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# Electronic structure, optical and dielectric constant of compounds Indium-based: $InAlP_2$, and $InGaP_2$ in its chalcopyrite, CuPt and CuAu-I structures


## Abstract

First principles calculations within the density functional theory framework were carried out to calculate electronic structures and dielectric constant predictions of $InGaP_2$ and $InAlP_2$ compounds. We use three arrangements of these compounds: CuAu-I, CuPt and chalcopyrite ones. Different approximations have been dealt with in order to predict valuable bands gaps energy using DFT calculations. Electronics structure results are promising, due to the good agreement with a number of observable physical-chemistry properties. On the other hand, electron localization function and atom in molecule formalisms have been done to give more insight on the bonding properties. Capabilities that exhibit the $InAlP_2$ in its CuAu-I structure, such as the anisotropy and second harmonic generation, make it promising for an intensive optoelectronic application.


**Keywords —** Ab initio calculations, indium-based compounds, nonlinear optical properties