Electronic Structure of In$_{3-x}$Se$_4$ Electron Transport Layer for Chalcogenide/p-Si Heterojunction Solar Cells

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ABSTRACT: In this article, we perform density functional theory calculation to investigate the electronic and optical properties of newly reported In$_{3-x}$Se$_4$ compound using CAMbridge Serial Total Energy Package (CASTEP). Structural parameters obtained from the calculations agree well with the available experimental data, indicating their stability. In the band structure of In$_{3-x}$Se$_4$ (x = 0, 0.11, and 0.22), the Fermi level (E$_F$) crossed over several bands in the conduction bands, which is an indication of the n-type metal-like behavior of In$_{3-x}$Se$_4$ compounds. On the other hand, the band structure of In$_{3-x}$Se$_4$ (x = 1/3) exhibits semiconducting nature with a band gap of ∼0.2 eV. A strong hybridization among Se 4s, Se 4p and In 5s, In 5p orbitals for In$_3$Se$_4$ and that between Se 4p and In 5p orbitals were seen for β-In$_3$Se$_4$ compound. The dispersion of In 5s, In 5p and Se 4s, Se 4p orbitals is responsible for the electrical conductivity of In$_3$Se$_4$ that is confirmed from DOS calculations as well. Moreover, the bonding natures of In$_{3-x}$Se$_4$ materials have been discussed based on the electronic charge density map. Electron-like Fermi surface in In$_3$Se$_4$ ensures the single-band nature of the compound. The efficiency of the In$_{3-x}$Se$_4$/p-Si heterojunction solar cells has been calculated by Solar Cell Capacitance Simulator (SCAPS)-1D software using experimental data of In$_{3-x}$Se$_4$ thin films. The effect of various physical parameters on the photovoltaic performance of In$_{3-x}$Se$_4$/p-Si solar cells has been investigated to obtain the highest efficiency of the solar cells. The optimized power conversion efficiency of the solar cell is found to be 22.63% with V$_{OC}$ = 0.703 V, J$_{SC}$ = 38.53 mA/cm$^2$, and FF = 83.48%. These entire theoretical predictions indicate the promising applications of In$_{3-x}$Se$_4$ two-dimensional compound to harness solar energy in near future.

1. INTRODUCTION

Nowadays, the renewable energy sources are taking place over world’s finite dominant energy sources (oil, coal, uranium) to meet up the increasing demand of power supply. The need for inexpensive and large-scale, carbon-neutral energy sources has stimulated a search for revolutionary concepts in solar-electricity energy conversion. The silicon solar cell covers over 90% of the global market, although it has an indirect band gap with weak light absorption and extreme processing temperature of ∼1400 °C. Researchers are focusing on making alternative efficient and cheap solar cells.

Recently, silicon/organic hybrid solar cells have gained extensive research interest as they are promising to combine the benefits of organic materials being cheap and easy to process and inorganic materials possessing better charge carrier mobilities and low exciton binding energies. A number of promising heterojunction solar cells have been demonstrated based on this type of architecture, such as devices that use Si in conjunction with conjugated polymers. Specifically, the comprehensive studies on conductive polymer poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) to modify its properties, texturing of silicon, and interface engineering between Si/cathode have led to remarkable progress in efficiency (power conversion efficiency, PCE) of 12–15.9%. In addition, it is advantageous to use p-type Si compared to n-type one due to its low cost. The photogenerated carriers can be effectively collected using p-type silicon as minority carrier diffusion length is larger in p-type silicon than that in n-type silicon. This phenomenon provides low recombination rates, enhanced photocurrent, and improved solar cell performance when p-type silicon is used. However, proper n-type organic materials have not been found yet that can be combined with p-type Si for efficient device performance. So far, C$_{60}$ and its derivatives have been studied as candidates as n-type acceptors for use in Si/organic heterojunction solar cells with p-type Si without providing high power, although they displayed outstanding dark rectifying effect. Most recently, Yun et al. have reported this type of solar cells with
InSe provides a very high electron mobility\textsuperscript{37} and also high transport layer can be used. It has already been reported that conductivity.\textsuperscript{28} The In\textsubscript{3}Se\textsubscript{4} phase.\textsuperscript{28} Moreover, it is also reported that chalcogenide thin films can be fabricated by low-cost solution process, which indicates their potential in future solution-processed chalcogenide/c-Si heterojunction solar cell applications.\textsuperscript{23–25} Indium selenide (InSe) is a III–VI two-dimensional (2D) compound semiconductor composed of stacking of Se–In–In–Se atoms bonded with van der Waals force between quadruple layers.\textsuperscript{26,27} The In–Se system can exist in many phases such as InSe, In\textsubscript{2}Se\textsubscript{3}, In\textsubscript{3}Se\textsubscript{4}, In\textsubscript{4}Se\textsubscript{5}, and In\textsubscript{5}Se\textsubscript{6}.\textsuperscript{22} There are some reports showing that the In–Se system can also exist in the In\textsubscript{3}Se\textsubscript{4} phase.\textsuperscript{28–31} The study of InSe thin films is motivated by the potential applications in photovoltaic (PV) cells,\textsuperscript{32,33} solid-state batteries,\textsuperscript{4} phase-change memories,\textsuperscript{35} optoelectronic devices,\textsuperscript{37,38} field-effect transistors,\textsuperscript{37} and thermoelectric power conversion.\textsuperscript{39,40}

