics (MD) simulation. Once each structure was relaxed, the crystallites were linearly raised to a number of desired temperatures, from 300K to 5000K, with a 10,000 time-step MD simulation. Once each temperature was achieved a 10,000 time-step, totaling 10 ps, was performed on each structure. By computing the radial distribution function and the nearest neighbor distance, we have obtained data that indicates CdS nanocrystals naturally favor atomic distributions very similar to relaxed wurtzite nanocrystals. We will discuss the degree to which this correlates with experiment [3].

We believe that these are the first *ab initio* MD simulations to study nanocrystals of this size.

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- [1] M. G. Bawendi, M. L. Steigerwald, and L. E. Brus. The quantum mechanics of larger semiconductor clusters (“quantum dots”). *Anny. Rev. Phys. Chem.*, 41:477–496, 1990.
 - [2] J. Ouellette. Quantum dots for sale. *Ind. Phys.*, 9:14–17, 2003.
 - [3] B. Banerjee, R. Jayakrishnan, and P. Ayyub. Effect of the size-induced structural transformation on the band gap in CdS nanoparticles. *J. Phys.: Condens. Mat.*, 12:10647–10654, 2000.

*Electronic address: chad.junkermeier@mail.wvu.edu; Also at Dept. of Physics and Astronomy, Brigham Young University, Provo UT 84602