World Academy of Science, Engineering and Technology
International Journal of Electrical and Computer Engineering
Vol:16, No:04, 2022

Bandgap Engineering of CsMAPbI3-xBrx Quantum Dots for Intermediate Band Solar Cell

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Abstract : Lead halide perovskites quantum dots have attracted immense scientific and technological interest for successful photovoltaic applications because of their remarkable optoelectronic properties. In this paper, we have simulated CsMAPbI3-xBrx based quantum dots to implement their use in intermediate band solar cells (IBSC). These types of materials exhibit optical and electrical properties distinct from their bulk counterparts due to quantum confinement. The conceptual framework provides a route to analyze the electronic properties of quantum dots. This layer of quantum dots optimizes the position and bandwidth of IB that lies in the forbidden region of the conventional bandgap. A three-dimensional MAPbI3 quantum dot (QD) with geometries including spherical, cubic, and conical has been embedded in the CsPbBr3 matrix. Bound energy wavefunction gives rise to miniband, which results in the formation of IB. If there is more than one miniband, then there is a possibility of having more than one IB. The optimization of QD size results in more IBs in the forbidden region. One band time-independent Schrödinger equation using the effective mass approximation with step potential barrier is solved to compute the electronic states. Envelope function approximation with BenDaniel-Duke boundary condition is used in combination with the Schrödinger equation for the calculation of eigen energies and Eigen energies are solved for the quasi-bound states using an eigenvalue study. The transfer matrix method is used to study the quantum tunneling of MAPbI3 QD through neighbor barriers of CsPbI3. Electronic states are computed using Schrödinger equation with effective mass approximation by considering quantum dot and wetting layer assembly. Results have shown the varying the quantum dot size affects the energy pinning of QD. Changes in the ground, first, second state energies have been observed. The QD is non-zero at the center and decays exponentially to zero at boundaries. Quasi-bound states are characterized by envelope functions. It has been observed that conical quantum dots have maximum ground state energy at a small radius. Increasing the wetting layer thickness exhibits energy signatures similar to bulk material for each QD size.

Keywords : perovskite, intermediate bandgap, quantum dots, miniband formation
Conference Title : ICAN 2022 : International Conference on Advanced Nanophotonics
Conference Location : New York, United States
Conference Dates : April 25-26, 2022