THE ELECTRONIC STRUCTURE OF $Ga_x In_{1-x} As$ and $InAS_x P_{1-x}$ USING THE RECURSION METHOD*

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ABSTRACT

The calculaion of the electronic structure of Gax In*1-x* As and In Asx P*1-x* alloys using the recursion method is reported . A five-orbitals, sp3s*, per atom model is used in the tight-binding representation of the Hamiltonian .

The local density of states is calculated for Ca, In, As and P-sites in a cluster of 216 atoms. The results are in good agreement with other calculations .

ملخص

استعملت طريقة الارتداد (Recursion Method) لدراسة البنيه الالكترونيه للمخاليط الثلاثيه $Ga_x In_{1-x} As$, $In As_x P_{1-x}$ وذلك باستعمال نموذج ذي خمسة مدارات sp^3s^* لكل ذره في تمثيل الترابط المحكم للهاملتونيه .

فحسبت كثافة الحاله الموضعيه لذرات Ga, In, As, p في عنقود يتكون من 216 ذره وكانت النتائج متوافقه الى حد ما مع نتائج منشوره لنفس المخاليط والتي حسبت بطرق اخرى.

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I- INTRODUCTION

There have been extensive experimental studies of the electronic structure of ternary alloys because of their importance in opto- electronic device applications (1-5).A quantitative understanding of the main features of the band structure, such as the compositional variations of band gaps, has been obtained. The theoritical work on the other hand, has not been extensive, mainly due to the difficulty in handling the disorder effects (6).

The virtual-crystal (VCA) and coherent -potential (CPA) approximations are used to study semiconducting ternary alloys. (7-10). Chen and Sher (7), in their CPA calculations, found at most no difference from the VCA results. The CPA theory is capable no of reproducing the compositional variations of band gaps, while most other models may give a rough estimate of bowing at various symmetry points.

In this work, the recursion method is a pplied to study the electronic properties of $Ga_{0.5}In_{0.5}As$ and $InAs_{0.5}P_{0.5}$. The paper is organized in the following manner. A brief summary of the most important aspects of the recursion method is given in section II. The details of the calculation and the results are summarized in section III.

II THE RECURSION METHOD.

The recursion method is amply discussed in the literature(12) Therefore, only a brief discussion of the essentials is given here. The main quantity of interest in this method is the local density of states (LDOS) defined by:

$$N\alpha(E,R) = \sum | \langle n|\alpha R\rangle |2\ \delta(E-En). \qquad (1)$$

Where $|n>$ and En are eigenfunctions and aigenvalues of the system, and $|\alpha R>$ is localized orbital α localed at R. Using the Green function $G(E)=(E-H)^{-1}$,one can write Eq (1) as:

$$N\alpha\,(E,R) = -(1/\pi)\lim \delta\to 0\ \mathit{Im} <\alpha R|G(E+i\delta)|\alpha R> . \quad (2)$$

The method generates by means of the following algorithm, an orthogonal basis $|n\}$, , which contains the orbital $|\alpha R>$ as starting element $|0>$, and in which the hamiltonian *H is tridiagonal.*

$$bn+1|n+1> = (H - an)|n> + bn|n-1>, \quad (3)$$

$$<n|H|m = \begin{cases} an, & \text{if } m=n; \\ bn, & \text{if } m=n+1; \\ bn^*, & \text{if } m=n-1; \\ 0, & \text{otherwise.} \end{cases}$$

The 0-0 element of G

$$< 0|G|0 > = \cfrac{1}{E - a0 - \cfrac{|b1|2}{E - a1\ldots}} \quad (5)$$

is equal to the local density of states $N\alpha(E,R)$. Thus, the essential information needed for LDOS is contained in the set of coefficients a_n ,b_n .

Once the coefficients an, bn are determined, the continued fraction can immediately be calculated for any E.

III. RESULTS AND CONCLUSIONS

The recursion method does not of course provide detailed k-space information about structure; but it yeilds valuable information on (LDOS) at chosen atomic sites . Encouraged by the smallness of the alloys scalturing effects, we use an interpolation procedure and to make a reliable use of known properties of the constituent binaries GaAs, InAs and InP.

A cluster of 216 atoms in zincblende structure with a lattice constant a= 5.6536 A° is used for GaAs . The Slater - Koster (SK) parameters used in describing the Hamiltonian H were calculated using the semi- emperical matrix elements of the Hamiltonian of Vogl et al (13) and given Table1. The five orbitals, sp3s*, per atom are used so that there are 1080 orbitals in the system. Here s* is the extra s-orbital, originally introdused by Vogl et al (13) to correct the lower conduction bands instead of extending the interactions to second nearest neighbours.

