Principle Investigation of Structural, Electronics and Chemical Properties of Sn Doped PbX (X=S, Se, Te)

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Abstract

The Structural, electronic and chemical bonding of the Sn doped PbX (X=S, Se, Te) are calculated by full potential linearized augmented plane wave method (FP-LAPW) within density functional theory (DFT). Generalized gradient approximation of Wu and Cohen (WC-GGA) is used for calculating the exchange correlation effects. The structural parameters changes with respect to doping. The calculations show that the band gap decreases with the increase of Sn concentration. It has observed that the s, p and d states of PbX (X=S, Se, Te) control their electronic properties. The alloys Pb1−xSnxS, Pb1−xSnxSe and Pb1−xSnxTe show covalent bonding nature which enhances by increasing the Sn concentration.

Keywords: Density functional theory; Generalized gradient approximation; Density of state; Structural properties; Electronic properties

Introduction

Computational materials science is an emerging field in condensed matter physics. Computational techniques have come to the level of experiment nowadays. One can determine the physical properties of a material even without the information of experimental data [1,2]. The recent development of computational power allows one to study very complex systems.

In 1874, IV–VI semiconductors were started to be utilized in solid state electronic devices after the Ferdinand Braun’s report on electrical rectification by PbS [3]. After this discovery, PbS also utilized as a rectifier in radios. In recent era, the IV–VI semiconductors have many applications in optoelectronic devices which are mainly utilized for emission and detection of mid-infrared radiations. The IV–VI semiconductors consist of binary compounds PbS, PbSe, and PbTe and their alloys i.e., PbSnS, PbSnTe, PbSrSe, PbEuTe etc. [4]. They are used in diode lasers [5], long wavelength imaging [6], and in also thermo photovoltaic devices [7]. They are also utilized to control pollution and gas spectroscopy, remote sensing, thermograph, chemical sensing etc. [8,9].

At normal temperature and pressure Lead sulfide (PbS) rock-salt structure is a narrow band gap semiconductor material. Its band gap is direct and equal to 0.45 eV at room temperature [10]. Lead selenide (PbSe) is also a direct band gap semiconductor material which has a stable rock-salt structure. The band gap of PbSe is equal to 0.16 eV at 4 K [11]. Lead telluride (PbTe) is direct band gap material and its band gap is equal to 0.29 eV. It also exists in rock salt structure at normal temperature and pressure [12]. Tin sulfide (SnS) is a narrow indirect band gap of 1.07 eV and the direct band gap occurs at energy of 1.3 eV [13]. The structure of SnS is orthorhombic but it changes to rock-salt structure at high temperature. Tin selenide (SnSe) is also an orthorhombic crystal and become rock-salt at high temperature as well [14]. Tin chalcogenide (SnTe) is a narrow direct band gap semiconductor with a value of 0.35 eV. It exists in rock-salt (RS) structure at ambient conditions [15].

With doping Sn in PbX (X=S, Se, Te), ternary compounds Pb1−xSnxTe, Pb1−xSnxSe, Pb1−xSnxS, Pb1−xSnxTe have been experimentally grown at various concentrations [9]. These materials are widely used for optoelectronic applications e.g., photovoltaic sensors. These photovoltaic IV–VI semiconductor infrared sensors (Pb1−xSnxTe, Pb1−xSnxSe, Pb1−xSnxS, PbTe etc.) are as sensitive as Hg1−xCdTe, and can fabricate easily especially on Si substrates. However, the technology of photovoltaic lead compound selection is behind that of Hg1−xCdTe alloy [9].

Density functional theory (DFT) [17] is usually used to investigate the electronic and structure properties of materials, it can also predict chemical, optical and magnetic properties of the materials i.e., metals, semi-metals, semiconductors and insulators. The density functional theory (DFT) was proposed by Hohenberg and Kohn to simplify the problem and got the noble price in chemistry in 1998. The density functional theory (DFT) is one of the important tools in computational material science for investigation of properties of material such as optical, structural, electronic and magnetic.

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Computational Details

This project is completed by performing the calculations through WIEN2K code. This software is based on DFT. FP-LAPW model is utilized in the Wien2k code [18], with different XC- potential. The main two parts are consisting in the Wien2k code. The first is the initialization and the second is the self consistent-field cycle (SCF). Then in every part there are still many programs which will be done step by step to complete these cycles and can be able to find the structural, electronic and Chemical properties of Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te compounds at concentrations x=0, 0.25, 0.5, 0.75, 1.

