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STRUCTURE OF THE MATTER

Electronic structure of Gallium Arsenide under pressure

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SUMMARY. – We present the structural and electronic properties of GaAs under the effect of pressure using large unit cell method within the framework of intermediate neglect of differential overlap (LUC-INDO) calculations. It is found that the results are consistent with the available experimental data and other theoretical results. Energy gap, valence bandwidth, bulk modulus and cohesive energy increase with increasing pressure, while the conduction bandwidth decreases. All the aforementioned properties are obtained by selecting empirical parameter sets for LUC-INDO calculation.

Key words: Electronic structure, gallium arsenide, pressure, LUC-INDO, Energy gap, valence bandwidth, bulk modulus and cohesive energy.

1. Introduction

Theoretical studies of properties continue to be of great importance. Among these are the complete (CNDO) and intermediate (INDO) neglect of differential overlap. The extension of the semi-empirical calculations to solids had begun in approximately one decade after its application to molecules (9). The extension made use of the large unit cell (LUC) method to implement periodic boundary of solid. LUC-INDO calculations have the ability to include large number of atoms including surfaces, interstitials, or vacancies. Previous LUC-INDO calculations for semiconductors had focused on diamond and silicon (14, 6). Other calculations applied the method to F centers (8) titanium oxides (10), etc. These methods were suggested in the seventies of the last century to overcome computational problems of *ab initio* methods for molecules (13). Vast literature accumulated on the use of semi-empirical methods in solid-state problems (20).

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The calculation of energy levels of electrons in solids, that is, the determination of energy bands, is central theoretical problem of solid state physics. Knowledge of these energies and electron wave functions is required, in principle, for any calculation of more directly observable properties including mechanical properties, vibrational spectra, magnetic order, electrical and thermal conductivities, optical dielectric function, and so on. On the other hand, calculation of the bulk ground state properties, such as lattice constants, bulk modulus, cohesive energy, and atomic positions, play an important role in the physics of condensed matter (37), bulk calculations help us to understand, characterize, and predict mechanical properties of materials in surroundings, under extreme conditions.

Gallium arsenide (GaAs) is the most technologically important and the most studied compound semiconductor material. Many band structure parameters for GaAs are known with a greater precision than for any other compound semiconductor. This is especially true of the fundamental energy gap with a value of 1.519 eV (32).

Gallium arsenide has been intensively investigated in recent years. Particular properties studied are its internally-carrier transport and higher mobility for generating microwaves (26), Nanotubes (12), its direct band gap for photonic applications (15), and atomic and electronic structure (35).

Pressure has been proved to be a valuable tool for studying the influence of the band-structure parameters on the electronic properties of semiconductors, bulk crystals, or two dimensional systems. Thus, we have studied the effect of pressure on the some properties of GaAs using the self-consistent large unit cell within intermediate neglect of differential overlap (LUC-INDO) method in the linear combination of atomic orbitals approximation (2).

2. Structural properties and phase transition of GaAs

GaAs crystallizes in the zinc-blende structure. Under ambient conditions and up to 13 GPa adopts the zinc-blende structure. At high pressures (Kelsey *et al*, 1998) it adopts a site-ordered (orthorhombic) Cmcm structure (25). Yu *et al* (Yu *et al*,1978) reported it to be orthorhombic, with an onset at about 17 GPa, and although it could not be conclusively solved at the time using EDX methods, all later experimental studies agreed on its orthorhombic symmetry (Baublitz and Ruoff, 1982). A second transition was reported by Weir *et al* (Weir *et al*, 1989) at about 24 GPa to another orthorhombic structure, Imm2, which then gradually approaches a “sh-type” structure. First-principles calculations by Mujica and Needs (Mujica and Needs, 1996) show that the Cmcm and Imm2 phases are close in enthalpy at high pressures and are clearly favored over other structures. First-principles studies had predicted the existence of a field of stability for a sc16 phase, which was, however, close to the numerical precision of the calculations (Mujica *et al*, 1995). Under compression, sc16 transforms into the Cmcm phase at 22 GPa, which remain stable up to at least 108 GPa (Weir *et al*, 1989). However,

it is believed that only in the range 13-14.5 GPa (where the temperature induced Cmcm→sc16 transition is observed) is the sc16 phase stable (Mujica *et al.*, 2003).