Table 1. Slater Koster parameters for GaAs,InP and InAs (eV).

Parameters	GaAs	InP	
-ssσ	1.6133	1.3403	1.4013
sapcσ	1.9399	0.9641	1.3144
-scpaσ	2.5045	2.4173	2.3551
ppσ	3.0276	2.5862	2.6946
-ppπ	0.7808	0.5881	0.6574
sa*pcσ	2.0967	1.4992	1.4612
-sc*paσ	2.0818	1.9401	1.6930
-E(s,c)	2.6569	1.4826	2.7219
E(s,a)	8.3431	8.5274	9.5381
E(p,c)	3.6686	4.0465	3.7201
E(p,a)	1.0414	0.8735	0.9099
E(s*,c)	6.7386	7.0665	6.7401
E(s*,a)	8.5194	8.2635	7.4099

The same model is used to study InAs and InP . The cluster, in these cases is arranged in the zincblende structure with a lattice constant a=5.8687 A°, and a= 6.036 A° respectively. The SK parameters used are given in Table 1.

The number of recursion coefficients an,bn2 calculated in all cases reported in this section is 17. We present the calculated LDOS curves for $Ga_{0.5}In_{0.5}As$ and $InAs_{0.5}P_{0.5}$. Figure 1-6 show the LDOS curves for Ga,In As, and p sites in the two alloys studied respectively .

Althogh we calculated the corresponding integrated DOS the structural energies, for simplicity we present here, in Figures 7 and 8 integrated DOS, structural energy for In in $Ga_{0.5}In_{0.5}As$. The last two Figures 9 and 10 show the orbital decomposition of LDOS for In-site in $Ga_{0.5}In_{0.5}As$.

In all calculations presented we used an averageing procedure where the interaction parameters and the lattice constant for the ternary $A_x B_{1-x} C$ are taken as:

$$Vallay = V_{AC} + (V_{BC} - V_{AC})(1-x). \quad (6)$$

$$aalloy = a_{AC} + (a_{Ba} - a_{AC})(1-x). \quad (7)$$

Self energies of same type of atoms are also averaged so that the concentration dependence of each environment is approximately taken into account . These two alloys systems have been studied among other ternery alloys . Magri et al (11) used special quasirandom structures (SQS's) to study the electeonic structure of these systems, but they calculate the total density of states . Gera et al (6) used CPA to calculate the electronic structure of these alloys and they reported the LDOS for these alloys . To compair with Gera et al (6), in all LDOS , we have extra peak on the right . It is due to the excited s state used in our calculation to produce the conduction band. Also the energy axis, must be rescaled, such that zero coinside with top of valance band. In this case our LDOS for anion sites Figure 1 , 2 , and 3 in good agreement with figure 1, of Gera et al (6).

The same for cation sites Figure 4 , 5 , and 6 are in good agreement with theirs Figure2 , in number of peaks and character . Our decomposed LDOS , Figure 9 and 10 are in good agreenment with their partial LDOS . Including an extra orbital, like Ga 3d for example, may affect the lower part of valane bands, but this would be neglibile since Ga 3d level lie about 6 eV below 4s levels .

To study the band gap variation with the concentration is not easy within the recursion methd because of the inherent difficulties with band gaps in this technique . They do not come out sharp enough for easy identification .