However, the use of n-type InSe with p-type Si to make solar cells has several drawbacks such as high series resistance and high defect density at the junction interface.\textsuperscript{22} Thus, a common thread in this system is the trade-off between efficient light absorption and charge collection. Charge can be effectively collected when highly conducting InSe electron transport layer can be used. It has already been reported that InSe provides a very high electron mobility\textsuperscript{37} and also high conductivity.\textsuperscript{28–31} Now, it is required to make InSe thin films with high mobility as well as high conductivity. This will make a pn junction with p-Si as well as effectively transport electron to cathode. To overcome this practical limit, new material synthesis approaches are needed. Although In\textsubscript{3}Se\textsubscript{4} has been synthesized and few physical properties have been reported by some researchers, the electronic and optical properties of this material are yet to be revealed.\textsuperscript{28–30} There is also a report unveiling that highly insulting \( \beta \)-In\textsubscript{3}Se\textsubscript{4} encounters a transition to metallic In\textsubscript{3}Se\textsubscript{4} phase.\textsuperscript{31}

In this article, we demonstrate the electronic structure of newly reported In\textsubscript{3}Se\textsubscript{4} 2D compound by first-principles study and its potential as an electron transport window layer for the chalcogenide/p-Si heterojunction solar cells as there are much scope for additional investigations to realize high power conversion efficiency of In\textsubscript{3}Se\textsubscript{4}/p-Si heterojunction solar cells.

2. RESULTS AND DISCUSSION

2.1. Structural Properties of In\textsubscript{3}Se\textsubscript{4} Compound. The optimization of lattice constants and atomic positions of In\textsubscript{3}Se\textsubscript{4} compound as a function of normal stress with minimum total energy has been performed by density functional theory (DFT) calculation using CAMbridge Serial Total Energy Package (CASTEP) code. The optimized crystal structure of the In\textsubscript{3}Se\textsubscript{4} (\( x = 1/3, 0 \)) compound is depicted in Figure 1 as unit cell and 2D view in the ab plane. The rhombohedral crystal structure with space group \( R \bar{3} m ( \#166) \) of In\textsubscript{3}Se\textsubscript{4} compound has already been confirmed by experimental studies. The calculated ground-state lattice constants are listed in Table 1. These calculated values agree well with the reported experimental results.\textsuperscript{29,41}

The rhombohedral structure (space group \( R \bar{3} m \)) of \( \beta \)-In\textsubscript{3}Se\textsubscript{3} has 15 lattice sites comprising the six In atoms forming trigonal pyramidal cages with three Se neighbors (Figure 1a), whereas the In\textsubscript{3}Se\textsubscript{4} structure has 21 lattice sites comprising the nine In atom sites forming octahedral cages with six Se neighbors and 12 Se atom sites forming trigonal pyramidal cages with three In neighbors (Figure 1b). The bond lengths in the octahedral (In–Se) and trigonal pyramidal (Se–In) planes for In\textsubscript{3}Se\textsubscript{4} structure are 2.61843 and 2.84135 Å, respectively. In contrast,
the only trigonal pyramidal bond (In−Se) length of 2.66773 Å is observed for the β-In2Se3 phase.

However, it is suitable to denote the unit cell as $3(R_{3-x}V_xX_4)$, where V is considered as vacancy in In atoms. For R2X3 compounds, $3/3$ sites of the nine In sites per unit cell are empty, i.e., $x = 1/3$, and for the R3X4 phases, there are no empty sites, i.e., $x = 0$. The ionic behavior of the In$_{3-x}$Se$_4$ lattice can be formulated as $(\text{In}^{3+})_{3-x}V_x(\text{Se}^{2-})_4(e^-)_{1+3x}$. In β-In$_2$Se$_3$, the two In$^{3+}$ ions provide six electrons to the chemical bonding, which are captured by the 3 Se$^{2-}$ ions. Therefore, there are no excess electrons for the electrical conduction, resulting in highly insulating In$_2$Se$_3$ compound.

