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Ab initio Theory of Semiconductor Nanocrystals[1]

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With blooming experimental synthesis of various nanostructures out of many semiconductor materials, there is an urgent need to calculate the electronic structures and optical properties of these nanosystems based on reliable ab initio methods. Unfortunately, due to the $O(N^3)$ scaling of the conventional ab initio calculation methods based on the density functional theory (DFT), and the >1000 atom sizes of the most experimental nanosystems, the direct applications of these conventional ab intio methods are often difficult. Here we will present the calculated results using our O(N) scaling charge patching method (CPM) [1,2] to nanosystems up to 10,000 atoms. The CPM yields the charge density of a nanosystem by patching the charge motifs generated from small prototype systems. The CPM electron/hole eigen energies differ from the directly calculated results by only ∼10-20 meV. We will present the optical band gaps of quantum dots and wires, quantum rods, quantum dot/quantum well, and quantum dots doped with impurities. Besides good agreements with experimental measurements, we will demonstrate why it is important to perform ab initio calculations, in contrast with the continuum model k.p calculations. We will show the effects of surface polarization potentials and the internal electric fields. Finally, a linear scaling 3 dimensional fragment (LS3DF) method will be discussed. The LS3DF method can be used to calculate the total energy and atomic forces of a large nanosystem, with the results practically the same as the direct DFT method. Our work demonstrates that, with the help of supercomputers, it is now feasible to calculate the electronic structures and optical properties of >10,000 atom nanocrystals with ab initio accuracy.

[1] L.W. Wang, Phys. Rev. Lett. 88, 256402 (2002).
[2] J. Li, L.W. Wang, Phys. Rev. B 72, 125325 (2005).

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