3. Method of calculation

We use large unit cell within intermediate neglect of differential overlap (LUC-INDO) method in the linear combination of atomic orbital (LCAO) approximation (2) to obtain a self-consistent solution for the valence electron. The iteration process was repeated until the calculated total energy of crystal converged to less than 1meV. A total of seven iteration was necessary to achieve self-consistency. The calculations are carried out, on the 8-atom LUC. The positions of atoms that constitute this LUC are calculated in the program according to zinc-blende structure for a given lattice constant. There are four electrons in average per each atom. Hence we have 32 eigenstates, two electrons per state, half are filled (valence band) leaving the other half empty (conduction band) in the ground state. The interaction of the atoms in the central Bravais with the surrounding atoms up to the fourth neighbors is included. These calculations require the determination of wave functions and positions of 864 electrons and 216 nuclei.

In our calculations, we have treated only valence orbitals of Ga ($4s^24p^1$) and As ($4s^24p^3$). The coordinates of the Ga atoms are chosen to be (0, 0, 0); (0, $\frac{1}{2}$, $\frac{1}{2}$); ($\frac{1}{2}$, 0, $\frac{1}{2}$); ($\frac{1}{2}$, $\frac{1}{2}$, 0) whereas the coordinates of the As atoms are chosen to be ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$); ($\frac{1}{4}$, $\frac{3}{4}$, $\frac{3}{4}$); ($\frac{3}{4}$, $\frac{1}{4}$, $\frac{3}{4}$); ($\frac{3}{4}$, $\frac{3}{4}$, $\frac{1}{4}$). The semicore 3d electrons of Ga were found to have as valence electrons and essential to describe accurately structural properties. Spin-orbit splitting will be used to obtain the original nonsplit levels, Experimental spin-orbit splitting Δ_{so} is given the value 0.341 eV for diamond (3).

The Fock matrix elements F_{pp} in their final forms in the LUC-INDO formalism are used in this work (29):

$$F_{pp(0)} = U_{op,op} - \sum_{A \neq B} \sum_v Z_B \gamma_{AB}^{ov} + \sum_v \beta_A^0 (S_{op,vp} - \delta_{ov}) + \sum_r \sum_v P_{rr}(0) \gamma_{AB}^{ov} - \frac{1}{2} \sum_{v \neq 0} P_{pp}(0) f(x) \gamma_{AA}^{ov} - \frac{1}{2} \sum_r P_{rr}(0) \left(\phi_p^r \phi_r^o \middle| \phi_p^o \phi_r^o \right)$$

$$F_{pq(0)} = \sum_v \beta_{AB}^0 S_{op,vp} - \frac{1}{2} \sum_v P_{pq}(0) f(x) \gamma_{AB}^{ov}$$

for p and q on different atomic centers, and

$$F_{pq(0)} = \sum_v \beta_A^0 S_{op,vp} - \frac{1}{2} \sum_{v \neq 0} P_{pq}(0) f(x) \gamma_{AA}^{ov} + \frac{1}{2} P_{pq}(0) \left[\left(\phi_p^o \phi_q^o \middle| \phi_r^o \phi_s^o \right) - \left(\phi_p^o \phi_r^o \middle| \phi_s^o \phi_q^o \right) \right]$$

for p and q on the same atomic center.

Here β_{AB} is the bonding parameter, P is the density matrix, Z is the nuclear

charge, S_{pq} is the overlap integral for atomic function ϕ_q and ϕ_p , γ_{AB}^{ov} is the average electrostatic repulsion between any electron on atom A and any electron on atom B , δ_{ov} is the Kronecker delta and U_{pp} is the local core matrix element, which can be written as (28):

$$[4] \quad U_{pp} = -\frac{1}{2}(I_p + A_p) + \left(Z_A - \frac{1}{2}\right)\gamma_{AA}$$

where I_p and A_p are the ionization potential and electron affinity, respectively, $f(x)$ is the modulating function and is given by (33):

$$[5] \quad f(x) = \left(\frac{\sin x}{x}\right)^2$$

For the 8 atoms LUC x is given by

$$[6] \quad x = \frac{\pi R_{AB}}{a}$$

Here R_{AB} is the distance between the atom A at the central lattice o and the atom B at the ν lattice. Many subroutines are written to simulate the crystalline solids. Position and properties of atoms, which compose these crystals, are entered as input data. The final modified LUC-INDO $k=0$ equations are embodied in these computer routines and solved by iterative methods.