On the other hand, in the In$_3$Se$_4$ phase, nine bonding electrons are provided by the three In$^{3+}$ ions, eight of which are captured by four Se$^{2-}$ ions, resulting in an excess of one electron to the conduction band per formula unit. The carrier concentration of In$_{3-x}$Se$_4$ phase is given by

$$n = \frac{N_A d}{M} (1 - 3x)$$ (1)

where $N_A$ denotes Avogadro’s number, $d$ represents the density, and $M$ denotes the molecular weight.

Mass density $d$ can be calculated by

$$d = \frac{Z M}{N_A V}$$ (2)

where $Z$ is the formula unit, $N_A$ is Avogadro’s number, $M$ is the molecular weight, and $V$ is the volume.

The reported and calculated values of $d$ for the In$_3$Se$_4$ phase are 6.11 and 6.6 g/cm$^3$, respectively.

Thus, the stoichiometric In$_3$Se$_4$ compound (with $x = 0$) gains a free-electron concentration of $6.01 \times 10^{21}$ cm$^{-3}$. The appearance of $x$ vacancies provides $(1 - 3x)$ electrons in the conduction band. Therefore, during the transition from β-In$_2$Se$_3$ to In$_3$Se$_4$ phase, there is a metallic transition as the empty sites are filled with In ions providing excess electrons. The carrier concentrations for different values of $x$ are shown in Table S1 in the Supporting Information.

The carrier can also be calculated theoretically by the formula

$$n = \frac{3}{V}$$ (3)

where $V$ is the volume of the unit cell in cm$^3$, as shown in Table 1, and coefficient 3 is introduced due the fact that every unit cell provides three free electrons to the In$_3$Se$_4$ system. Using this formula, the carrier concentration is found to be $6.01 \times 10^{21}$ cm$^{-3}$ similar to the value obtained from eq 1, which agrees well with the reported values.

2.2. Band Structure of In$_{3-x}$Se$_4$ Compound. The electronic properties of a compound are revealed by the band structure, partial density of states (PDOS), and total density of state (TDOS), which are also closely related to charge density distribution and Fermi surface. The results of band structure calculations along the high-symmetry directions within the Brillouin zone for In$_{3-x}$Se$_4$ are presented in Figure 2a−d. The horizontal dashed line is the signature of Fermi level, $E_F$, while the valence and conduction bands are indicated by blue and red, respectively. Figure 2a depicts a clear gap
between valence and conduction bands for the $\text{In}_{3-x}\text{Se}_4$ compound for $x = 1/3$. The valence band maxima occurs at $\Gamma$ point, whereas the conduction band minima occurs at $M$ point, so there exhibits an indirect band gap of $E_g \sim 0.2$ eV. On the other hand, it is seen from Figure 2b–d that with $x = 0.22, 0.11,$ and 0, the Fermi level ($E_F$) shifted to the conduction band is an implication of their metal-like n-type conductivity. However, this phenomenon might be rare but can happen due to the doping effect of In, which generates additional free electrons, and consequently, $E_F$ cuts the conduction band showing degeneracy of these materials.\(^{45}\)

The band structure and band gap of $\text{In}_{3-x}\text{Se}_4$ were calculated by the software CASTEP as shown in the figures using localized density approximation (LDA) function yielding a band gap of $\beta$-$\text{In}_2\text{Se}_3$ phase of about 0.2 eV, whereas the experimental band gap is reported to be 1.55 eV.\(^{46}\) This happens as the LDA function consistently underestimates the band gap of $\beta$-$\text{In}_2\text{Se}_3$ phase of about 0.2 eV, whereas the experimental band gap is reported to be 1.55 eV.\(^{46}\) This happens as the LDA function consistently underestimates the band gap.\(^{47}\) The optical band gap is normally calculated using hybrid functional HSE06 function based on DFT for accurate value, although it is reported that DFT-based hybrid functional cannot always give exact band gaps of the materials found in the experiments.\(^{48,49}\) However, HSE06 function was not performed in this study due to system limitations. The crystal structure of $\text{In}_2\text{Se}_3$ is similar to that of the $\beta$-$\text{In}_2\text{Se}_3$ phase, as reported another work.\(^{50}\) The relative shifts in $E_F$ to those of the $\beta$-$\text{In}_2\text{Se}_3$ phase are 1.06, 1.10, and 1.62 eV for the $x$ values of 0.22, 0.11, and 0, respectively, in $\text{In}_{3-x}\text{Se}_4$ compounds, as shown in Figure 2b–d. The optical band gap of the nonstoichiometric $\text{In}_{3-x}\text{Se}_4$ thin films is reported to be $\sim$1.8 eV with metallic conductivity.\(^{44}\) Therefore, from these figures, it can be concluded that the optical band gap of stoichiometric $\text{In}_3\text{Se}_4$ phase should not be less than 1.62 eV, consistent with the report as Fermi level must cross the conduction band for metallic characteristics,\(^{53}\) which indicates that $\text{In}_3\text{Se}_4$ is a semiconductor with finite energy gap.\(^{53}\) However, HSE06 function was not performed in this study due to system limitations.

