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FULL PAPER

First-principles Study of the Electronic and Optical Properties of Pristine and In-doped SnS_2 Monolayers

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Abstract

In a large scale first principles study we look at how substitutal indium (In) doping effects the structural, electronic, and optical properties of SnS_2 monolayers. We find that Indium incorporation at the Sn site is energetically favorable which in turn causes only local lattice distortions while the essential CdI_2-type layer framework is preserved. We report that pure SnS_2 is an indirect band gap semiconductor which has a 2.25 eV band gap which reduces to 1.89 eV upon Indium substitution. This band gap reduction is mainly from the In-p state hybridization with S-p and Sn-s/p orbitals at the band edge which the In-d states play a very small role in. Also we see from charge density difference maps and Bader charge analysis that there is a change in charge distribution which Indium donates electrons weakly than Sn does and instead deposits them on nearby sulfur atoms. Also Indium doping greatly improves the optical response of SnS_2 which we see in a red shift of the absorption edge, an increased dielectric response, and modified plasmonic behavior. We present that Indium doping is an effective method to tune the electronic structure and optical performance of SnS_2 mon layers which in turn puts them forward for use in next generation optoelectronic and plasmonic applications. .

Keywords: Monolayer SnS_2; In-doping; Density functional theory; HSE06; Electronic properties; Optical properties

1. Introduction

Two-dimensional (2D) materials have attracted remarkable attention in recent years due to their reduced dimensionality, strong quantum confinement effects, and exceptional tunability of electronic and optical properties[1-3]. Since the isolation of graphene, layered materials belonging to the transition metal dichalcogenides (TMDs) family have emerged as versatile platforms for applications in nanoelectronics, optoelectronics, catalysis, and energy conversion technologies[4-6]. Their characteristic features including weak van der Waals (vdW) interlayer interactions, structural anisotropy, and chemically stable surfaces enable property engineering down to the atomic scale[7, 8].

In Group IV dichalcogenides, tin disulfide (SnS_2) has become of great interest as a very common, environment friendly, and chemically stable semiconductor[9, 10]. In a hexagonal structure which is that of CdI_2, SnS_2 has a layer of tin atoms between two layers of sulfur,[11]. In the monolayer scale we see that the interaction between layers is reduced which in turn widens the indirect band gap which has a reportable range of 2.2 to 2.4 eV. This makes monolayer SnS_2 very promising for use in photodetectors, photocatalytic and thin film optoelectronic applications[9, 12]. However in the case of pristine SnS_2 which has a large band gap and low intrinsic carrier concentration it's optical absorption in the visible range is reduced and it's electrical conductivity is decreased which in turn motivates us to look into methods of electronic structure modulation[13, 14].

In that which regards tailoring SnS_2 electronic properties many approaches have put forth strain engineering, layer number control and the development of van der Waals heterostructures[15, 16]. In that which these techniques do very well in terms of modifying band dispersion and charge transfer, we see also that they require very precise experimental control and at time introduce structural instability. In that which substitutional doping does so very directly and at large scale is in which it introduces localized impurity states, changes carrier concentration, and at the atomic level restructures charge[17, 18].

In certain reports we see that cation substitution at the Sn site is a very effective approach to modify both the conduction band minimum and valence band maximum in SnS_2[19, 20]. Indium is a very attractive dopant choice we see because of its ($4d^{10}5s^25p^1$) electronic configuration that which allows for partial hybridization with host orbitals also it's a relatively weak donor as compared to Sn[21]. As opposed to lighter nonmetal dopants, in substitution we see that impurity level states near the band edges are introduced which at the same time do not produce deep trap levels. This in turn enables what we see is a controlled band gap narrowing and improved electronic delocalization[22, 23].

In recent time we have seen from both theoretical and experimental studies that foreign elements in tin disulfide create large changes in the electronic, magnetic, and optical properties[24-26]. Also, we have not yet fully understood at a detailed microscale how In substitution changes the band structure, orbital hybridization, and charge redistribution in monolayer SnS_2 which also includes study using both semilocal and hybrid exchange correlation functionals[27, 28]. Also we have seen that study of In-doping's role in the optical response which includes dielectric behavior and plasmonic excitations is required to determine structure property relationships[29, 30].

