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First principles electronic structure calculation of interstitial P doped C_{60} solid. SHIZHONG YANG, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Physics Department, Southern University and A&M College, Baton Rouge, LA70813 — C_{60} solid has a very low thermo-conductivity that can be utilized to improve the *figure-of-merit* of thermo-electric devices. The selection of suitable doping elements and doping concentrations in C_{60} bulk semiconductors, for best performance in thermoelectric applications, is of great interest. In this work, we calculated the electronic structure of solid C_{60}, interstitially doped with P, at concentrations varying from 1:240 to 1:60. We employed a density functional potential and the plane wave method. Both local density approximation (LDA) and generalized gradient approximation (GGA) potentials were considered. The stability, the electron densities of states, dopant location, carrier type, volume change, and charge transfers of P doped C_{60} were calculated and compared to those of B, N, and Co doped C_{60} solids. In the 1:60 doping case, we found that P doped C_{60} solid is an n-type semiconductor with the dopant energy levels in the band gap, close to the top of conduction band. This work was supported in part by the Department of the Navy, Office of Naval Research (ONR, Grant No. N00014-4-1-0587) and by the National Science Foundation (Award No. HRD0503362).

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