In this study, thereby showing the ionic nature. The ionic nature of these compounds unveils the structural stability. It is seen that for $x = 1/3$, the PDOS around $E_F$ is found to be mainly spherical around all of the atoms for $\text{In}_3\text{Se}_4$ (Figure 4a). For $x = 0.22, 0.11,$ and 0, as shown in Figure 4b–d, three central sheets are the electron-like sheets with spherical cross section centered along the $A’G$ direction of the Brillouin zone. A star-shaped sheet is also surrounding the central sheets. Far from the central sheets, three distinguished middle-sagged U-shaped close sheets are observed along the $G’M$ direction and expanded along the $M’L$ direction in the same sheet as well. The surfaces also include two V-shaped holelike sheets centered at the corners of the Brillouin zone along the $G’K$ direction, which are further expanded along the $K’H$ direction. However, these Fermi surfaces are predominantly constructed due to the dispersion of In and Se 4s, Se 4p orbitals resulting in the higher electrical conductivity of the compounds that can also be ensured from DOS (Figure 3b–d).

![Figure 3. DOS of $\text{In}_3\text{Se}_4$ compound for different ($x$) values: $x = 1/3$ (a), $x = 0.22$ (b), $x = 0.11$ (c), and $x = 0$ (d).](image)

2.5. Electron Charge Density Map of $\text{In}_3\text{Se}_4$ Compound. Figure 5a–d shows the valence electron charge density maps (in the units of $e/\text{Å}^3$), which delineate the distribution of the total electronic charge density of $\text{In}_{3-x}\text{Se}_4$ materials. The right-hand-side scale represents the intensity of the electron concentration. Low concentration of electrons is presented by blue, whereas high concentration of electrons is presented by red. It is seen from Figure 5b–d that the distribution of charge is mainly spherical around all of the atoms for $\text{In}_3\text{Se}_4$ ($x = 0, 0.11,$ and 0.22) compounds under this study, thereby showing the ionic nature. The ionic nature is an effect of metallic characteristics,\(^{53}\) which indicates that In-Se bonds in the aforementioned compositions manifest metallic nature. Thus, a strong isotropic combination of ionic and metallic interactions stands for $\text{In}_{3-x}\text{Se}_4$ compounds. On
the other hand, for \( x = 1/3 \) (\( \beta \)-In\(_2\)Se\(_3\)) compound, the electronic charge density of In/Se atoms shows potential overlapping of charge and they are not perfectly spherical rather somewhat zigzag in shape. This nonideal shape of atoms and their potential overlapping are an indication of covalent bonding nature of the materials. This covalent nature might also be correlated to the insulating property of the \( \beta \)-In\(_2\)Se\(_3\) material, as seen from the electronic properties calculations (Figure 3).
2.6. Optical Properties of In$_{3-x}$Se$_4$ Compound. The optical properties of a material are determined by a number of parameters such as dielectric function, refractive index, loss function, conductivity, reflectivity, and absorption coefficient, which completely depend on the energy of the incident electromagnetic radiation. The frequency-dependent optical properties of In$_{3-x}$Se$_4$ are investigated, where various optical parameters fairly agree with the characteristic features of the electronic properties. Both the electronic band structure and optical conductivity reveal strong metal-like conductivity for the In$_{3-x}$Se$_4$ (x = 0, 0.11, and 0.22) compound.

Figure 6a shows the calculated spectra of the dielectric function of In$_{3-x}$Se$_4$. The dielectric constant at zero frequency is known as the static dielectric constant. The static dielectric constant of In$_{3-x}$Se$_4$ is found to be 16.93, 30.81, 30.35, and 30.72, respectively, for x = 1/3, 0.22, 0.11, and 0.

