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Nowotny–Juza NaZnX (X = P, As and Sb) as photovoltaic materials

A.H. Reshak *

New Technologies – Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic
Center of Excellence Geopolymer and Green Technology, School of Material Engineering, University Malaysia Perlis, 01007 Kangar, Perlis, Malaysia

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Abstract

The electronic band structures of Nowotny–Juza NaZnX (X = P, As and Sb) compounds suggest that the valence band maximum (VBM) and the conduction band minimum (CBM) are located at the center of the Brillouin zone, resulting in a direct band gap of about 1.80, 1.47 and 0.25 eV, respectively. The total and the partial density of states explore the type of orbitals which rule the band gaps and to classify the hybridizations between the orbitals. The VBM is formed mainly by P-p, As-p, Sb-p, Zn-p and Na-p states with substituting P → As → Sb. The CBM of NaZnP is formed by Zn-s, Na-s/p, while the CBM of NaZnAs (NaZnSb) is formed by Zn-s and As-d (Zn-s and Sb-d), one can see that As-d and Sb-d orbitals govern the CBM of NaZnAs and NaZnSb, hence these orbitals rule the energy gaps. It is clear that there exists a strong hybridizations between Na-s/p and As-d states, Zn-s/p and P-p states, Sb-p and Zn-s states and also between Sb-d and Na-s states. The strong hybridization may led to form a strong covalent bonding between these atoms. For more detail and to get deep insight into the electronic structures, the optical properties were investigated. The uniaxial anisotropy and the birefringence values confirm the existence of the considerable anisotropy between the two components of the optical properties. The calculation confirm that these compounds are promising candidates for optoelectronics devices.
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Keywords: Nowotny–Juza compounds; Photovoltaic; Structure properties; Optical properties

1. Introduction

The filled tetrahedral Nowotny–Juza NaZnX (X = P, As and Sb) compounds are direct band gap semiconductors, therefore these compounds are promising candidates for photovoltaic and efficient thermoelectric applications (Wood et al., 1985; Carlsson et al., 1985; Bacewicz et al., 1988; Wei and Zunger, 1986; Kuriyama et al., 1994a,b; Beleanu et al., 2011; Madsen, 2006). There are several experimental and theoretical investigation were reported for the other Nowotny–Juza compounds for instance LiXY (X = Mg, Zn and Y = N, P, As), LiCdP, LiCdAs and AgMgAs. It was found that LiZnP possess a direct band gap, despite that its binary GaP is indirect band gap semiconductor (Wood et al., 1985). The measured optical gap of LiZnAs founds to be a direct gap of about 1.51 eV at 300 K which is grater than the gap for GaAs (1.42 eV at 300 K) (Ul Haq et al., 2014; Reshak et al., 2013a). Gallium arsenide (GaAs) solar cell shows superior conversion efficiency and radiation resistance when compared to silicon solar cells (Kumar et al., 2004; Deshmukh and Nagaraju, 2005; Minwoo et al., 2013; Davis and Knight, 1975). We should emphasize that there are dearth information concerning the NaZnX (X = P, As and Sb) compounds especially the investigation of the

* Address: New Technologies – Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic. Tel.: +420 777 72 9583; fax: +420 377 63 4702.
E-mail address: maalidph@yahoo.co.uk

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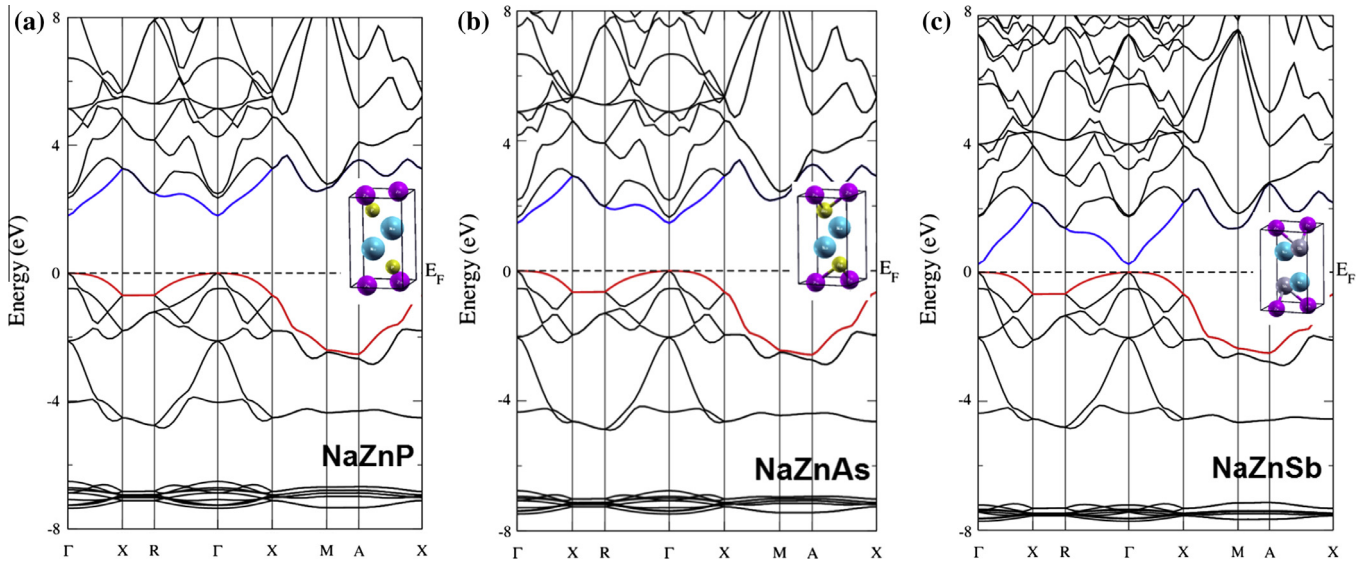