4. Results and discussion

4.1 – Choice of parameters

The number of parameters in the LUC-INDO method is four. These are the orbital exponent ζ , the bonding parameter β , the electronegativity of s -orbital E_s , and the electronegativity of p -orbital E_p . The value of the orbital exponent determines the charge distribution of electrons around the nucleus or in the solid.

These parameters are varied firstly to give nearly the exact value of the equilibrium lattice constant, cohesive energy, band gap and valence bandwidth. The remaining of the output data of the programs is a result of the theory that is used in the present work. We found that the investigated properties were sensitive to the aforementioned parameters. Our suggested parameters are shown in Table 1.

The main assumptions of these methods can be summarized by considering only valence electrons, replacing the overlap matrix by unit matrix, neglecting differential overlap in two-electron repulsion integrals, reducing the remaining set of two-electron integrals to one value per atom pair, neglecting monatomic differential overlap in the interaction integrals involving the cores of other atoms, and finally taking diatomic off-diagonal core matrix elements to be proportional to the corresponding overlap integrals (2).

Table 1The adjusted parameters for *GaAs* in the Zinc-Blende (ZB) structure.

Parameter	Ga	As
Orbital exponent $\zeta_{4s,4p}$ (a.u) ⁻¹	1.7038	2.3240
Bonding parameter β (eV)	-5.7127	-4.0113
Electronegativity of s-orbital E_{4s} (eV)	14.9800	19.4300
Electronegativity of p-orbital E_{4p} (eV)	11.9000	16.000

4.2 – The electronic and structural properties

The second step after the choice of parameters is to examine the structural properties of *GaAs* at the equilibrium lattice constant in order to test the accuracy of the cohesive energy, band gap, and valence bandwidth.

The cohesive energy is calculated from the total energy of the LUC. Since the large unit cell is composed of eight atoms, the cohesive energy is given by (1):

$$[7] \quad -E_{\text{coh}} = \frac{1}{8} E_{\text{tot}} - E_{\text{free}} - E_0$$

where E_{tot} is the total energy, E_{free} is the energy of (*sp*) orbitals for the free atom and equals to 113.394 eV, which value is taken from ionization potential of *GaAs*, and E_0 is the correction of cohesive energy for the zero-point motion of the nuclei. This is a pure quantum mechanical effect and is directly related to the uncertainly principle (7). So $E_0 = 0.067$ eV, is calculated by the formula $E_0 = (9/8) k_B \theta_D$ (per atom) (5), where k_B is Boltzmann constant, θ_D being the Debye temperature which is equal to 360 K (27).

The results of cohesive energies as a function of lattice constant are obtained by the above method at $0k$ and zero pressure. Figure 1 displays the cohesive energy versus lattice constant of *GaAs*, obtained using the same set of parameters. The curve is fitted to the Murnaghan's equation of state (24), from which we obtain the equilibrium lattice constant a_0 , the bulk modulus B , and its derivative B'_0 .

The results of structural and electronic properties of *GaAs* are given in Table 2, along with the experimental measurements and other results. The lattice constant and the cohesive energy for *GaAs* are in a good agreement with experimental results. For example, the calculated lattice constant and the cohesive energy are 5.6542 Å and -6.50 eV/atom, respectively, in good agreement with the corresponding experimental values of 5.65 Å and -6.52 eV/atom, respectively. The lattice constant for *GaAs* presented here is slightly larger than experimental calculations, the difference between the experimental data and our results is very small, i.e., only 0.0042 Å. The results of B and B'_0 are essentially identical to those obtained by using other method. Fig. 2 shows the band structure in the vicinity of the energy gap of *GaAs* throughout the first Brillouin zone (36).

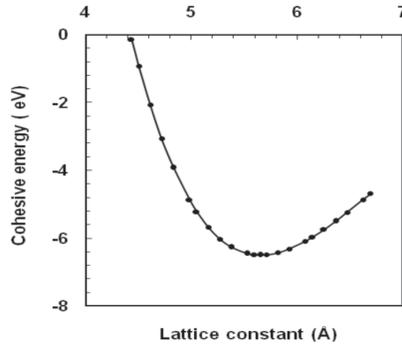


FIG. 1

Cohesive energy as a function of lattice constant for *GaAs*.

