C atom endohedral doping effect on the bond lengths in the crystal structure of fcc-C\(_{60}\)

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(Received 25 August 2009, in final form 1 August 2010)

Abstract

Single and double equilibrium bond lengths of the fcc-C\(_{60}\) crystal were calculated in the absence and presence of the endohedral C atom as an impurity doped into each C\(_{60}\) cluster, i.e., fcc-C@C\(_{60}\), by means of fully-relaxed self-consistent calculations within the density functional theory (DFT) employing the full potential-augmented plane waves plus local orbital (FP-APW+lo) method. The result shows that the single and double bond lengths were decreased for the doped case of fcc-C@C\(_{60}\) when compared with the pure fcc-C\(_{60}\). The reduction in the bond lengths by the carbon impurity doping is attributed to the bond alternation effect and reduction of the symmetry in the C\(_{60}\) molecule. The result shows that the impurity injection gives rise to change in the electron charge distribution and as a result to change in electronic properties.

Keywords: fcc-C@C\(_{60}\), density functional theory, endohedral doping of C\(_{60}\) crystal, bond length, PBE_GGA, Wien2k code

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