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Study of Bulk Modulus in Zincblende Nitrogen doped Gallium Phosphide Alloys Using Density Functional Theory BRANDON BUTLER, MUHAMMAD HUDA, Department of Physics, University of Texas Arlington — Solar energy is seemingly the most attractive prospect in renewable energy technology. The problem arises in the ability to convert and store this source of energy into usable electrical energy. Development of solar cell materials has become an object of focus among scientists. In this work, a theoretical analysis will be employed to a study investigating elastic properties, namely bulk modulus, and electronic properties of GaP alloys doped with varying concentrations of nitrogen. The total energy calculation for each periodic system has utilized the principles of density functional theory (DFT) and its' generalized gradient approximation (GGA). Once the total energy calculation was performed, we obtained the bulk modulus, B_0 , and its first pressure derivative, B_0' , by fitting the Birch-Murnaghan equation of state. The bulk modulus was calculated for a few extensively studied materials, namely GaN and un-doped GaP. The results of these prototype calculations compared well with the published experimental values as well as other GGA calculated values. Our computational method of determining the bulk modulus was then used for the $\text{GaP}_{1-x}\text{N}_x$ alloy with varying concentrations of nitrogen. The bulk modulus for these alloys was found to be notably higher than un-doped GaP and further increases with higher concentrations of nitrogen.

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