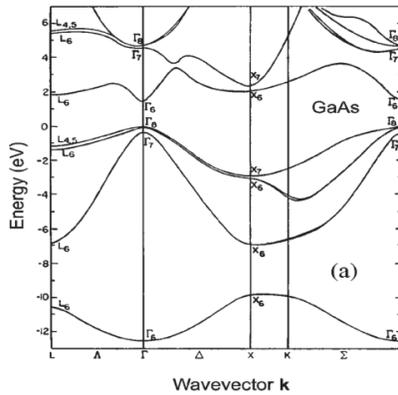


FIG. 2

Diagram of the band structure in the vicinity of the energy gap of *GaAs* throughout the first Brillouin zone (36).

The valence band in *GaAs* consists of four sub-bands when spin is neglected in the Schrodinger equation, and each band is doubled when spin is taken into account. Three of the four bands are degenerate at $k=0$ (Γ point) and form the upper edge of the band, while the fourth band forms the bottom. Furthermore, the spin-orbit interaction causes a splitting of the band at $k=0$. The conduction band consists of a number of sub-bands. The bottom of the conduction band can appear at the center $k=0$, or off center along different k axes. Symmetry considerations alone do not determine the location of the bottom of the conduction band. The conduction-band minimum can be aligned or misaligned in k -space in determining the band gap.

We obtain an energy gap of 1.91eV which is larger than the other results (39, 19) (see Table 2); this is, mainly, a consequence of two approximations made in

this calculation. First, the core structure was ignored, through some compensation results from using semiempirical parameters. Second, using minimal basis set atomic orbitals (without considering any excited levels). However, the INDO method predicts a one-electron eigenvalues band gap that is too large and conduction bands that is much narrower than the band model values. This result in energy gap for *GaAs* bears significant consequences when carriers transfer between this minimum gap in that momentum is conserved for energy gap.

Table 2

Electronic and structural properties calculated within LUC-INDO method at ground state (zero pressure and 0 temperature) compared to experiment and other references.

Property	This work	Experimental	Others
Lattice constant (Å)	5.6542	5.65 (Ref. 19)	5.51 (5.56 Refs. 18, 30)
Cohesive energy (eV/atom)	-6.50	-6.52 (Ref16)	-6.21, -6.51 (Ref.18)
Conduction bandwidth (eV)	6.709
Valence bandwidth (eV)	13.22	13.21 (Ref. 11)	12.69 (Ref. 11)
Energy gap (eV)	1.91	1.42 (Ref. 39) 1.52 (Ref. 40)	1.062, 1.717 (Ref. 30)
Bulk modulus (GPa)	79,8	74.7 (Ref. 19)	75.4, 60.4 (Ref.18)
B'_0	3,686	3.36 (Ref. 42)	...

The valence-band maximum occurs at Γ , the total valence bandwidth or the difference between the top of the valence bands (Γ_{15v}) and the lowest energy of valence band (Γ_{1v}) is 13.22 eV for *GaAs*. The obtained total valence bandwidth is in agreement with previous results. Our work gives a value of the conduction bandwidth to be 6.709eV, but no experimental results are found to the conduction bandwidth of the ZB of *GaAs*.

The energy eigenvalues for *GaAs* crystal are calculated at various high symmetry points of the Brillouin zone and the results are listed in Table 3, along with the results of the GW method (31).

Table 3

Eigenvalues (eV) at Γ and X high-symmetry points from the present LUC-INDO method, compared with other results.

Symmetry point	LUC-INDO	Experimental	Theoretical (Ref. 31)
Γ_{1v}	-13.22	-13.21	-12.69
Γ_{15v}	0.0	0.0	0.0
Γ_{1c}	2.251	1.52	0.57
Γ_{15c}	6.41	4.61	3.57
X_{1v}	-9.521	-10.68	-10.37
X_{5v}	-6.88	-6.81	-6.79
X_{1c}	3.90	1.90	1.8
X_{5c}	8.96	10.33

We also include experimental data in Table 3, for comparison to theoretical results. For folding reasons, the electronic structure is only studied at Γ and X points of the fcc Brillouin zone. The most important band states are considered. They are the valence bands Γ_{1v} , Γ_{15v} , X_{1v} , and X_{5v} . In the case of the conduction bands we consider the states X_{1c} , X_{5c} , Γ_{15c} , and Γ_{1c} . The agreement between the present calculations, LUC-INDO results, and the experimental data is in a good agreement.

