
The Study of Structural and Electron Properties of Gase Using the Fundamental Principles

somayeh kashefi aji bisheh*,

Gallium Selenide (GaSe) has been of interest to researchers, and due to its good semi conductivity properties, nonlinear optical properties, photovoltaic conductivity, and also having a suitable energy gap, have many industrial applications. Due to the use of this material in the manufacture of lasers, extensive laboratory research has been carried out, but the theoretical studies performed on it are limited. In this research, the structural properties of the material will be studied theoretically. Using the principles of the functional density theory, we will try to optimize the structure of the material using various potentials; and then will examine the electron and optical properties of the two-phase χ and ϵ of this useful combination. The calculation of the band gap, the state of Electron equilibrium, the distribution of electrical charges around the atoms and the network, and the comparison of results with experimental values are one of the main objectives of this research. This research can be considered as the basis for more extensive research on this useful substance. Therefore, the electron properties, the effect of adding various impurities on the electron and optical properties can be considered for further studies.

Keywords : GaSe

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