In this work we report a detailed first principles study of pristine and In-doped SnS_2 monolayers using density functional theory. We use a 6x3x1 supercell that has 54 atoms in it which includes one Sn atom that is replaced by In, this corresponds to ~1.85% total atomic concentration (5.56% on the cation sublattice). We calculate electronic band structures and density of states within the PBE-GGA framework which we then refine via the HSE06 hybrid functional to correct for band gap underestimation[31, 32]. In order to determine the microscopic cause of band gap modification we analyze projected density of states, perform Bader charge analysis and present charge density difference maps. Also we study the optical properties which we evaluate via the frequency dependent dielectric function and energy loss spectra to see how In doping plays a role in optical absorption and plasmonic behavior[33].

In this work we present a study that looks at how electronic structure modification plays out in terms of charge redistribution and optical response which in turn we use to present a very clear picture of the physical mechanism Indium substitution uses to do effective band gap engineering in SnS_2 monolayers. We also report fundamental insight into how doping with Indium tunes 2D chalcogenides and put forth In-doped SnS_2 as a very promising material platform for the next generation of optoelectronic and energy related applications.

2. Computational Details

In the present study we used density functional theory (DFT) within the quantum ESPRESSO package for all first principles calculations[34, 35]. In this work we used ONCVP pseudopotentials for electron-ion interaction[36], In the present study we used the Perdew-Burke-Ernzerhof (PBE) functional which is a form of (GGA) to account for exchange and correlation effects[37].

We made a 6x3x1 supercell of monolayer SnS_2 which includes 54 atoms to study both pristine and In-doped configurations. We introduced Indium substitution by trade in one Sn atom for one In atom which is equal to total dopant concentration of about 1.85% (which is 5.56% on the cation sublattice). Also we applied a vacuum spacing of $\geq$ 15 Å in the out of plane (z) direction to avoid interaction between periodic images.

In our study we fully relaxed all atomic structures until we achieved a residual force of less than 10^-3 Ry/Bohr which in turn ensured we had reached the minimum energy configuration. We did structural optimization prior to all electronic and optical calculations and we used the optimized geometries which we found to be the most stable throughout the study.

In our work we did SCF calculations that used a plane wave kinetic energy cutoff of 50 Ry for wave functions and 400 Ry for charge density. We used a 4 x 4 x 2 Monkhorst Pack k point mesh for SCF calculations which in turn was used for sampling the Brillouin zone. For the accurate evaluation of band structure and density of states (DOS/PDOS) we performed non self-consistent field calculations which we did with a denser 8 x 8 x 2 k-point grid.

In order to overcome the issue of band gap underestimation which is a known issue of semi local exchange correlation functionals we calculated certain cases with the Heyd-Scuseria-Ernzerhof (HSE06) screened hybrid functional[38]. In the HSE06 approach we put in a bit of short range Hartree-Fock exchange into the PBE functional which in turn gives us a better description of band edges and electronic excitation energies. We report band gaps from both PBE and HSE06 calculations for direct comparison.

In our work we calculated total density of states (DOS) and projected density of states (PDOS) which we did to determine the role of orbitals of Sn, S and In atoms. We used orbital projections to see what the S-p, Sn-s/p, and In-s/p/d states are doing in the formation of the valence band maximum (VBM) and conduction band minimum (CBM). Also we aligned all energy spectra with respect to the VBM which we set at zero energy.

In order to determine charge redistribution caused by In substitution we performed Bader charge analysis of real space charge density grids which were from converged SCF calculations[39]. In the present study we determined effective atomic charges as pseudo valence charges which in turn enabled us to directly compare pristine and doped systems. Also we calculated charge density difference maps which we visualized using VESTA to present areas of electron accumulation and depletion around the dopant site[40].

In pristine and In-doped SnS_2 monolayers we looked at the optical properties which we did via the epsilon.x post processing utility in Quantum ESPRESSO[25]. In order to improve the convergence of the optical spectra we used a very dense 12x12x1 k point mesh for the Brillouin zone. Also we looked at the complex dielectric function, performed electron energy loss spectroscopy (EELS) and studied related optical properties which in turn we did to look at interband transitions, dielectric response and plasmonic effects of In-doping

3. Structural optimization

In our study we performed full geometric optimization of pristine and In-doped SnS_2 monolayers using density functional theory in a 6x3x1 supercell which we did so to accurately model local structural relaxations. We found that the optimized pristine SnS_2 mon layer still has the typical CdI_2-type hexagonal layered structure in which each Sn atom is coordinated with six S atoms which indicates no lattice distortion post relaxation as seen in Figure 1a. Also in Figure 1b we see the preserved layered geometry and structural integrity in the out of plane direction. Upon doping with In into the Sn sites we note the overall framework is maintained without structural breakdown; what we do see are very small very local changes around the dopant which present as a slight extension of the nearest In – S bonds due to In's larger atomic radius as compared to Sn as is shown in Figure 1c. Thus we report that Indium substitution is a geometric fit into the SnS_2 monolayer.