Results and Discussion

Structural properties

The calculated structural properties of the studied materials are lattice constant a (Å$^2$), Bulk modulus B (GPa), derivative of bulk modulus B’ unit cell energy $E_0$. Before the discussion of structural properties of ternary compounds Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te at concentrations x=0, 0.25, 0.5, 0.75, 1, we first start the structural properties of binary compounds PbS, PbSe, PbTe, SnS, SnSe and SnTe in rock-salt phase. The Birch-Murnaghan’s equation [19] is used to minimize the total energy with respect to unit cell volume which is given as:

$$E(V) = E_0 + \frac{9V_0B_0}{16} \left[ \left( \frac{V}{V_0} \right)^{2/3} - 1 \right]^2 - \frac{1}{36} \left( \frac{V}{V_0} \right)^2 \left( \left( \frac{V}{V_0} \right)^{2/3} - 1 \right)^3$$ (1)

The structure of all binary compounds PbS, PbSe, PbTe, SnS, SnSe, SnTe and ternary compounds Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te are in sodium chloride (rock-salt) structure. The sodium chloride structure represented a face centered cubic lattice. The structure of binary compounds and ternary compounds are shown in Figure 1. Plots of total energy as a function of volume of Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te at different concentration of Sn gives unit cell volume $V_o$, lattice constant a (Å$^2$), Bulk modulus B (GPa), derivative of bulk modulus B’ and unit cell energy $E_0$ as shown in Figure 2. So the lattice constant and bulk modulus values are in good agreement with experimental values as shown in Tables 1 and 2 and from the tables lattice constant is decreasing as we adding the concentration of Tin (Sn) in PbX (X=S, Se, Te). The maximum lattice constant is at zero doping in the PbX (X=S, Se, Te) and minimum at the doping concentration of x=1. In Pb$_x$Sn$_{1-x}$S the bulk modulus is maximum when Sn is doped at the concentration of x=1 and minimum when the Tin (Sn) is doped at concentration of x=0.

Also the energy of Pb$_x$Sn$_{1-x}$S is maximum at concentration of x=0.25 and minimum at the doping concentration of Tin (Sn) at x=1 as shown in Table 1. In Pb$_x$Sn$_{1-x}$Se the bulk modulus is maximum at doping concentration of x=1 and minimum at the doping concentration of x=0.25. Also the energy of Pb$_x$Sn$_{1-x}$Se is maximum at concentration of x=0.25 and minimum at concentration of x=1 as shown in Table 2. In Pb$_x$Sn$_{1-x}$Te the bulk modulus is maximum at concentration of x=1 and minimum at doping concentration of Tin (Sn) at x=0.25 as shown in Table 3. The energy of Pb$_x$Sn$_{1-x}$Te is maximum at concentration of x=0.25 and minimum at concentration of x=1. The bulk modulus and energy of Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te are changing in same way as in both samples the bulk modulus is maximum at concentration of x=1 and minimum at concentration of x=0.25, also in the energy case in both samples it is maximum at concentration of x=0.25 and minimum at concentration of x=1 but the parameters i.e., bulk modulus and energy of Pb$_x$Sn$_{1-x}$S is changing in different concentration then Pb$_x$Sn$_{1-x}$Se and Pb$_x$Sn$_{1-x}$Te.

Electronic properties

Band structure: The band structure gives useful information about the structure of materials. The band structure of Sn doped PbX (X=S, Se, Te) compounds at different concentration are calculated and shown in Figures 4a-4o respectively. For PbS the band structure is shown in Figure 4a which is in rock salt phase, from figure the minimum of conduction band (CB) and the maximum of valance band (VB) are at $E_g = 0.48$ eV and $E_g = 0.8$ eV as shown in Figures 4b and 4c. From Figures 4d-4f it is clear that SnS, SnSe and SnTe have zero band gap, so they have large direct band gap values 0.09 eV, 0.1 eV and 0.07 eV respectively. The compounds Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se are zero band gap material as shown in Figure 4g and 4j. The Pb$_x$Sn$_{1-x}$Te has a narrow direct band gap 0.082 eV as shown in Figure 4m. In Pb$_x$Sn$_{1-x}$S, Pb$_x$Sn$_{1-x}$Se, Pb$_x$Sn$_{1-x}$Te compounds have zero band gap.

