Band structure of fcc-C\(_{60}\) solid state crystal study

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(Received 22 July 2008 ; in final form 31 December 2008)

Abstract

We studied the architecture of the C\(_{60}\) cluster to drive its atomic positions which can be seen at room temperature. We then used the obtained carbon positions as a basis set for the fcc structure to construct the fcc-C\(_{60}\) compound. Self consistent calculations were performed based on the density functional theory (DFT) utilizing the accurate WIEN2K code to solve the single-particle Kohen-Sham equation within the augmented plane waves plus local orbital (APW+lo) method. The cohesive energy has been found to be 1.537 eV for the fcc-C\(_{60}\). The calculated small cohesive energy that results from the weak Van der Waals-London interactions among a C\(_{60}\) cluster with its nearest neighbors is in good agreement with experiment. The electron densities of states (DOSs) were calculated for a C\(_{60}\) macromolecule as well as the fcc-C\(_{60}\) compound and the results were compared with each other. The band gap from DOS calculations has been found to be 0.7 eV. Band structures were also calculated within the generalized gradient approximation (GGA). The band structure calculation results in 1.04 eV for the direct band gap. Two kinds of \(\sigma\) and \(\pi\) bonds were determined in the band structure. Our results are in good agreement with experiment and pseudopotential calculations.

Keywords: C\(_{60}\) cluster, Wien2k, APW+lo, cohesive energy, density functional theory, electron densities of states, charge density, band structure

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