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Some physical properties of GaX (X = P, As and Sb) semiconductor compounds using higher-order perturbation theory

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Abstract

Recently proposed model potential for describing the electron–ion interaction is employed to calculate total energy, energy band gap at Jones-zone face at X, equation of state and bulk modulus of GaP, GaAs and GaSb compounds using higher-order perturbation theory. The covalent correction term corresponding to third- and fourth-order perturbation energy terms are used to take account of covalent bonding effect in such semiconductors. The significant value of the covalent bonding term shows the essentiality of higher-order correction for zincblende-type crystals. We have employed five different screening functions alongwith the latest screening function proposed by Sarkar et al. in the present work. The numerical results for the total energy, energy band gap at Jones-zone face and bulk modulus of these compounds are in good agreement with the experimental data and found better than other such theoretical findings. The pressure and bulk modulus at different volumes are obtained by using such higher-order perturbation theory with the application of our model potential. The pressure obtained by this method is compared with pressure obtained by equations proposed by Murnarghan and Vinet et al. The present study also shows that the incorporation of different screening functions generates distinct effects.

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Keywords: Pseudopotential method; Total energy; Equation of state; Bulk modulus

1. Introduction

Groups III–V, II–VI semiconductor compounds and ternary alloys are used in fabrication of optoelectronics devices such as light emitting diodes, photovoltaic cells, photo detectors, lasers,

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modulators, integrated circuits and filters. Due to technological importance of these materials it is essential to understand various properties of such semiconductor compounds and hence it is the current topic of interest for theoretical investigations as well as experimental research. It is also true that the interest of the research has increased on high-pressure behaviors of above materials [1–6].

From the ground state total energy calculation of the system it is possible to calculate various electronic and mechanical properties like binding energy, equation of state and bulk modulus, etc., of crystalline materials. The higher-order perturbation scheme had been proved a simple and successful theory to compute various properties of covalent crystals [7]. Recently, we had successfully employed model potential proposed by Jivani et al. [7] to calculate total energy, equation of states and bulk modulus for Si and Ge. We have also used the similar model potential to evaluate some physical properties of few III–V and II–VI semiconductor compounds [8–10]. The analytical form of our model potential [7] is

$$W_i(r) = \begin{cases} -\dfrac{Z_i e^2}{R_{C_i}}\left[\dfrac{3r}{2R_{C_i}} - \dfrac{r^2}{2R_{C_i}^2}\right], & r < R_{C_i}, \\ -\dfrac{Z_i e^2}{r}, & r \geqslant R_{C_i}, \end{cases} \tag{1}$$

where suffix i denotes element species. In Eq. (1), Z_i is ion valency, e is the electronic charge and R_{C_i} is the parameter of the potential. It is clear from Eq. (1) that our model potential is continuous in real space. This model potential combines both linear and quadratic types of interactions in such a way that additions of quadratic term within the core cancels the linear contribution and make the potential weaker as $r \to 0$ within the core R_{C_i}.

Momentum-space representation of our model potential [7] is

$$W_{i_b}(q) = -\frac{12\pi Z_i e^2}{\Omega q^3 R_{C_i}}\left[\frac{\sin(qR_{C_i})}{2} - \frac{1}{qR_{C_i}} + \frac{\sin(qR_{C_i})}{(qR_{C_i})^2}\right]. \tag{2}$$

Here Ω is the atomic volume and q is the wave vector. The value of potential parameter R_{C_i} is determined by using zero-pressure equilibrium condition. The potential contains only a single parameter and it is better in the sense that it has minimum parameters. In the present study, we have extended the application of model potential proposed by Jivani [7] to study various properties for the GaP, GaAs and GaSb semiconductor compounds. We have not used any historical model potentials and any adjustable parameters like those used by others [11–14].

2. Method of computations

For a covalent crystal with zincblende structure, based on the higher-order perturbation theory, the total energy per atom of the crystal [7,11,14] is given by

$$E = E_i + E_0 + E_1 + E_2 + E_{\mathrm{cov}}. \tag{3}$$

In Eq. (3) E_i is electrostatic energy of point ions immersed in the uniform gas of valence electrons, E_0 is the sum of the kinetic, exchange and correlation energies of the valence electron, E_1 is the first-order perturbation energy of the valence electron due to the pseudopotential. E_2 and E_{cov} are second-order perturbation term and the covalent correction term [11,15], respectively. The covalent correction term is approximately equal to third- and fourth-order energy perturbation terms [13,16].

For the incorporation of exchange and correlation effects to the dielectric function, we adopted five approximations, Hartree (H) [17], Taylor (T) [18], Ichimaru et al. (UI) [19], Farid et al. (F) [20] and Sarkar et al. (S) [21].

2.1. Equation of state and bulk modulus under pressure

The pressure (P) at low temperature is obtained from the first derivative of the crystal energy with respect to the atomic volume Ω_0 which is given by

$$P = \frac{\mathrm{d}E}{\mathrm{d}\Omega_0} = -\frac{r_s}{3\Omega_0}\frac{\mathrm{d}E}{\mathrm{d}r_s} \tag{4}$$

and the bulk modulus (B) is obtained from the second derivative of the crystal energy with respect