Figure 1: Structure of (a) PbS (b) PbSe (c) PbTe (d) SnS (e) SnSe (f) SnTe (g) Pb$_{0.50}$Sn$_{0.50}$S (h) Pb$_{0.50}$Sn$_{0.50}$Se (i) Pb$_{0.50}$Sn$_{0.50}$Te (j) Pb$_{0.50}$Sn$_{0.50}$Se (k) Pb$_{0.50}$Sn$_{0.50}$Te (l) Pb$_{0.25}$Sn$_{0.75}$S (m) Pb$_{0.25}$Sn$_{0.75}$S (n) Pb$_{0.25}$Sn$_{0.75}$Se (o) Pb$_{0.25}$Sn$_{0.75}$Te.
Figure 2: Total energy as a function of volume of (a) PbS (b) PbSe (c) PbTe (d) SnS (e) SnSe (f) SnTe (g) Pb$_{0.75}$Sn$_{0.25}$S (h) Pb$_{0.50}$Sn$_{0.50}$S (i) Pb$_{0.75}$Sn$_{0.25}$Se (j) Pb$_{0.50}$Sn$_{0.50}$Se (k) Pb$_{0.75}$Sn$_{0.25}$Te (l) Pb$_{0.50}$Sn$_{0.50}$Te (m) Pb$_{0.75}$Sn$_{0.25}$Te (n) Pb$_{0.50}$Sn$_{0.50}$Te.
as shown in Figure 4g, 4h, 4k, 4l, 4n and 4o. So the semiconductor materials become metallic at doping concentration of x= 0.25, 0.50, 0.75 but at doping concentration of x=1 then again there is again narrow band gap. All the band gap values for different compounds at different doping concentration are mentioned in the Table 4. As the band gap occurs in the range of 0-0.8 eV, the fundamental edge occurs in the infrared region. The result matches with experimental one because it’s also show metallic nature at different doping concentrations as mentioned in Table 4 As there are less materials on the band gap of Sn doped PbX(X=S, Se, Te) with which we compare it with our results but we are confident about our results due to use of Wu-Cohen GGA at high k-point value of 5000.

**Density of states:** Density of states (DOS) describes the number of states of a system per unit interval of energy which are occupied by the electrons. Study of band structure, dielectric function, bond character

| Table 1: Calculated structural parameters of Sn doped PbX(X=S) at variation of Sn concentration along with experimental and other calculations. |

| Compound   | a(Å) | B(GPa) | B’ | E_f(Ry.) |
|------------|------|--------|----|----------|
| PbS        | 5.8893 | 60.7348 | 7.13 | -42652.61 |
| This work  | 5.95 | 52.9$^a$ | - | - |
| Other works| 6.012$^a$ | 52.1$^a$ | 4.10$^a$ | - |
| Experiment | 5.8717 | 62.26 | 5.0 | -141112.67 |
| Pb$_{0.75}$Sn$_{0.25}$S | 5.835 | 60.08 | 5.0 | -111614.78 |
| This work  | 5.796 | 62.01 | 4.12 | -82116.89 |
| Other works| 5.7492 | 5.848$^a$ | 64361 | 4.034 | -13154.73 |
| Experiment | 5.8717 | 62.26 | 5.0 | -141112.67 |

| Table 2: Calculated structural parameters of Sn doped PbX(X=Se) at variation of Sn concentration along with experimental and other calculations. |

| Compound   | a(Å) | B(GPa) | B’ | E_f(Ry.) |
|------------|------|--------|----|----------|
| PbSe       | 6.095 | 56.6262 | 4.5911 | -46714.19 |
| This work  | 6.222$^a$ | 47.5$^a$, 49.1$^a$ | 4.35$^a$ | - |
| Other works| 6.117$^a$ | 54.1$^a$ | - | - |
| Experiment | 6.081 | 52.5234 | 4.4792 | -157359.025 |
| Pb$_{0.75}$Sn$_{0.25}$Se | 6.035 | 55.94 | 4.12 | -127861.13 |
| This work  | 5.997 | 56.2424 | 4.4051 | -98362438 |
| Other works| 5.954 | 6.062$^b$ | 60798 | 5.0 | -17216.3178 |
| Experiment | 5.8717 | 62.26 | 5.0 | -141112.67 |

*Ref [20], *Ref [21], *Ref [22], *Ref [23], *Ref [24].