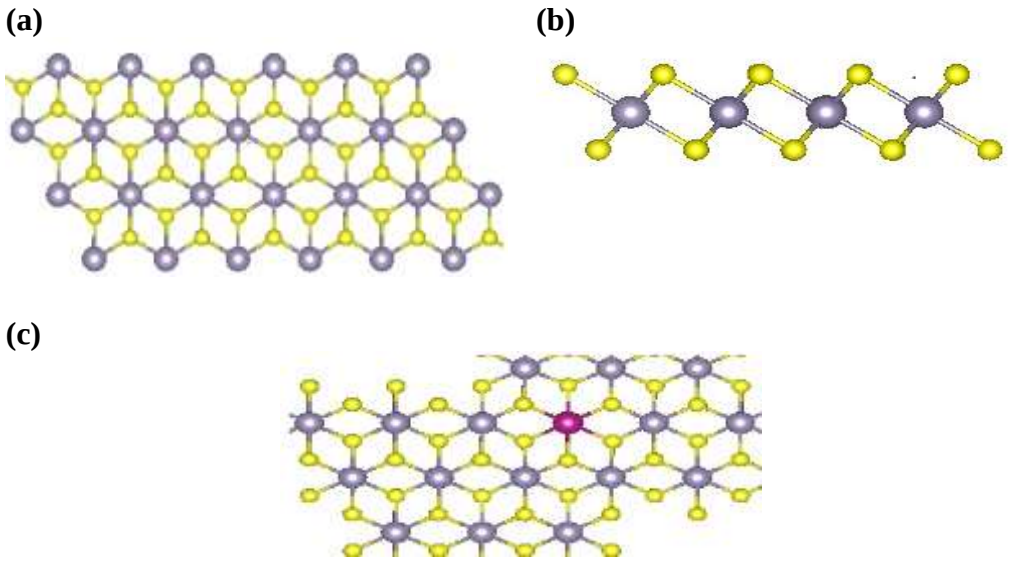


Figure 1. Optimized geometries of SnS_2 monolayers after full structural relaxation: (a) pristine SnS_2 monolayer, (b) side view of the pristine SnS_2 monolayer, and (c) In-doped SnS_2 monolayer highlighting localized geometric distortion around the Indium dopant.

4. Results and Discussion

4.1 Electronic properties

In this section we look at the electronic properties of pristine and In-doped SnS_2 monolayers which we do so to report on the effect of substitutional indium doping on that which is of primary electronic behavior. We focus on the gap's evolution, the role of elements and orbitals at the band edges, and also the charge redistribution brought about by the dopant which in turn gives us a full picture of the changes in electronic structure.