The calculated refractive index values $n(0)$ of In$_{3-x}$Se$_4$ for x = 1/3, 0.22, 0.11, and 0 are 4.11, 5.57, 5.52, and 5.56, respectively, as shown in Figure 6b. The refractive index varies with the applied energy, revealing that the In$_{3-x}$Se$_4$ compound has the photorefractive effect.

The optical conductivity ($\sigma$) spectrum of In$_{3-x}$Se$_4$ is shown in Figure 6c. The maximum photoconductivity for this compound is 6.43 found at 4.16 eV for x = 1/3 and ~6 found at 3.75 eV for x = 0.22, 0.11, and 0.

Figure 6d illustrates the absorption spectra of In$_{3-x}$Se$_4$. Normally, the low-energy infrared part of the spectra originated by the intraband transition. On the other hand, the interband transition may contribute to the appearance of the peaks in the high-energy region of the absorption and conductivity spectra. Notably, it is observed in Figure 6c that the change in the conductivity spectra is identical to that in the absorption spectra. Therefore, we may conclude that the photoconductivity of the In$_{3-x}$Se$_4$ compound rises as a result of photon absorption.

The reflectivity (R) spectra of In$_{3-x}$Se$_4$ are displayed in Figure 6e. A higher reflectivity is seen in the infrared region approximately 37% for x = 1/3 and 48% for x = 0.22, 0.11, and 0 of the total radiation, and in the high-energy region, some peaks arise due to interband transition. However, the high reflectivity spectra of this material indicate that it could be used as a promising coating material to diminish solar heating. The high value of reflectivity in the low-energy region reveals the characteristics of high conductance in the low-energy region.
The energy loss spectra ($L$) of In$_{3-x}$Se$_4$ are exhibited in Figure 6f. The energy loss function is a significant index to express the loss of energy of a fast moving electron when it goes through a material.35 In the graph of loss function, the highest peak is related to the plasma resonance and its associated frequency is called plasma frequency, $\omega_p$. The highest peak is observed at about 15.97 eV for $x = 1/3$ and 16.34 eV for $x = 0.22, 0.11, and 0$, which reveal the plasma frequency of compounds. The In$_{3-x}$Se$_4$ compounds become transparent when the incident light frequency is higher than the plasma frequency.

Figure 6a–f shows that all of the curves of In$_{3-x}$Se$_4$ for $x = 0.22, 0.11, and 0$ overlap with each other, which means there is no change of optical properties at those compositions but showing a different picture for $x = 1/3$.

2.7. In$_{3-x}$Se$_4$/p-Si Heterojunction Solar Cells. Figure 7a,b delineates the schematic structure and energy band diagram of In$_{3-x}$Se$_4$/p-Si heterojunction solar cell, respectively. In In$_{3-x}$Se$_4$, the Fermi energy ($E_F$) and electron affinity of indium selenide are about $\sim 4.4$ and $4.55$ eV, respectively.51,57 Therefore, Fermi level will reside within the conduction band in In$_{3-x}$Se$_4$. On the other hand, the electron affinity of Si is $\sim 4.05$ eV. As a result, In$_{3-x}$Se$_4$ builds a favorable junction with Si, as schematically depicted in Figure 7b. Moreover, it has also been reported that the band gap as well as the conductivity of the chalcogenides can be modulated using electron beam irradiation, which may also play an important role in the formation of favorable chalcogenide/p-Si heterojunction for the photovoltaic (PV) applications.58

2.7.1. Thickness- and Doping Concentration-Dependent PV Performance. The simulated $J$–$V$ curves of the In$_{3-x}$Se$_4$/p-Si heterojunction solar cells with the variation of thicknesses of In$_{3-x}$Se$_4$ and silicon substrate are shown in Figure 8a,b, respectively. Figure 8a delineates that the highest PCE, $\eta$, of the solar cell is $20.69\%$ with $J_{SC} = 38.96$ mA/cm$^2$, $V_{OC} = 0.683$ V, and FF = $82.55\%$, for solar cell having In$_{3-x}$Se$_4$ and Si layer thicknesses of $0.10$ and $300$ $\mu$m, respectively. However, the thickness of In$_{3-x}$Se$_4$ with $\eta = 20.32\%$ is set to $0.20$ $\mu$m for the simulation as thinner transport layer introduces huge defects resulting in poor PV performance of the solar cells. Figure 8b reveals that the efficiency of the In$_{3-x}$Se$_4$/p-Si heterojunction solar cells increases with the increase of thickness of Si substrate that happens due to the fact that thicker Si absorber layer absorbs higher number of photons. The summarized PV parameters of the corresponding In$_{3-x}$Se$_4$/p-Si heterojunction solar cells are shown in Table 2. The higher $J_{SC}$ and FF of the solar cells can be attributed to the high transparency and metallic behavior of the In$_{3-x}$Se$_4$ layer.56,59 The high open-circuit voltage instigates the better junction properties of the solar cells. The change in PV parameters with respect to the thicknesses of In$_{3-x}$Se$_4$ and Si is also shown in Figure S1 in the Supporting Information.