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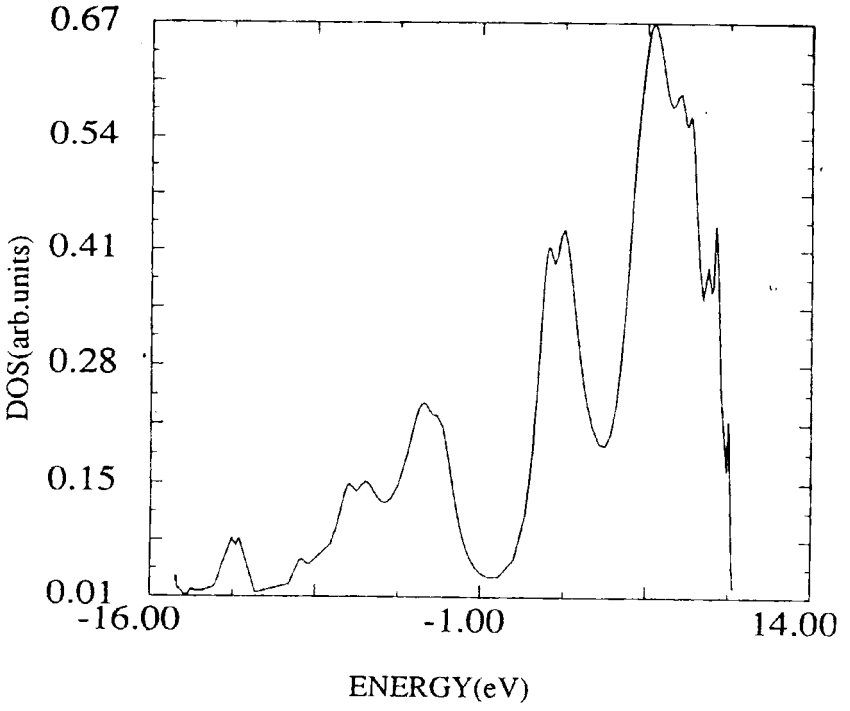
FIGURE CAPTIONS:

Figure (1) Partial LDOS at Ga-site in $Ga_{0.5}In_{0.5}As$.
Figure (2) Parial LDOS at In-site in $GA_{0.5}In_{0.5}As$.
Figure (3) Partial LDOS at In-site in $InAs_{0.5}P_{0.5}$.
Figure (4) Partial LDOS at P-site in $InAs_{0.5}P_{0.5}$.
Figure (5) Partial LDOS at As-site in $Ga_{0.5}In_{0.5}As$.
Figure (6) Partial LDOS at As-site in $InAs_{0.5}P_{0.5}$.
Figure (7) Partial integrated DOS at In-site in $Ga_{0.5}In_{0.5}As$
Figure (8) Partial structural energy at In-site in $Ga_{0.5}In_{0.5}As$.
Figure (9) Partial SDOS at Ga-site in $Ga_{0.5}In_{0.5}As$.
Figure (10) Partial PDOS at $Ga_{0.5}In_{0.5}As$.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0.54
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0.28
0.15
0.01
DOS(arb.units)
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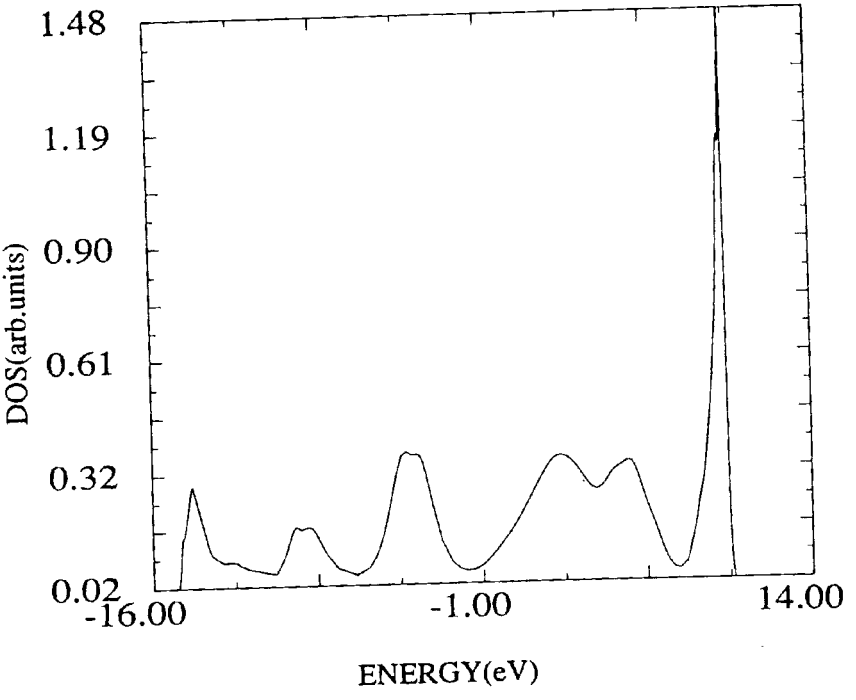
-1.00
14.00
ENERGY(eV)