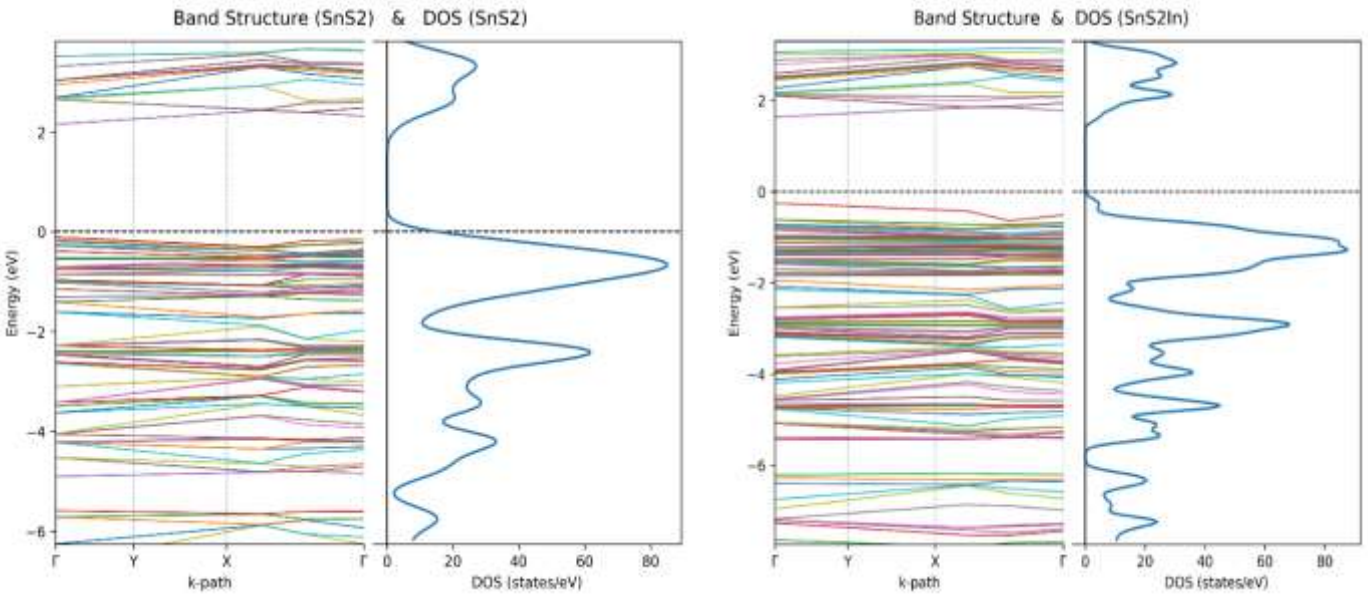
4.1.1 Band Structure and Total Density of States (DOS)

In our study we analyzed the electronic band structure and total density of states (DOS) of both pristine and In-doped SnS_2 monolayers using the HSE06 hybrid functional which we found to do a better job in the description of band gap characteristics as compared to semi local exchange – correlation functionals. Hence in this section we present only the HSE06 results to properly assess the effect of Indium substitution on the electronic properties of SnS_2.

In pristine SnS_2 monolayer, the HSE06 band structure we see is of an indirect band gap semiconductor which has the valence band maximum (VBM) at one high symmetry point and the conduction band minimum (CBM) at another in the Brillouin zone. As reported in Figure 2(a) we see the band gap is of 2.25 eV which is in agreement with past hybrid functional studies of monolayer SnS_2. Also the total DOS we note has a clear gap at the Fermi level which in turn confirms the semi conducting character of the pristine system also reporting no mid gap states.

In the study we see that upon the introduction of Indium large changes in the electronic structure take place. As we can note in Figure 2(b) the In-doped SnS_2 monolayer still displays a large band gap but this is reduced in size to 1.89 eV within the HSE06 model. This reduction is due to the defect induced states that pull the conduction and valence band edges towards the Fermi level but also do not produce any deep localized states in the gap. Also of note is the variation of the total DOS for the doped system in which we see an increase in electronic density at the band edge as opposed to the pure system.

In looking at Figure 2(a) and Figure 2(b) we see that Indium substitution changes the electronic structure of SnS_2 by reducing the band gap but at the same time preserves the material's overall semiconducting character. Also we note that there are no deep trap states present in the DOS which indicates that In-doping does not degrade the electronic quality of the monolayer which is a key requirement for optoelectronic device applications. We report that In-doping is indeed a very efficient method for band gap engineering in SnS_2 mon layers within our hybrid functional description.



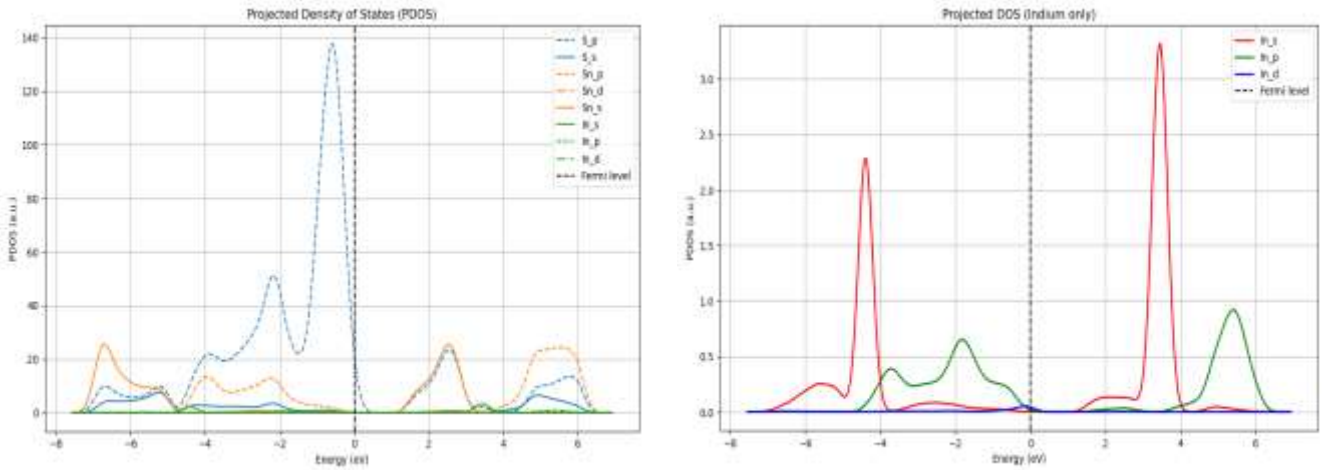
(a) (b)