4.3 – Effect of pressure on the properties

The pressure is a continuously varying parameter which can be used in systematic studies of the properties of solids as a function of interatomic distances. An interesting phenomenon that may occur at the applied pressure is a sudden change in the arrangement of the atoms, i.e., a structural phase transition. The effect of pressure on the electronic structure and other properties can be calculated from the present theory and computational procedure. The conversion from pressure dependence to the relative lattice change is performed using the following equation:

$$P = \frac{B_0}{B'_0} \left[\left(\frac{V_0}{V} \right)^{B'_0} - 1 \right]$$

where V is the lattice volume at pressure P , V_0 is the equilibrium volume at zero pressure, B_0 the bulk modulus equal to 79.8 GPa, and its pressure derivative B'_0 which is equal to 3.686. We use a pressure up to 14 GPa, because this structure transforms to another phase, Cmcm structure, when pressure exceeds nearly 14 GPa (25). The calculated lattice constant as a function of pressure is shown in Fig. 3. The relative pressure changes of the unit cell constant were found to be linear.

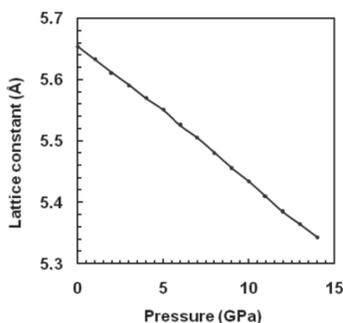


FIG. 3

Lattice constant as a function of pressure for GaAs.

The pressure dependence of the cohesive energy and the bulk modulus are illustrated in Fig. 4. It is shown that the absolute value of the cohesive energy de-

creases as the pressure increases. On the other hand, the bulk modulus increases linearly with pressure.

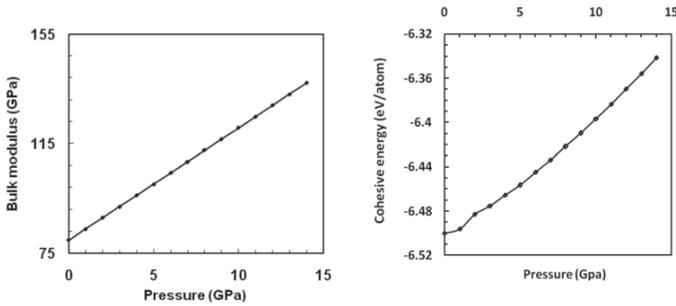


FIG. 4

Effect of pressure on (a) the bulk modulus, and (b) Cohesive energy of for $GaAs$.

The pressure derivative of the high symmetry points (Γ_{1v} , Γ_{15v} , X_{1v} , X_{5v} , X_{1c} , X_{5c} , Γ_{15c} , and Γ_{1c}) is shown in Figure 5, from this figure one can see that the eigenvalues at conduction band (X_{5c} , Γ_{15c} , Γ_{1c} , X_{1c}) are increase with pressure, whereas eigenvalues at valence band (X_{5v} , X_{1v} , Γ_{1v}) decrease with pressure. However, the decrease of X_{5v} , X_{1v} , and Γ_{1v} with pressure is very small.

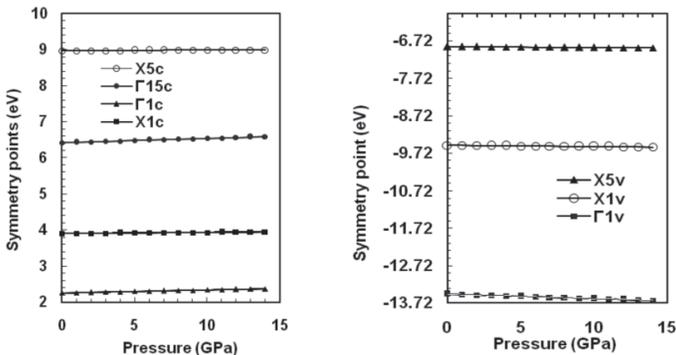


FIG. 5

Effect of pressure on the high symmetry points in (a) conduction band (X_{5c} , Γ_{15c} , Γ_{1c} , X_{1c}), and (b) valence band (X_{5v} , X_{1v} , Γ_{1v}).