Fig. 1. Calculated electronic band structures of Nowotny–Juza NaZnX (X = P, As and Sb) compounds using mBJ; (a) NaZnP; (b) NaZnAs; (c) NaZnSb.

Table 1
Calculated energy band gaps, $\varepsilon_1^{\parallel}(0), \varepsilon_1^{\perp}(0), \varepsilon_1^{tot}(0), \delta\varepsilon(0), R^{\parallel}(0), R^{\perp}(0), n^{\parallel}(0), n^{\perp}(0)$ and $\Delta n(0)$ of Nowotny–Juza NaZnX (X = P, As and Sb) compounds using mBJ in comparison with previous calculations at ambient pressure and high pressure (α, β, γ-phases).

	NaZnP	NaZnAs	NaZnSb
E_g (eV)	1.80, 0.79[a], 0.77[b],1.30[c], 0.64[d], 0.73[e], 0.75[f], 0.45[g], 1.0[h], 0.71[i], 0.66[j], 0.35[k], 0.85[l], 0.0[m,n]	1.47, 0.44[a], 0.39[b], 0.79[c], 0.163[d], 0.0[f,j,o]	0.25, 0.0[a,b,c,d,f,j,o]
$\varepsilon_1^{\parallel}$ (0)	6.41	7.40	8.90
$\varepsilon_1^{\perp}$ (0)	7.15	8.40	10.50
ε_1^{tot} (0)	6.78	7.90	9.70
$\delta\varepsilon$ (0)	−0.109	−0.126	−0.164
$R^{\parallel}$ (0)	0.189	0.214	0.247
$R^{\perp}$ (0)	0.207	0.237	0.279
$n^{\parallel}$ (0)	2.54	2.72	2.98
$n^{\perp}$ (0)	2.69	2.89	3.23
$\Delta n(0)$ (0)	0.15	0.17	0.25

[a] Reference Charifi et al. (2014) using FPLAPW within LDA.
[b] Reference Charifi et al. (2014) using FPLAPW within GGA.
[c] Reference Charifi et al. (2014) using FPLAPW within EVGGA.
[d] Reference Jaiganesh and Merita (2008) using TB-LMTO method within LDA.
[e] Reference Charifi et al. (2014) for α-phase (high pressure phase) using FPLAPW within LDA.
[f] Reference Jaiganesh and Merita (2008) for α-phase (high pressure phase) using TB-LMTO method within LDA.
[g] Reference Charifi et al. (2014) for α -phase (high pressure phase) using FPLAPW within GGA.
[h] Reference Charifi et al. (2014) for α -phase (high pressure phase) using FPLAPW within EVGGA.
[i] Reference Charifi et al. (2014) for β -phase (high pressure phase) using FPLAPW within LDA.
[j] Reference Jaiganesh and Merita (2008) for β-phase (high pressure phase) using TB-LMTO method within LDA.
[k] Reference Charifi et al. (2014) for β -phase (high pressure phase) using FPLAPW within GGA.
[l] Reference Charifi et al. (2014) for β -phase (high pressure phase) using FPLAPW within EVGGA.
[m] Reference Charifi et al. (2014) for γ-phase (high pressure phase) using FPLAPW within LDA, GGA, EVGGA.
[n] Reference Jaiganesh and Merita (2008) for γ-phase (high pressure phase) using TB-LMTO method within LDA.
[o] Reference Charifi et al. (2014) for α, β, γ-phases (high pressure phase) using FPLAPW within LDA, GGA, EVGGA.

photovoltaic properties of such important candidates. Recently Charifi et al. (2014) reported a theoretical study on the structural, electronic, elastic and phonon properties of NaZnX (X = P, As and Sb) compounds using the full-potential linear augmented plane wave and pseudopotential plane wave method. They used the generalized-gradient approximation (GGA), the local density approximation (LDA) and Engel–Vosko (EVGGA) formalism, to calculate the lattice constant, bulk modulus, second-order elastic constants, the electronic band structures and the related total density of states and charge density. They studied three high-pressure phases and found that phase transition pressure occurs from tetragonal to high-pressure phase. Their calculations predict that NaZnSb is a metal in all phases. In 2008, Jaiganesh and Merita, performed first-principles tight-binding linear muffin-tin orbital

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