Figure 2. HSE06 band structure and DOS of pristine and In-doped SnS_2 monolayers.

4.1.2 Projected Density of States (PDOS)

HSE06 hybrid functional we used to determine the atomic and orbital contributions to the electronic states at the band edges. In Figure 3(a) we see that in pristine SnS_2 the valence band is mainly a result of S-p states, and that the conduction band edge which we see is mostly from hybridized Sn-s and Sn-p states which is the typical electronic structure for CdI_2-type layered materials. Upon Indium substitution we see an increase in total PDOS at the valence and conduction band edges which we interpret as an increase in orbital hybridization, also no deep localized states within the gap appear which we take as a sign that the semi conducting character is preserved.

In order to present the specific dopant related results we have separated out the Indium atom's orbital resolved PDOS in Figure 3(b). What we find is that In-p states play the primary role near both the VBM and CBM which in turn are responsible for the which we see is the band gap narrowing in the HSE06 framework, also In-d states play an almost non role across the energy range of interest. Also of note is the combined analysis of Figure 3(a) and Figure 3(b) which we see to report that substitutional In-doping what it does is it tunes the electronic structure of SnS_2 via p – p hybridization also it does so without introducing what we would term in gap states which in turn highlights In's great suitability for use in band gap engineering in optoelectronic applications.



(a) (b)

Figure 3. HSE06 projected density of states (PDOS) of SnS_2 monolayers: (a) PDOS of all constituent elements and (b) orbital-resolved PDOS of the In-dopant.

4.1.3 Charge Redistribution and Bader Analysis

In-dopants' introduction we see that the electronic structure changes which in turn causes charge redistribution in the SnS_2 lattice. We looked at this via Bader charge analysis in the doped systems. What we found is that the In atom has an effective charge of +1.308 e which is lower than that of the Sn at (+1.559 e) which means In is a less effective electron donor. This reduced charge donation leads to enhanced electron accumulation on neighboring sulfur atoms, which acquire an average charge of approximately (− 0.773 e). The resulting local charge imbalance modifies the electrostatic potential around the dopant site and promotes orbital hybridization near the band edges.

4.2 Optical properties

In pure as well as In-doped SnS_2 monolayers we report which inelastic In-doping does to their interaction with light. We focus at the frequency variable dielectric response along with associated optical properties which in turn we are using to see how changes in electronic structure play out in terms of improved light absorption and plasmonic properties.

4.2.1 Imaginary Part of the Dielectric Function $\varepsilon_2(\omega)$

In the dielectric function's imaginary part, which we see in reference to the optical absorption in both pristine and In-doped SnS_2 monolayers' case that is through interband electronic transitions. From the data in Figure 4, we see that the absorption in case of pure SnS_2 takes place at high photon energies as expected from the wide band gap. But when Indium is introduced we observe a large shift towards lower energy for the absorption edge along with increase of low energy

absorption, that is a result of new allowed optical transitions at the band edges brought about by dopant induced orbital hybridization. We note also that In-doping does in fact improve SnS_2 monolayers' ability to absorb visible light.