Doping concentrations of In$_{3-x}$Se$_4$(N$_D$)- and Si(N$_A$)-dependent simulated $J$–$V$ characteristics of In$_{3-x}$Se$_4$/p-Si heterojunction solar cells are depicted in Figure 9a,b, respectively. Figure 9a reveals that both short-circuit current and open-circuit voltage are almost independent of donor concentration of the In$_{3-x}$Se$_4$ layer. The highest PCE, $\eta$, of the solar cell is found to be $22.69\%$ with $J_{SC} = 38.53$ mA/cm$^2$, $V_{OC} = 0.703$ V, and $FF = 83.48\%$, for solar cell having In$_{3-x}$Se$_4$ and Si layer thicknesses of $0.10$ and $300$ $\mu$m, respectively. On the other hand, Figure 9b shows that open-circuit voltage significantly increases with the increase of doping concentration of Si substrate. Table 3 delineates the summarized photovoltaic performances of the corresponding In$_{3-x}$Se$_4$/p-Si heterojunction solar cells. It is observed from the table that $J_{SC}$ reduces with the increase of doping density for both the cases. These results are the consequences of recombination losses in the absorber and transport layers due to higher doping.60,61 The change in solar cell parameters due to the variation of doping concentration of In$_{3-x}$Se$_4$ and Si, respectively, is also depicted in Figure S2 in the Supporting Information.

Figure S3a,b in the Supporting Information represents the simulated quantum efficiency (QE) of the In$_{3-x}$Se$_4$/p-Si heterojunction solar cells with the variation of thickness of In$_{3-x}$Se$_4$ and Si substrate, respectively. It is observed from the figures that QE of the solar cells is highly dependent on the In$_{3-x}$Se$_4$ layer thickness, which arises due to the parasitic absorption of light in the In$_{3-x}$Se$_4$ layer. It is also found that QE increases with Si substrate thickness. These results are due to the fact that longer-wavelength light is absorbed at longer distance from the junction.60,62 The simulated quantum efficiencies (QE) with doping concentrations of In$_{3-x}$Se$_4$ and Si substrate of the CuInSe$_2$/n-Si heterojunction solar cells are also shown in Figure S4a,b, respectively. The figures show that QE of the solar cells is lower for $N_D = 10^{14}$ cm$^{-3}$ of Si substrate; on the contrary, it is almost independent of other doping, indicating that $J_{SC}$ is almost independent of In$_{3-x}$Se$_4$ and Si substrate doping concentrations, which can also be observed from Figure 9a,b.

The simulated PV performances of In$_{3-x}$Se$_4$/p-Si solar cells with the change in defect density of In$_{3-x}$Se$_4$ layer are shown in Figure S5 in the Supporting Information. It is seen from the figure that PV performance of the In$_{3-x}$Se$_4$/p-Si solar cells does not significantly change up to a defect density, $N_0$, of $10^{17}$ cm$^{-3}$. The efficiency greatly decreases for $N_0$ of $10^{18}$ cm$^{-3}$. The defect-density-dependent PV parameters of In$_{3-x}$Se$_4$/p-Si solar cells are also depicted in Figure S6.
2.7.2. Junction Formation at In$_{3-x}$Se$_4$/p-Si Interface. The built-in potential ($\psi_{bi}$) at the In$_{3-x}$Se$_4$/p-Si junctions has been investigated by the capacitive ($C$−$V$) response employing the Mott−Schottky analysis of the solar cells in Solar Cell Capacitance Simulator (SCAPS) simulation software.$^{63}$ The built-in potential, $\psi_{bi}$, at the junction can be determined from the intercept of the $1/C^2$ vs. $V$ plot of the following equation$^6$

$$ \psi_{bi} = -\frac{2kT}{q} \frac{E_p - E_F}{\varepsilon_{Si}} N_D $$

where $A$ denotes the diode area, $\varepsilon_{Si}$ denotes the permittivity of silicon, and $V$ denotes the applied voltage.