![](image1.png)
Figure 4: Band structure of (a) PbS (b) PbSe (c) PbTe (d) SnS (e) SnSe (f) SnTe (g) Sn$_{0.25}$Pb$_{0.75}$S (h) Sn$_{0.25}$Pb$_{0.75}$Se (i) Sn$_{0.25}$Pb$_{0.75}$Te (j) Sn$_{0.50}$Pb$_{0.50}$S (k) Sn$_{0.50}$Pb$_{0.50}$Se (l) Sn$_{0.50}$Pb$_{0.50}$Te (m) Sn$_{0.75}$Pb$_{0.25}$S (n) Sn$_{0.75}$Pb$_{0.25}$Se (o) Sn$_{0.75}$Pb$_{0.25}$Te.
Figure 5: DOS of PbS.

Figure 6: DOS of PbSe.

Figure 7: DOS of PbTe.
and reflectivity require the knowledge of electron density of states. The DOS of PbS, PbSe, PbTe, SnS, SnSe, SnTe and ternary compounds of Sn_{1-x}Pb_{1-x}S, Sn_{1-x}Pb_{1-x}Se and Sn_{1-x}Pb_{1-x}Te by using GGA scheme are shown in Figures 1 and 5-12. There are four regions in the fundamental density of states. The lower region of VB, the upper region of VB, the lower region of CB and the upper region of CB. DOS of PbS in rock salt are shown in Figure 5. The lower part of VB is started around -8.75 eV and the major contribution at this part is Pb-s state, also a little contribution by the states of S-s and S-p. Now the upper part of VB start about -5.8 eV. The VB near Fermi level is dominated by S-p and also a little contribution by the states of Pb-s and Pb-p. Now the third region is the CB in which the lower part dominated by Pb-p and S-p states and the upper part is due to S-d state. For PbSe the lower part of VB is dominated by Pb-s state and also a little contribution of Se-p state. Then after the lower part is the upper part of VB which is near to the Fermi level and has a major contribution due to Se-p state and also a little contribution due to Pb-s, Pb-p, and Pb-d states. Then near to the Fermi level is the CB whose lower part is dominated by the Pb-p and Se-p states. For the upper part of CB the major contribution is due to Se-d state and also little contribution of Pb-s, Pb-p and Pb-d as shown in Figure 6.

DOS for PbTe is the lower part of CB, dominated by Te-s state and also little contribution due to Pb-s state is shown in Figure 7. The upper part of VB is dominated due to Te-p state and also little contribution of Pb-s, Pb-p, and Pb-d states. Then in CB the lower part is dominated due to Pb-p and Te-p states and the small contribution is due to Pb-s, Pb-p and Te-d states. The upper level of CB is mainly contributed due to Pb-p and Te-d states. From figure of SnS it is clear that the lower part of VB is dominated due to Sn-s state and small contribution of Sn-p, S-s and S-p states. Then the upper part is dominated due to Sn-s and Sn-p states and also small contribution is Sn-p state. The lower part of CB is dominated due to Sn-p and Sn-s states near the Fermi level and the upper part is dominated due to Sn-p, Sn-d and S-d states. Then after the lower part there is the upper part of VB which is near to Sn-p, Sn-d and S-d states and also small contribution of Sn-s, Sn-f and S-p states as shown in Figure 8.

DOS of SnSe is shown in Figure 9. The lower part of VB is dominated by Sn-S state and also small contribution of Se-s, Se-p states. Then the upper part has a major contribution of Sn-s and Se-p states and also small contribution of Sn-p and Sn-d states. Then the lower part of CB near the Fermi level is dominated by Sn-p and Se-p states and the upper part is dominated due to Sn-p and Se-d states and also small contribution of Sn-s, Sn-d, Sn-f, Se-s and Se-p states.

It is clear from Figure 10 that the lower part of VB is dominated by Te-s state and also small contribution of Sn-s and Sn-p states. The upper part of VB is due to Sn-s and Te-p states. After Fermi level is the lower part of CB which is dominated by Sn-p and Te-p states and for the upper part it is dominated by Sn-d and Te-d states.

For the compound Sn_{1-x}Pb_{1-x}Se the DOS is shown in Figure 11. The lower part of the VB is dominated due to Sn-s and Pb-s states and also small contribution of S-s and S-p states. Then the upper part of VB is dominated due to S-p state and also a small contribution of Sn-p, Sn-s, Sn-p, Pb-p and Pb-d states. Then for lower part of CB which is near to Fermi level is dominated by Sn-p, Pb-p and S-p states and also small contribution of Sn-s, Sn-d, Pb-d and S-d states. For upper part of CB is dominated by S-d state.