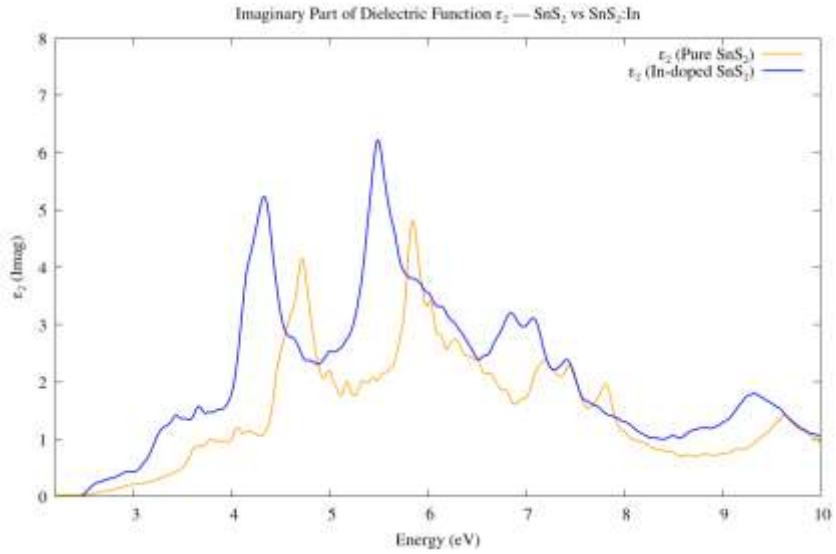


Figure 4. Imaginary part of the dielectric function ε₂(ω) for pristine and In-doped SnS_2 monolayers.

4.2.2 Real Part of the Dielectric Function ε₁(ω)

In the pristine state, the dielectric function's real part, ε₁(ω), we see the electronic polarisation and dielectric screening of pure as well as In-doped SnS_2 monolayers. As reported in Figure 5, for the native SnS_2 we note a typical dielectric response at low photon energies related to its base electronic structure. With Indium substitution that feature changes we see an enhanced low energy response and the characteristic features have a shift towards lower energies which in turn indicates better electronic screening and greater polarizability. Also these changes are in agreement with the Indium induced band gap reduction we report and also point out the In-doping role in the tuning of the dielectric properties of SnS_2 monolayers.

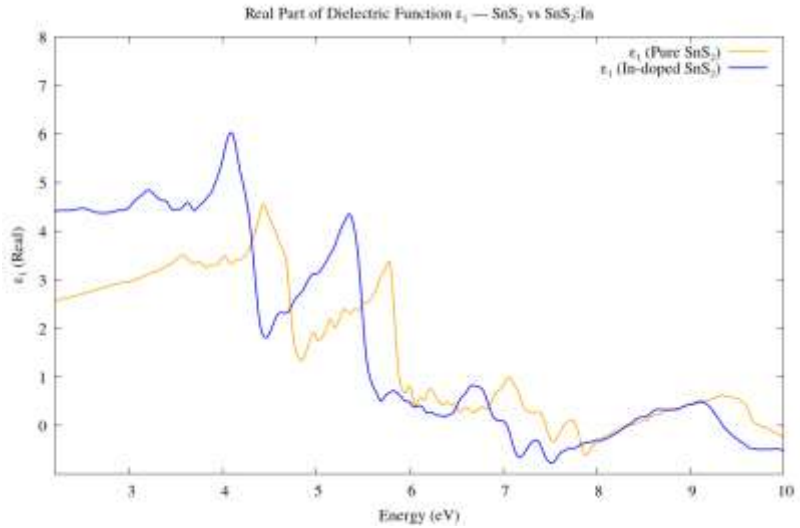


Figure 5. Real part of the dielectric function $\varepsilon_1(\omega)$ for pristine and In-doped SnS_2 monolayers.

4.2.3 Electron Energy Loss Spectrum and Energy Loss Function

In pristine and In-doped SnS_2 monolayers we see that (EELS) and energy loss function present to us information on collective electronic excitation and plasmonic behavior[41]. In theory EELS intensity is a function of the imaginary part of the inverse dielectric function which may be put as:

$$EELS(\omega) = Im\left[\frac{1}{\varepsilon(\omega)}\right]$$

where the complex dielectric function is defined as:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$$

In Figure 6 we present EELS spectra which for pristine SnS_2 show a large loss peak at higher energies that is a tell-tale of intrinsic plasmon excitations. Upon Indium doping we see this peak shift to lower energies along with a change in intensity which we interpret as a sign of enhanced collective electronic response. Also in Figure 6(b) we see the energy loss function which supports our view that we have improved electronic screening and enhanced plasmonic action in the doped system. We present that In-doping does in fact play a large role in tuning the plasmonic response of SnS_2 monolayers.