Fig.1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1.19
0.90
0.61
0.32
0.02
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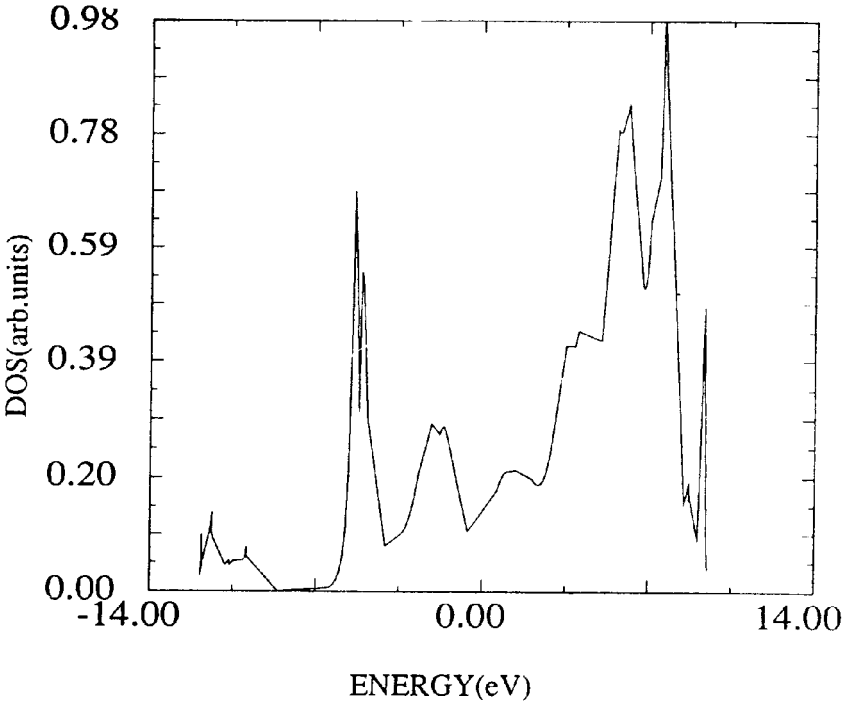
14.00
ENERGY(eV)

Fig.2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0.78
0.59
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0.00
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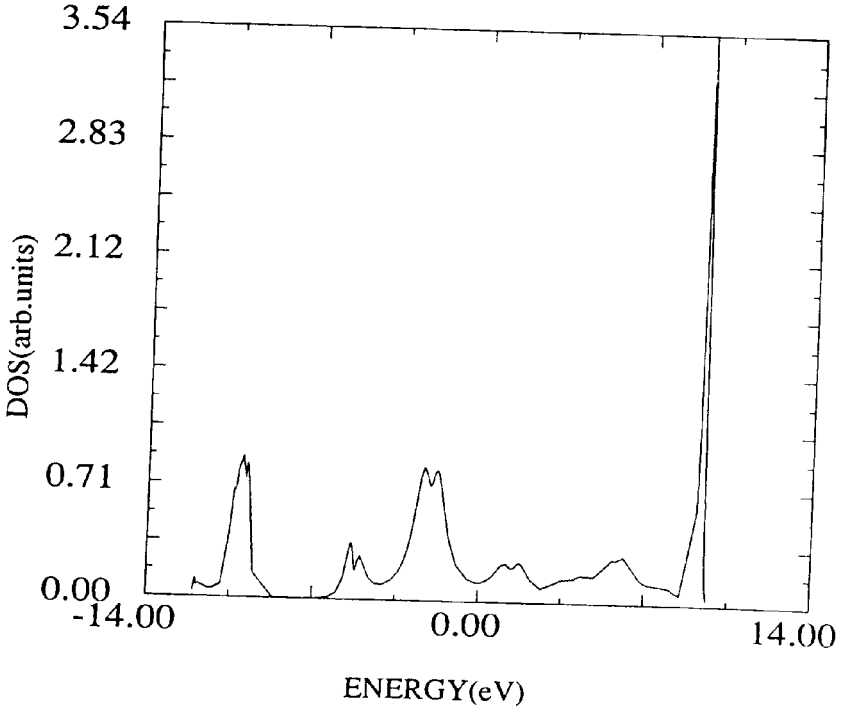
0.00
14.00
ENERGY(eV)

