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Effects of doping on the band gap of iron pyrite[1] JUN HU, YANNING ZHANG, MATT LAW, RUQIAN WU, University of California, Irvine — Iron pyrite (FeS_2), a highly abundant materials in Earth's upper continental crust, is of great interests in photovoltaic and photo-electrochemical applications, due to its wide band gap of 0.9 - 0.95 eV and large absorption coefficient of $\alpha > 10^5$ cm-1 for $\lambda < 10^3$ nm. However, its electron/hole mobility is typically very low, caused by the presence of sulfur deficiency in crystalline FeS_2 bulks or nanostructures. In principle, doping electrons or holes by exotic elements may not only compensate sulfur deficiency but also create mobile carriers. In this work, we systematically studied the dopabilities of N, P, F and Cl in bulk FeS_2, by using the first-principles calculations. First of all, we found that these elements substitute S under sulfur poor condition in the FeS_2 bulk and nanostructures. While N, P and F dopants merely induce deep localized defect levels, doping 1.6% Cl not only generates a 0.996 μ_B local magnetic moment per Cl and but also increases the carrier density by $3x10^{18}/cm^{-3}$. The defect states are delocalized and hence doping of Cl also improve the carrier mobility in FeS_2. We found that incorporation of Cl also leads to significant structural distortions around Cl atom.

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