First principles electronic structure calculation of interstitial P doped C\textsubscript{60} solid. SHIZHONG YANG, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Physics Department, Southern University and A&M College, Baton Rouge, LA70813 — C\textsubscript{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\textsubscript{60} bulk semiconductors, for best performance in thermoelectric applications, is of great interest. In this work, we calculated the electronic structure of solid C\textsubscript{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\textsubscript{60} were calculated and compared to those of B, N, and Co doped C\textsubscript{60} solids. In the 1:60 doping case, we found that P doped C\textsubscript{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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