

Abstract Submitted  
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**3D Simulation of Phonon Modes in Semiconductor Nanocrystals<sup>1</sup>**

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— The goal of this current research is the visualization of different phonon modes of NCs with 3D simulation to help in the understanding of their behavior. In order to realize this goal, the numeric data output from the previous atomistic model calculations is used that provides a list of positions of atoms in NCs, the vibration frequencies and the displacement vectors of atoms in each phonon mode. These phonon modes are organized in different symmetries. Methods of visualizing the movement of these atoms are searched, and VMD from the University of Illinois is chosen as the best method to carry out it. VMD can create a 3-D image based on the positions and displacements of atoms, and it allows the user to rotate the structure around and to also “fly” through the structure. To use VMD, a program to convert the output of the simulation program into something that VMD can read is created. In this presentation, how VMD is used to carry out the 3D simulation of phonons in NCs will be discussed, and some interesting simulation results will be presented. These simulations can be used to understand more about the phonons and their related properties of NCs.

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