Figure 9 shows the characteristic $1/C^2$ vs. $V$ plots for In$_{3-x}$Se$_4$/p-Si devices with different doping concentrations of In$_{3-x}$Se$_4$ and silicon substrate. The $\psi_{bi}$ value is determined from the intercepts of the curves of eq 4. The calculated built-in potentials of the In$_{3-x}$Se$_4$/p-Si heterojunction solar cells are summarized in Table 4.

The built-in potentials of In$_{3-x}$Se$_4$/p-Si devices are almost independent of In$_{3-x}$Se$_4$ doping concentration, as seen in Figure 10a, whereas, they gradually increase with the silicon substrate doping, as delineated in Figure 10b. These findings reveal an abrupt pn$^+$ junction at the In$_{3-x}$Se$_4$/p-

### Table 2. Thickness-Dependent PV Performance of In$_{3-x}$Se$_4$/p-Si Heterojunction Solar Cells

| thickness ($\mu$m) | $J_{SC}$ (mA/cm$^2$) | $V_{OC}$ (V) | FF (%) | $\eta$ (%) |
|-------------------|----------------------|-------------|--------|------------|
| In$_{3-x}$Se$_4$ (Si, $N_A = 10^{18}$ cm$^{-3}$) | | | | |
| 0.05              | 39.01                | 0.643       | 81.54  | 20.46      |
| 0.10              | 38.96                | 0.643       | 82.55  | 20.69      |
| 0.15              | 38.27                | 0.634       | 83.34  | 20.24      |
| 0.20              | 38.22                | 0.643       | 82.69  | 20.32      |
| 0.25              | 37.83                | 0.634       | 83.91  | 20.12      |
| Si (In$_{3-x}$Se$_4$, $N_D = 10^{20}$ cm$^{-3}$) | | | | |
| 100               | 36.11                | 0.608       | 81.40  | 17.88      |
| 150               | 36.67                | 0.625       | 81.43  | 18.66      |
| 200               | 37.32                | 0.627       | 82.19  | 19.22      |
| 250               | 37.69                | 0.629       | 83.49  | 19.81      |
| 300               | 37.99                | 0.632       | 83.57  | 20.07      |
| 350               | 38.94                | 0.634       | 83.66  | 20.66      |

### Table 3. Doping Concentration-Dependent PV Performance of In$_{3-x}$Se$_4$/p-Si Heterojunction Solar Cells

| doping concentration (cm$^{-3}$) | $J_{SC}$ (mA/cm$^2$) | $V_{OC}$ (V) | FF (%) | $\eta$ (%) |
|----------------------------------|----------------------|-------------|--------|------------|
| In$_{3-x}$Se$_4$ (Si = 350 $\mu$m) | | | | |
| $10^{18}$                        | 37.79                | 0.634       | 84.46  | 20.24      |
| $10^{19}$                        | 37.45                | 0.642       | 82.99  | 19.95      |
| $10^{20}$                        | 37.37                | 0.644       | 83.78  | 20.16      |
| $10^{21}$                        | 37.37                | 0.634       | 85.43  | 20.23      |
| Si (In$_{3-x}$Se$_4 = 0.20$ $\mu$m) | | | | |
| $10^{14}$                        | 40.26                | 0.494       | 70.99  | 14.12      |
| $10^{15}$                        | 39.30                | 0.573       | 80.67  | 18.15      |
| $10^{16}$                        | 38.22                | 0.643       | 82.69  | 20.32      |
| $10^{17}$                        | 38.53                | 0.703       | 83.48  | 22.63      |

Figure 10. $C$−$V$ characteristic curves of In$_{3-x}$Se$_4$/p-Si heterojunction solar cells with varying In$_{3-x}$Se$_4$ (a) and Si substrate (b) doping concentration.
ensured the metallic conductivity of In\textsubscript{3}Se\textsubscript{4} through dispersion from the band structure calculation. The DOS calculations exchange correlation in this work.\textsuperscript{66} The Broyden localized density approximation (LDA) of a Perdew threshold of 5 eV/atom for the total energy, 0.01 eV was found for In\textsubscript{3}Se\textsubscript{4} p-Si heterojunction solar cells, which agrees well with the calculated value of carrier concentration. The chemical bonding in In\textsubscript{3}Se\textsubscript{4} materials shows mainly the ionic or metallic and covalent nature from the electronic charge density map. Electron-like Fermi surface appeared in the compound, which implies its single-band character. The calculated value of carrier concentration is ~6.01 × 10\textsuperscript{18} cm\textsuperscript{-3}, which agrees well with the reported values. The optical study of In\textsubscript{3}Se\textsubscript{4} indicates that band gap of stoichiometric In\textsubscript{3}Se\textsubscript{4} should be >1.62 eV, which is consistent with the reported values. We also demonstrate the highly efficient In\textsubscript{x}Se\textsubscript{4−x} p-Si heterojunction solar cells by SCAPS software using experimental data. These results indicate the potential of the In\textsubscript{3}Se\textsubscript{4} compound in solar energy harvesting in future.

