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Study of Bulk Modulus in Zincblende Nitrogen-doped Gallium Phosphide Alloys Using Density Functional Theory BRANDON M. BUTLER, University of Texas at Arlington, JOHN A. TURNER, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, University of Texas at Arlington — The prospect of solar energy as a renewable resource is ever-increasing. Density functional theory (DFT) calculations can elicit reliable behavior predictions in energy conversion materials to achieve higher efficiencies. Chemical stability of the photocatalysts in aqueous solution is of particular interest for its long term performances. The bulk modulus is a mechanical property that is a good indicator of material stability. GaP has a low band gap and is a good candidate for use as a photocatalyst for hydrogen evolution by splitting water. Unfortunately, it is not stable and highly susceptible to corrosion over a very short time period, making it unfeasible for long-term use. GaN has too high of a band gap but a good stability factor. While these materials both possess desirable qualities, they cannot be used solitarily. We will report electronic properties and bulk moduli from the total energy calculations of the zincblende and wurtzite species using DFT-GGA and DFT+U as a function of doping concentration x. We will also present the density of states and charge density distribution of the alloy materials to study the localization/delocalization effects of N defects levels and their impact on the alloys' stability.

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