Simulation of Electronic Structure and some Properties of CdTe Crystals Using DFT

Abstract:

The current study investigated the electrical properties of Cadmium Telluride (CdTe)by using the first principle of density functional theory (DFT). The nanocrystals suggested being varied constantly over the network systematically so that the lowest value for energy is obtained, through which stability is obtained and through this exceptionality, the measurements of the properties are in their exact state. The conduction and the valence bandwidths were also studied. The investigations targeted the "highest occupied molecular orbital" (HOMO) [Ionization Potential], and the "lowest unoccupied molecular orbital" (LUMO) [Electron Affinity]. Total and cohesive energies, the atomic iconicity, electron affinity, energy gap (Eg), and the density of states (DOS) for 8, 16, 54, and 64 atoms. The results showed that the shape of the conduction and valence affect the crystal groups significantly, and the energy gap exhibited very close results to their practical counterparts that were previously conducted. When the lattice constant decreases the modulus of bulk and the waves of sound speed increase with the increase of the core atoms number. Subsequently, the applied pressure increases the Plasmon energy and bulk modulus. The key of study is to inspect if using materials in their nanoscale state gives special physical, electronic and optical properties through which devices are manufactured with high efficiency in the solar cell industry. Where the compound becomes a point of a sleeve, and the fluorescent peak shifts across the visible field to the UV field. This was obtained by controlling the size of the compound in 54 and 64, at which the energy gap showed an increase, which would make it more preferred to stimulate the electron from the valence band to the conduction band.