Fig. 3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2.83
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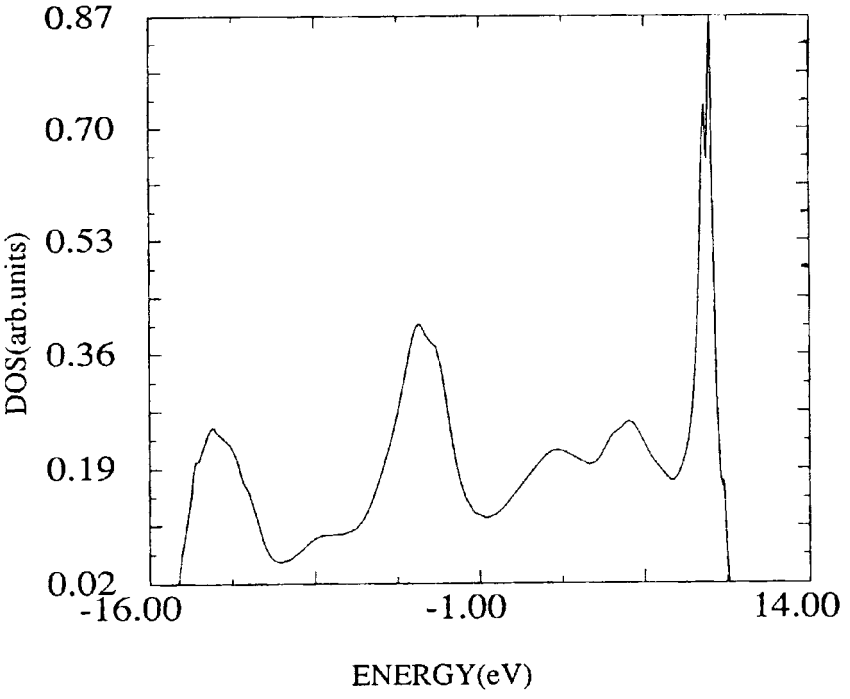
0.00
DOS(arb.units)
-14.00
0.00
14.00
ENERGY(eV)

Fig. 4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0.70
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DOS(arb.units)
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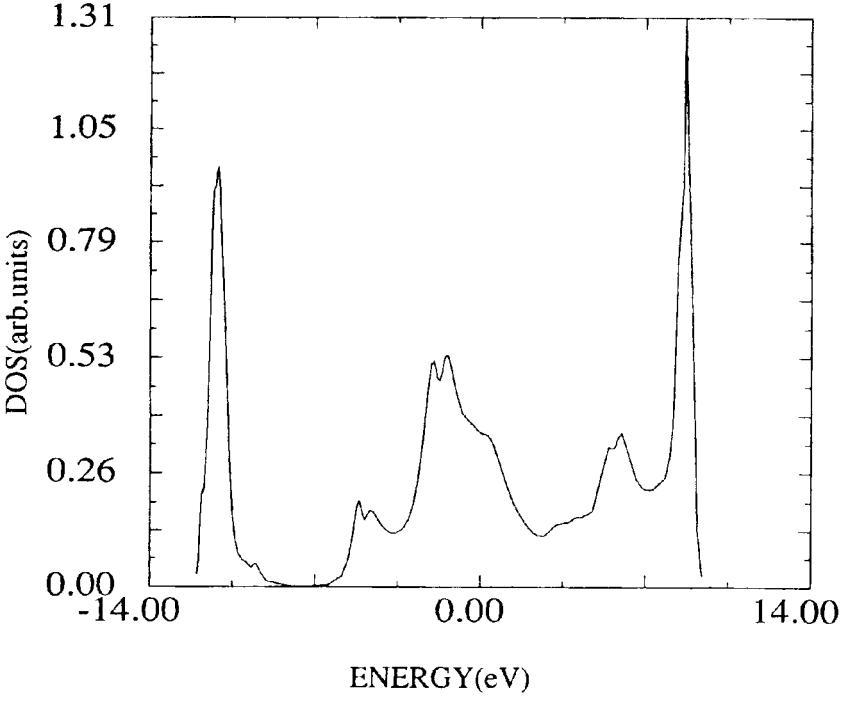
-1.00
14.00
ENERGY(eV)