The DOS of Sn_{1-x}Pb_{1-x}Te is shown in Figure 12. In figure the lower part of VB is dominated by Sn-s and Pb-s states and also small contribution of Se-s and Se-p states. Then after the lower part there is the upper part of VB which has a major contribution of Se-p state and also small contribution of Sn-s, Sn-p, Pb-s and Pb-p states. The lower part of CB is dominated by Sn-p state and the upper part is dominated by Se-d state.

The lower Te-s state band is dominated and the small contribution of Sn-s and Pb-s states is shown in Figure 13. Then near Fermi level is the upper part of VB which is dominated by Pb-s and Te-p states and also small contribution of Sn-s, Sn-p and Pb-p states. After the Fermi level is the lower part of CB which is dominated by Sn-p and Pb-p states and also little contribution of Sn-s, Sn-d and Te-d states. The upper part of CB is dominated by Sn-d, Pb-d and Te-d states.

**Electron density:** The chemical bonding properties can be defined by the charge density distribution in a solid. The nature of bonding can be described by electron density i.e., ionic or covalent bond between the cation and anion. The electron density plots of Sn doped PbX(X=S,

|              | a(A) | B(GPa) | B'    | E_(eV) |
|--------------|------|--------|-------|--------|
| PbTe         |      |        |       |        |
| This work    | 6.43 | 44.44  | 5.0   | -55466.977 |
| Other works  | 6.55 | 39.95  | 4.32  |        |
| Experiment   | 6.47 | 39.8  | -     | -      |
| Sn_{1-x}Pb_{1-x}Te |   |        |       |        |
| This work    | 6.409 | 46.1301 | 4.4436 | -192290.1989 |
| Other works  | 6.373 | 46.29  | 5.00  | -162792.31 |
| Experiment   | 6.33  | 47.1526 | 4.6470 | -133294.4232 |
| SnTe         |      |        |       |        |
| This work    | 6.28  | 6.312  | 50.0925 | 4.9679 |
| Other works  | 6.327  | 6.327  | -25949.032 | - |
| Experiment   | -     | -      | -     | -      |

*Ref [26], **Ref [22], ***Ref [24], ****Ref [27].

Table 3: Calculated structural parameters of Sn doped PbX(X=S, Te) at variation of Sn concentration along with experimental and other calculations.
Table 4: Energy band gaps (in eV) for Sn doped PbX (X=S, Se, Te) compounds at (0 ≤ X ≤ 1) in the rock salt phase along with the experimental and other calculations.

| Compounds       | This work (GGA) | Experimental | Other Calculations |
|-----------------|-----------------|--------------|--------------------|
| PbS             | Eg 0.28         | 0.42, 0.286  | 0.448, 0.380, 0.380 |
| Pb_{1-x}Sn_{x}S | Eg 0            | -            | -                  |
| SnS             | Eg 0.09         | -            | -                  |
| PbSe            | Eg 0.48         | 0.279        | 0.318, 0.340       |
| Pb_{1-x}Sn_{x}Se| Eg x=0…0.2,0.18–0 eV T=77k | -            | -                  |
| SnSe            | Eg 0.1          |              |                    |
| PbTe            | Eg 0.8          | 0.33, 0.19   | 0.649              |
| Pb_{1-x}Sn_{x}Te| Eg 0.082        | x=0…0.4,0.22–0 eV T=77k | -                  |
| SnTe            | Eg 0.07         | 0.35         | 0.19 (300k)        |

Pb_{1-x}Sn_{x}S, Pb_{1-x}Sn_{x}Se, Pb_{1-x}Sn_{x}S, Pb_{1-x}Sn_{x}Se, Pb_{1-x}Sn_{x}Te are zero band gap due to our result. aRef [28], bRef [29], cRef [30], dRef [23], eRef [31], fRef [32], gRef [33]

Conclusion

The Structural, electronic and chemical bonding, of the Sn doped PbX (X=S, Se, Te) are calculated by full potential linearized augmented plane wave method (FP-LAPW) within density functional theory (DFT). The Sn doping concentration for Pb_{1-x}Sn_{x}S, Pb_{1-x}Sn_{x}Se, and Pb_{1-x}Sn_{x}Te is in the range x=0 to x=1 in step of 0.25 in the rock salt phase. By doping Sn in PbX (X=S, Se, Te) the lattice constants decreases linearly by increasing the concentration. The electronic properties also changes with respect to the composition of the materials. The band gap plots of PbX (X=S, Se, Te) show the direct band gap (L-L) nature. The direct band gap is found to vary by doping Sn in PbX (X=S, Se, Te). So the direct band gap of the ternary alloys varies in the range 0–0.8 eV. It has observed that the s, p and d states of PbX (X=S, Se, Te) control their...
Figure 9: DOS of SnSe.