### 3. CONCLUSIONS

The electronic and optical properties of the In\textsubscript{3}−xSe\textsubscript{x} compound have been studied employing CASTEP based on the DFT method. The band structure of the In\textsubscript{3}−xSe\textsubscript{x} compound (for x < 1/3) exhibits that the Fermi level (E\textsubscript{F}) crossed over several bands, which is an indication of highly degenerate n-type semiconducting or metallic behavior. On the contrary, a band gap of ~0.2 eV was found for In\textsubscript{3}−xSe\textsubscript{x} (x = 1/3) from the band structure calculation. The DOS calculations ensured the metallic conductivity of In\textsubscript{3}Se\textsubscript{4} through dispersion of In\textsubscript{3}Se\textsubscript{4}. The occupancy of In\textsubscript{1} atom in 3a site of the In\textsubscript{3}Se\textsubscript{4} phase as the metallic behavior comes from the excess In of the phases.\textsuperscript{45,51,52} The structure of the β-In\textsubscript{2}Se\textsubscript{3} compound was used for the value of x = 1/3 in the calculation. The occupancy of different sites in the unit cell of the In\textsubscript{3}Se\textsubscript{4} compounds is shown in Table S2 in the Supporting Information.

#### 4. EXPERIMENTAL DETAILS

4.1. First-Principles Study. The density functional theory (DFT) calculation using CASTEP software was performed for demonstrating the band structure and optical properties of the In\textsubscript{3}−xSe\textsubscript{x} compound.\textsuperscript{64} The crystal structures of the In\textsubscript{3}−xSe\textsubscript{x} material system were visualized by the software VESTA.\textsuperscript{65} The data of optical transmittance spectra, as shown in Figure S7, band gap, and carrier concentration were used in this simulation obtained from the experimental data, as reported elsewhere.\textsuperscript{51} The device simulation parameters used in this study are shown in Table S3 in the Supporting Information.

### 3. CONCLUSIONS

The electronic and optical properties of the In\textsubscript{3}−xSe\textsubscript{x} compound have been studied employing CASTEP based on the DFT method. The band structure of the In\textsubscript{3}−xSe\textsubscript{x} compound (for x < 1/3) exhibits that the Fermi level (E\textsubscript{F}) crossed over several bands, which is an indication of highly degenerate n-type semiconducting or metallic behavior. On the contrary, a band gap of ~0.2 eV was found for In\textsubscript{3}−xSe\textsubscript{x} (x = 1/3) from the band structure calculation. The DOS calculations ensured the metallic conductivity of In\textsubscript{3}Se\textsubscript{4} through dispersion of In\textsubscript{3}Se\textsubscript{4}. The occupancy of In\textsubscript{1} atom in 3a site of the In\textsubscript{3}Se\textsubscript{4} phase as the metallic behavior comes from the excess In of the phases.\textsuperscript{45,51,52} The structure of the β-In\textsubscript{2}Se\textsubscript{3} compound was used for the value of x = 1/3 in the calculation. The occupancy of different sites in the unit cell of the In\textsubscript{3}Se\textsubscript{4} compounds is shown in Table S2 in the Supporting Information.

#### 4.2. Device Simulation. For the device simulation of In\textsubscript{3}−xSe\textsubscript{x}/p-Si heterojunction solar cells, we essentially utilized SCAPS (Solar Cell Capacitance Simulator) simulation software developed by Burgelman and his team at University of Gent.\textsuperscript{67–70} The data of optical transmittance spectra, as shown in Figure S7, band gap, and carrier concentration were used in this simulation obtained from the experimental data, as reported elsewhere.\textsuperscript{51} The device simulation parameters used in this study are shown in Table S3 in the Supporting Information.

### ASSOCIATED CONTENT

#### Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acsomega.9b02210.

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