Fig.5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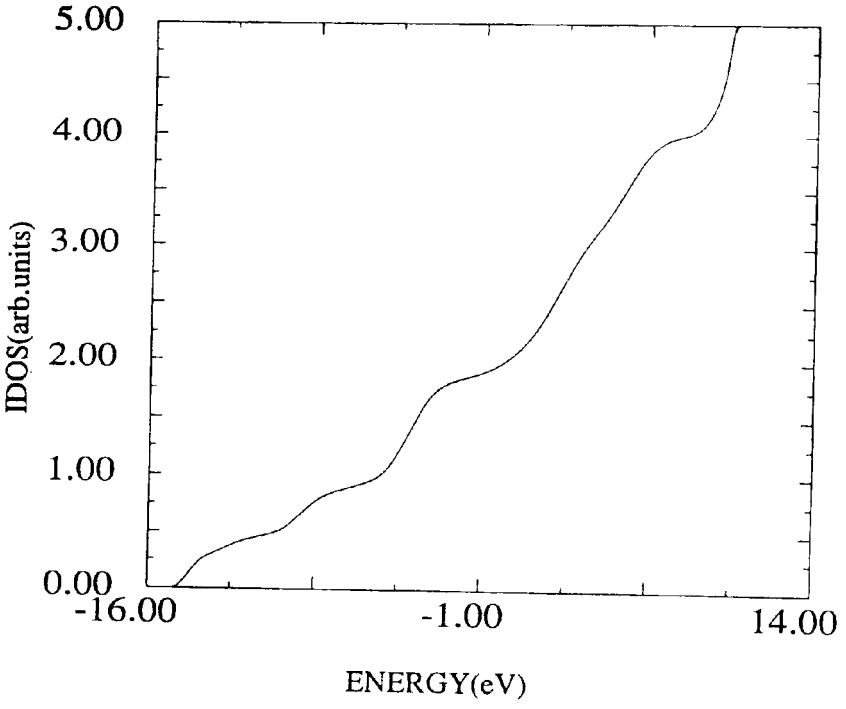
14.00
ENERGY(eV)

Fig. 6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4.00
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2.00
1.00
0.00
IDOS(arb.units)
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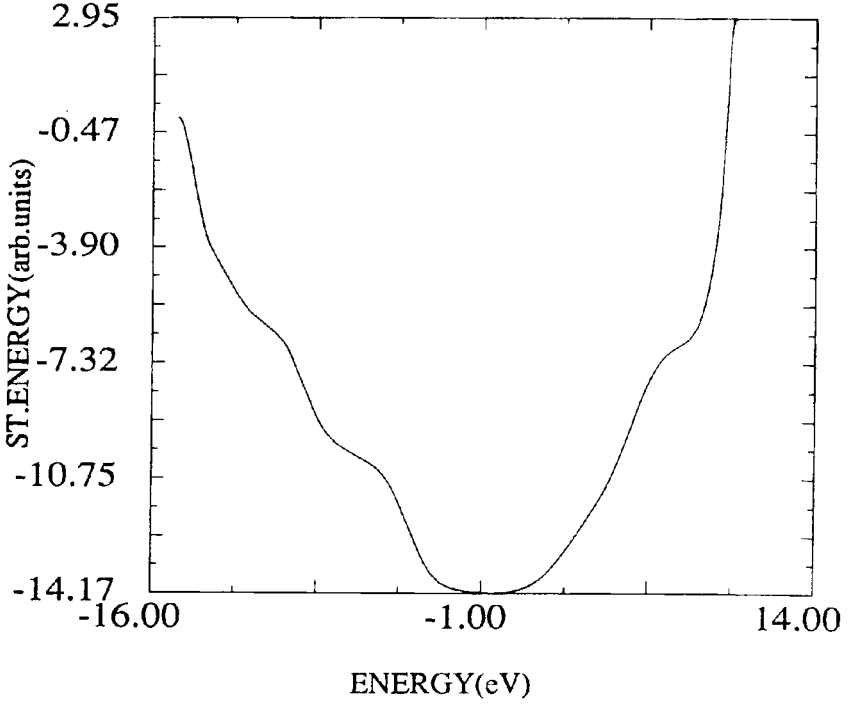
-1.00
14.00
ENERGY(eV)