Figure 10: DOS of SnTe.

Figure 11: DOS of Sn_{0.50}Pb_{0.50}S.
Figure 12: DOS of Sn$_{0.5}$Pb$_{0.5}$Se.

Figure 13: DOS of Sn$_{0.5}$Pb$_{0.5}$Te.

Figure 14(a): Electron charge density of PbS at (110) plane.

Figure 14(b): Electron charge density of PbSe at (110) plane.
Figure 14(c): Electron charge density of PbTe at (110) plane.
Figure 14(d): Electron charge density of SnS at (110) plane.

Figure 14(e): Electron charge density of SnSe at (110) plane.
Figure 14(f): Electron charge density of PbTe at (110) plane.

Figure 14(g): Electron charge density of Pb$_{0.75}$Sn$_{0.25}$S.
Figure 14(h): Electron charge density at (110) plane of Pb$_{0.75}$Sn$_{0.25}$Se at (110) plane.
electronic properties. The alloys Pb$_1-x$Sn$_x$S, Pb$_1-x$Sn$_x$Se and Pb$_1-x$Sn$_x$Te show covalent bonding nature which enhances by increasing the Sn concentration. Hence it is concluded from this study that the Sn doing PbX(X=S, Se, Te) varies the physical properties widely and the resulted materials become more suitable to use in Infrared detectors, Braggs reflectors and optical devices working in lower frequency regime.

References
1. Mun Wong K, Alay-e-Abbas SM, Shaukat A, Fang Y, Lei Y (2013) First-principles investigation of the size-dependent structural stability and electronic properties of O-vacancies at the ZnO polar and non-polar surfaces. Journal of Applied Physics 113: 014304.
2. Mun Wong K, Alay-e-Abbas SM, Fang Y, Shaukat A, Lei Y (2013) Spatial distribution of neutral oxygen vacancies on ZnO nanowire surfaces: An investigation combining confocal microscopy and first principles calculations. Journal of Applied Physics 114: 034901.
3. Braun F (1874) On Current Flow through Metallic Sulfides. Annalen der Physik und Chemie 153: 556.
4. McCann PJ (2006) IV–VI semiconductors for mid-infrared optoelectronic devices. InMid-infrared Semiconductor Optoelectronics 237-264.
5. Preier H (1979) Recent advances in lead-chalcogenide diode lasers. Applied Physics A: Materials Science & Processing 20: 189-206.
6. Zogg H, Fach A, Maissen C, Masek J, Blunier S (1994) Photovoltaic lead-chalcogenide on silicon infrared sensor arrays. Optical Engineering-Billingham 33: 1440-1449.
7. Chaudhuri TK (1992) A solar thermophotovoltaic converter using PbS photovoltaic cells. International Journal of Energy Research 16: 481-487.
8. Abe S, Masumoto K, Mochizuki K, Suto K (1994) Growth and characterization of PbI$_2$-xCaxS$_1$-ySe$_x$ thin films prepared by hot wall epitaxy. Journal of Crystal Growth 144: 54-58.
9. Kumar S, Khan MM, Zulfequar M, Husain M (2007) Optical, structural and electrical investigations on PbTe$_{1-x}$S$_x$ alloys. Journal of Materials Science 42: 363-367.
10. Gadi SB, Singh A, Yousuf M (2003) Structural stability of PbS films as a function of temperature. Thin Solid Films 431: 506-510.
11. Paul A, Klimeck G (2011) Atomic-scale study of electronic structure of PbSe nanowires. Applied Physics Letters 98: 212105.
12. Leitsmann R, Bechstedt F, Groiss H, Schäffler F, Heiss W, et al. (2007) Structural and electronic properties of PbTe (rocksalt/CdTe (zinc-blende) interfaces. Applied Surface Science 254: 397-400.
13. Rajagopalan M, Kalpana G, Priyamvadha V (2006) Pressure induced structural phase transition in SnS-An ab initio study. Bull Mater Sci 29: 25-28.
SnY (Y=S, Se, and Te). Royal Institute of Technology.

33. Zogg H, Arnold M, Felder F, Rahim M, Ebneter C, et al. (2008) Epitaxial Lead Chalcogenides on Si for Mid-IR Detectors and Emitters Including Cavities. Journal of Electronic Materials 37: 213-219.