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Adjustment of the Band Gap Energy According to Sizes of some Cubic Nanosemiconductors of IV, III-V and II-VI Groups

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Abstract

The present work focuses on the modeling of the quantum confinement for several cubic semiconductors of the IV, IV-IV, III-IV, II-VI groups. In this way, we improve the actual methods of the band gap energy adjustment as function of the nano-semiconductors sizes. First, we used the Effective Mass Approximation (EMA) to investigate several confinement regimes such as weak, medium and strong. Then to ensure a good adjustment of this band gap energy, we recalculated the holes and the electrons effective masses of the cubic semiconductors via the K-P theory, the Luttinger parameters, and various interpolations. The results are compared with two other methods: a theoretical model of the Hyperbolic Band (HBM) and experimental method of the absorption spectra and photoluminescence. We found a better adjustment of the band gap energy according to nanosemiconductors size. These results may enhance considerably the efficiency of solar cells based on quantum dots by optimizing the nano-semiconductors size for each junction and converting the maximum of the solar spectrum. Indeed, we have found that the optimal quantum dot radii of all silicon tandem solar cells are 1.1nm for the upper junction and 1.5nm for the middle junction.