Investigation of properties for the commun compounds employed in Photovoltaics

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***Abstract*—The III-V semiconductors are the most used compounds high-efficiency for solar cells, In this work we aim, to study the structure and band structure properties for Indium–V semiconductor, The development of new model of solar cells from those semiconductors materials are very promising technology to give high conversion efficiency. To investigate the electronic and optical properties of binary compounds Indium -V (InAs, In Sb, InN and InP) in Zinc blend structure we have used the density functional theory (DFT), with Full-potential linearized Augmented Plane Wave. For exchange and correlation energy treatment we employed the local density approximations (LDA) as proposed by Wang and Pedrew and the generated gradient approximation (wc-GGA) from Wu and Cohen to calculate the accurate band structure we used the mBjexchange potential. These results show that those materials have wide range of bandgap and that its hold promise for the potentiel application in optoelectronic devices as a results we have found that thoses materials could convert these structures capable of converting wavelength between [810 nm and 3500 nm] from solar spectrum into electrical energy. Furthermore, we could have very interesting material by making alloys with those binary compounds.**

Keywords: Solar cell, FP-LAPW, mBJ, III-V semiconductor.

I. Introduction

The most promising technologies for solar cells is multijunction technology wich gives the highest efficiency for solar cells as it is demonstrates by NREL laboratory [1] . The III-V semiconductor is one of the most interesting materials to use in multijunction solar cells applications because of their structure , electronic and optical properties.

The III-V solar cells combine the advantage of high-efficiency. The materials most suitable for multijunction designs are the III-V semiconductors families, given their range of optical and material properties where incompatibilities, especially due to lattice constants, may be managed or even eliminated. We had chosen to study the zinc blend binary compounds Indium -V (InAs, In Sb , InN and InP) because its widely used .

II. COMPUTATIONAL *DETAIL:*

The III-V solar cells technology necessities three basic design to take in considerations: band gap differentiation, lattice constant matching, and current matching. Two of that criteria, lattice and bandgap parameters could be investigated by using the WIEN2k code ; This code employs a scalar relativistic full potential linear augmented plane wave (FP-LAPW) method . For exchange and correlation energy treatment we employed the local density approximations (LDA) as proposed by Wang and Pedrew , the generated gradient approximation (wc-GGA) from Wu and Cohen and PBE-GGA to calculate the accurate band structure we used the mBj exchange potential.

*A. **Structural study:***

The lattice constant of semiconductor materials is the distance between atoms locations in a crystal. To make an effective multijunction solar cell (III-V solar cell) it is important that the materials used have a similar lattice constant. If there is a mismatch in the lattice structures of the material defects or dislocations can occur. These defects can cause recombination which is when electrons in the conduction band drop back down into the valence band. The equilibrium lattice constant (a) has been determined by calculating the total energy at a number of lattice constants around the experimental value. we had use LDA , WC-GGA and PBE-GGA as showing in table1.

Comparing our results to the other works we found a small difference owing to the different used approximation. The wc-GGA by Wu and Cohen is very suitable for the structural properties of solids according to a lot of calculation for semiconductors that have confirmed it.

Table1 : Calculated lattice parameter (a) for the binary compounds (InP, InAs , InN and InSb) with wc-GGA , LDA and PBE-GGA.

	Lattice parameter a (A°)				
	Our work			Other work	exp
	LDA	WC-GGA	pbe-GGA		
InP	**5,84**	**5,84**	**5,97**	**5,84 ; 6,01[e]**	**5,86[a]**
InAs	**6,03**	**6,09**	**6,18**	**6,05[c]**	**6,05[a]**
InSb	**6,42**	**6,45**	**6,63**	**6,50[e]**	**6,47[a]**
InN	**4,96**	**4,98**	**4,88**	**4,99[c]**	**4,95[b]**

a: [2] b : [3] c : [4] e : [5]

*B. **Band structure properties:** :*

The four materials have direct band gap where the valence band peak and the lowest conduction band are in the same point of symmetry Γ as showing in the figure1.

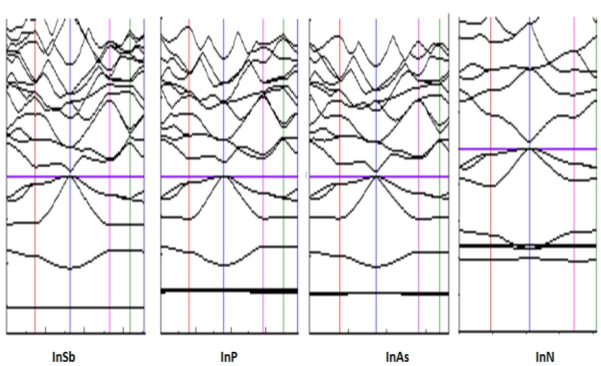

Fig 1- band structure of the four materials traced by mbj-GGA

As known GGA and LDA giving under estimate values of band gap parameters so we had used mBJ to to correct band gap parameters (for the values look Table2).

Table2 : Calculated band gap energy (Eg) for the binary compounds (InP, InAs , InN and InSb) with wc-GGA , LDA and PBE-GGA and mBJ.

	Bandgap Eg (eV)					
	Our work				Other work	exp
	LDA	WC-GGA	pbe-GGA	mBJ		
InP	**0,51**	**0,45**	**1,01**	**1,53**	**1,43[e]**	**1,35**
InAs	**0**	**0**	**0**	**0,57**	**0,70[c]**	**0,41[h]**
InSb	**0**	**0**	**0**	**0,36**	**1,02[e]**	**0,63[g]**
InN	**0**	**0**	**0**	**0,66**	**0,60[e]**	**0,7[f]**

h: [6] f:[7] g:[8] l:[2]

The following equation could calculate the wavelength from the bandgap parameters,

$$Eg(eV) = 1240/\lambda(nm) \qquad \text{Eq (1)}$$

The wavelengths calculated from Eq. (1) are 810.475 nm, 1878.7878 nm, 2175.4385 nm and 3444.4444 nm for InP, InN , InAs ans InSb binary compounds, respectively.

These wavelengths are between the UV range and the infrared range , which confirms that our compounds can be incredibly engaging to fabricate solar cells materials that could be convert a large part from the solar spectrum.

CONCLUSIONS

Our computations with LDA, PBE-GGA and wc-GGA generally give a good agreement with the experimental data for structural properties. We observe that in general, GGA estimate the experimental data while LDA underestimates. However, they agree with the experiment between 2 and 5%. For electronic band structure, our results with LDA and GGA, although in good agreement with other computational work, are lower than the experimental results. This is due to a simpler form of the exchange-correlation functional. However, band gap calculated with mBJ is closer to the experimental values .These results indicate that those materials have wide range of band gaps and that its hold promise for the potential application in optoelectronic device such as solar cells

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