Fig. 7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-3.90
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ST.ENERGY(arb.units)
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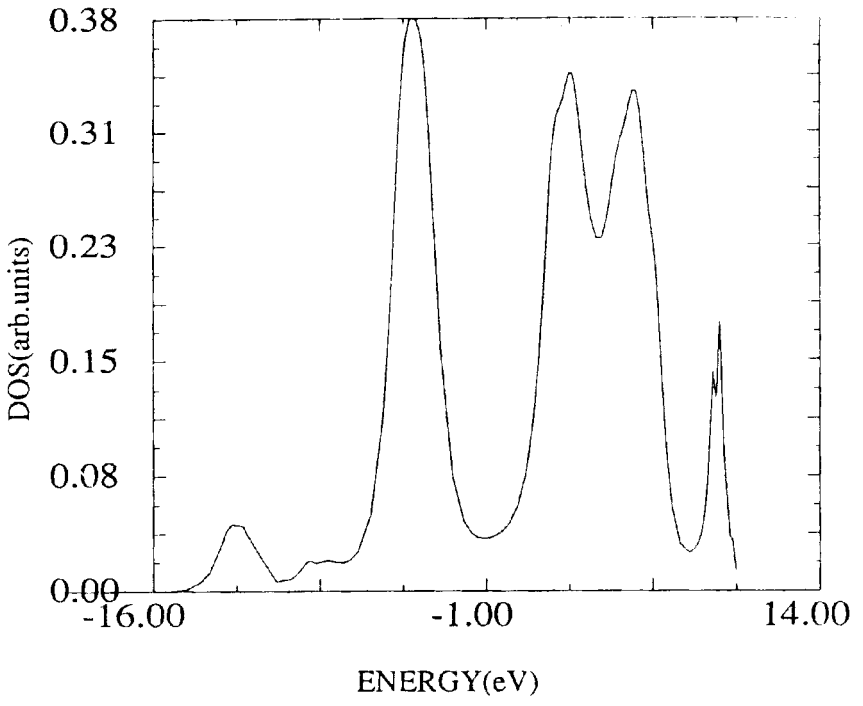
-1.00
14.00
ENERGY(eV)

Fig. 8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0.08
0.00
DOS(arb.units)
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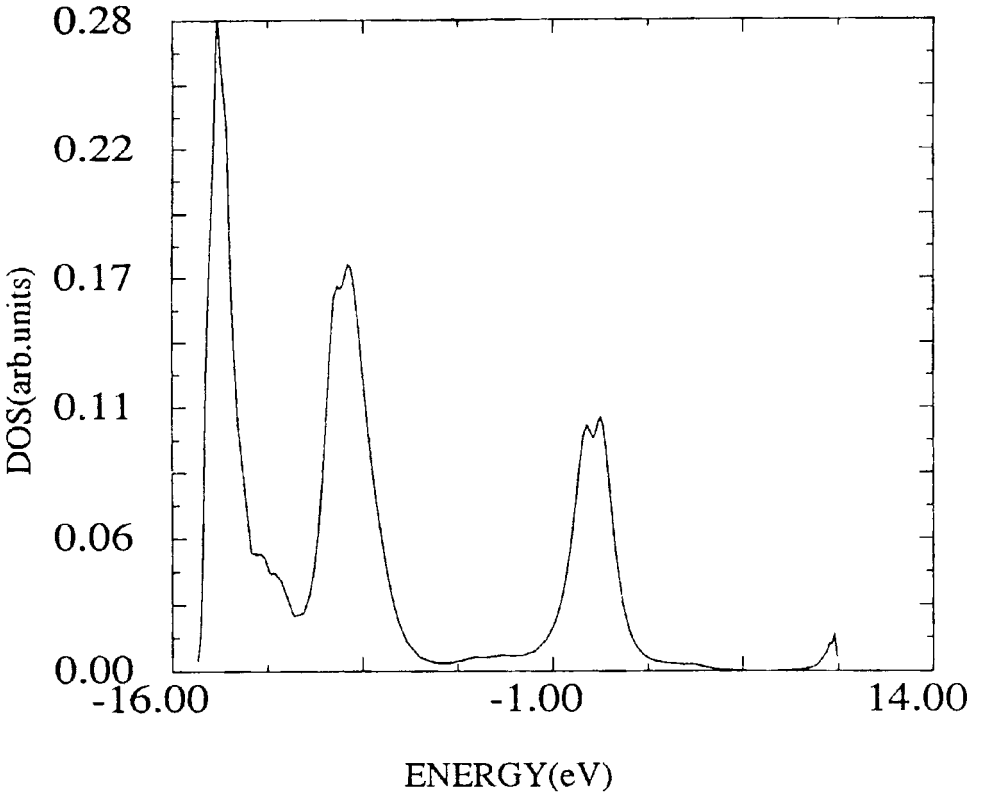
-1.00
14.00
ENERGY(eV)

Fig 9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0.22
0.17
0.11
0.06
0.00
DOS(arb.units)
-16.00
-1.00
14.00
ENERGY(eV)

Fig. 10