The pressure derivative of the direct band gap is shown in Fig. 6. From this figure we can see that the direct band increase with the increase of pressure. The predicted effect of pressure on the valence bandwidth and conduction bandwidth is illustrated in Fig. 7. The valence bandwidth increases with the increase of pressure, while the conduction bandwidth decreases with the increase of pressure.

Our calculations give pressure derivative of ~ 0.136 eV/GPa for the valence bandwidth, and ~ -0.63 eV/GPa for the conduction bandwidth.

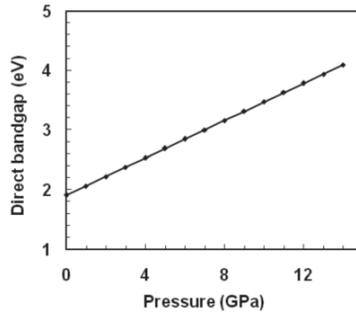


FIG. 6

Effect of pressure on direct gaps for GaAs, calculated within the LUC-INDO method.

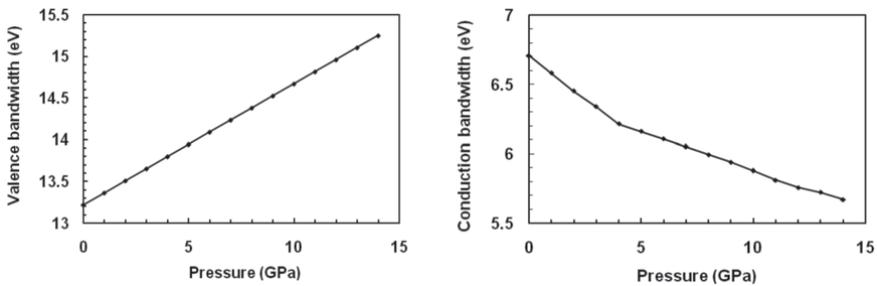


FIG. 7

Effect of pressure on (a) the valence bandwidth, and (b) conduction bandwidth.

We found that the s -state occupation for Ga and As decreases with the increase of pressure, whereas the p -state occupation for Ga and As increases in this case. The occupation of s and p states for Ga and As with pressure is shown in Fig. 8.

The increase of pressure causes an increase of the probability of electron transition from s -orbital to p -orbital. This phenomenon is known and leads to a phase transition due to the change of electronic distribution such as the s - d transition in alkali metals (34).

5. Conclusions

We applied large unit cell within the intermediate neglect of differential overlap method to studies the structural and electronic properties of $GaAs$ semi-

conductor under effect of pressure. The properties obtained are in very good agreement with the existing experimental data and with others results except the energy gap which is greater than the experimental data, this difference is due to the neglect to the core states and to the approximations incorporated with the computational formalism and INDO methods neglect a large number of two electron integrals. The increasing of pressure on *GaAs* is predicted to cause the following effects; an increase of the valence bandwidth and energy gap, a decrease of the conduction bandwidth. In addition to this we have found that the parameter values resulting from the fittings by this method are as a rule physically reasonable and the present self-consistent semiempirical theory can be applied successfully to account for the band structure and physical properties of semiconductors using appropriate parameters. Transforming the calculations to larger unit cells gives generally acceptable results. Relativistic effect is added to the calculation of the energy gap, also zero point energy is added to the calculation of the cohesive energy. Finally, this method is shown to give a good description to the charge density and it is expected that this method could give reliable description for other materials that have zinc blende and cubic structure.

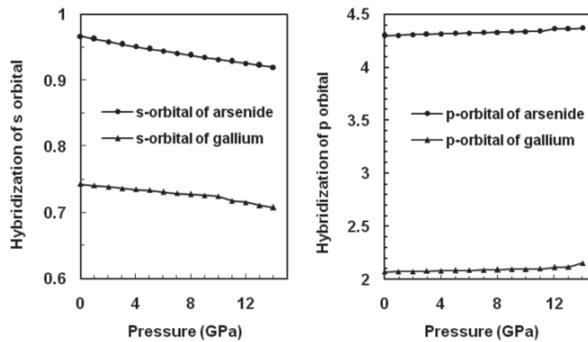


FIG. 8

Effect of pressure on the hybridization of (a) *s*-state and (b) *p*-state.

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