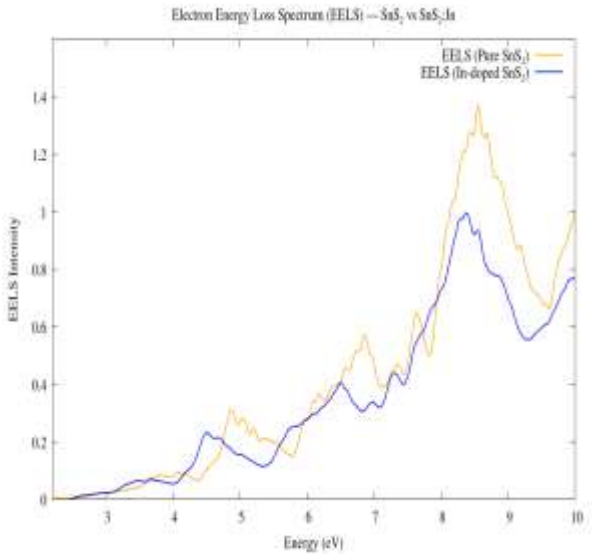
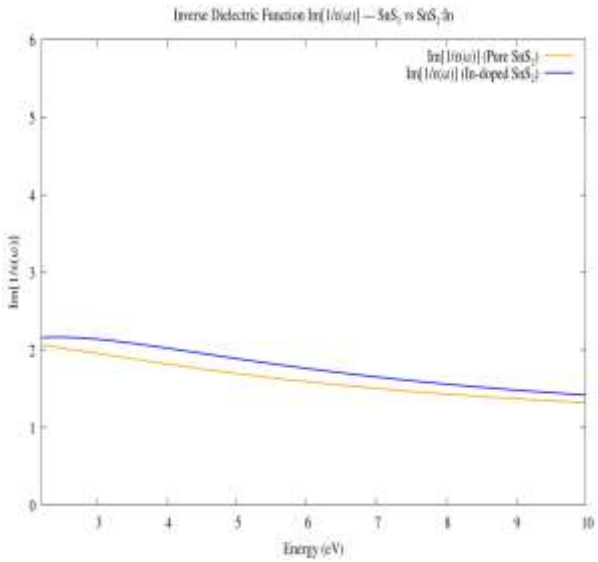


Figure 6. **(a)** Electron energy loss spectrum (EELS)



(b) energy loss function of pristine and In-doped SnS_2 monolayers.

5. Conclusion

As a whole we did an in depth first principles study looking at the effect of indium doping into SnS_2 monolayers. We see that In inclusion at the Sn site is both energy and geometry favorable which in turn causes local lattice distortions but at the same time preserves the base CdI_2-type layered structure. Also we looked at the electronic structure which via HSE06 hybrid functional we determined for pure SnS_2 to be that of an indirect band gap semiconductor which is 2.25 eV. Upon introduction of Indium we see a large and intrinsic band gap reduction to 1.89 eV which at the same time preserves the overall semiconducting character of the system.

In our study we found out that what causes the band gap reduction is mainly the hybridization of In-p orbitals with the nearby S-p and Sn s/p states at the band edges which in turn see almost no contribution from In-d states in the low energy range. Also we noted via charge density difference maps and Bader charge analysis that there is a large scale charge redistribution which the dopants bring about in this case Indium which we note is a less effective electron donor as compared to Sn and what we see is that it promotes greater electron accumulation on nearby sulfur atoms. What we also find is that Indium substitution does in fact modify the electronic structure through a controlled orbital hybridization which we see does not introduce what we term as harmful deep trap states.

In-dopants play a large role in the optical response of SnS_2 monolayers which we see via a red shifted absorption edge, greater dielectric response, and modified plasmonic resonances which in

turn indicate improved electronic screening and carrier dynamics. As a whole our results present In-doping as very that which tuned the electronic structure and optical performance of SnS_2 mon layers which in turn we put forth In-doped SnS_2 as a very promising 2D material for use in next generation of optoelectronic and plasmonic applications.

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Data Availability

All data supporting the findings of this study are available from the corresponding author upon reasonable request. Additional supporting information is included within the article and its supplementary materials.

Author Contributions

Hassan Karm: Conceptualization, Methodology, Validation, writing—original draft, Writing—review & editing.

Mujahid Eldaw: Computational analysis, Software, Data curation, Visualization, draft, & editing.

Rawia Elobaid: Conceptualization, Supervision, Formal analysis, Investigation, Resources, Writing—review & editing. Ismael A Wadi: review & editing.

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