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Effects of electronic correlations on the mechanical properties of Gallium Phosphide using density functional theory (DFT+U)[1]

PRASHANT KHATRI, BRANDON BUTLER, University of Texas at Arlington, JOHN A. TURNER, National Renewable Energy Laboragory, MUHAMMAD N. HUDA, University of Texas at Arlington — Developing an efficient material for solar energy conversion and storage has been an important task for many scientists working on renewable energy technology. Gallium phosphide (GaP) alloys are among the materials that have potential to be used in the solar technology. Hence, we investigate the elastic property, mainly the bulk modulus, and electronic properties of GaP. The goal of this work is to study the effect of electron correlation on the mechanical stability of GaP. The calculation of energy as a function of cell volume has been performed using density functional theory with U-parameter (DFT+U) The Birch-Murnaghan equation of state is used to calculate equilibrium cell volume, total energy, bulk modulus, B_0, and its first pressure derivative, B_0'. The bulk modulus obtained using different U-parameter was compared with published experimental values. The use of U-parameter in Gallium d-orbital has increased the theoretical value of bulk modulus, making it closer to the experimental value. On the other hand, increasing values of U on Phosphorus p-orbital decreases the bulk modulus further. The physical consequences of these results will be discussed.

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Prashant Khatri
University of Texas at Arlington

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