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Curriculum Vitae

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EXPERIENCE

Postdoctoral Fellow

Indian Institute of Technology, Bombay

Feb 2019 – Feb 2022

Mumbai, India

- Development and characterization of 2D materials like Ruddlesden Popper perovskites, TMDs for photonic and optoelectronic applications.
- Fabrication of nanoparticles and nanostructures for nanophotonic applications.
- Integrating Plasmonics with 2D materials for optoelectronic and energy applications.
- Mentoring PhD, MTech and MSc students for their thesis work.
- Teaching assistantship for BTech and MSc batches in Physics and Nano- laboratory.

Guest Lecturer

S.G.T.B. Khalsa College, University of Delhi

Jan 2018 – Dec 2018

Delhi, India

- Taught two subjects (a) Semiconductor devices (b) C Programming to undergraduate BSc(H.) Electronics students.
- Mentored lab sessions and annual projects.
- Wrote popular/academic science articles for Physics Education India and UK magazine.

Guest Lecturer

S.G.T.B. Khalsa College, University of Delhi

Sept 2016 – Dec 2016

Delhi, India

- Taught the subject of Basic Circuit Theory and Network Analysis to undergraduate BSc(H.) Electronics students.

PROJECTS

Plasmonics and Nanophotonics

Institute PDF, IIT Bombay

2019 - ongoing

- Fabrication of gold nanostructures and perovskite quantum dots.
- Integrating plasmonic nanostructures with 2D materials to study energy and charge transfer phenomenon.

Photovoltaics

Institute PDF, IIT Bombay

2019 - ongoing

- Study of 2D and quasi-2D perovskite thin films for optoelectronic applications.
- Mechanical study of perovskite for usage in flexible electronics.

OBJECTIVE

Help make a better world with sustainable development.

KEY ACHIEVEMENTS



Institutional Postdoctoral fellowship by IIT Bombay

Feb 2019 - ongoing



INSPIRE fellowship by Department of Science and Technology, INDIA.

2014-2018



Gold Medal

Smt. Shanti Devi Bhargava Memorial Gold Medal for securing First rank in University in master program.



Gold Medal

for securing First rank in graduation by Hansraj College, University of Delhi.



Junior Research Fellowship by University Grant Commission (UGC), India.

Fellowship offered for pursuing Doctoral studies in India.



Sh. Vijay Malhotra Prize and Dr. Rajbeer Singh Prize

for academic excellence in university examinations in graduation.

SKILLS

Hard-worker

Strong working relationships

Motivator & Leader

Python

Lumerical

C/C++

Linux

Data analysis softwares like Origin, WSXm etc.

Thermal Evaporation

Sputtering (DC/RF)

Wet Bench Chemical synthesis like Hydrothermal

Spin Coating

Glovebox Usage

LANGUAGES

English



Hindi



- Fabrication and characterization of Quasi-2D Ruddlesden Popper Perovskite based solar cells.

Advanced Material Synthesis and Thin Film fabrication INSPIRE Fellowship, Department of SCinece and Technology (DST), India

📅 2014-2018

- Fabrication and study of Inorganic Chalcogenide (CdS, SnS) and Perovskite (CsPbI₃) thin films.

EDUCATION

Ph.D. in Electronics University of Delhi, India

📅 2014 - 2019

Area: Applied Physics, Thin film, Photovoltaics

Thesis title: Development, Characterization and Optimization of p-SnS Thin Films for Photovoltaic Applications.

M.Sc. Electronics Department of Electronic Science, University of Delhi

📅 2011 - 2013

Percentage : 86.14%

B.Sc. Electronics (H) Hansraj College, University of Delhi

📅 2008 - 2010

Percentage : 83.16%

MAIN PUBLICATIONS

15+ publications in International peer reviewed journals

- "Tailoring the mechanical response of Ruddlesden Popper lead halide perovskites" **Yashika Gupta**, S.Rathore, A.Singh, A.Kumar, Journal of Alloys and Compounds 901 (2022) 163575.
- "Gate tunable light-matter interaction in natural biaxial hyperbolic van der Waals heterostructures" A.Bapat, S.Dixit, **Yashika Gupta**, A.Kumar, arXiv preprint arXiv:2110.07526, 2021.
- "A Novel Route for Fabrication of Stable CsPbI₃ Perovskite Thin Film by Thermal Evaporation" **Yashika Gupta**, Arun Palakkandy, Stepan V.Syrotyuk, Kuldeep Kumar, Smriti Arora ChemistrySelect 4 (2019) 1.
- "Mitigating Reasons for the Poor Performance of n-CdS/p-SnS Solar Cells" **Yashika Gupta**, Chhaya Ravikant, P.Arun Global Challenges 2 (2018) 1800017.
- "Analysis of Zener-like Behaviour of p-SnS/ZnO and p-SnS/ZnS Heterojunctions" **Yashika Gupta**, P.Arun Materials Research Express, 5 (2018) 036409.
- "Contribution of Lattice Parameter and Vacancies on Anisotropic Optical Properties of Tin Sulphide" C.I.Zandalazini, J.Navarro Sanchez, E.A.Albanesi, **Yashika Gupta**, P.Arun Journal of Alloys and Compounds, 746 (2018) 9 .

- "Optimization Of SnS Active Layer Thickness For Solar Cell Application" **Yashika Gupta**, P.Arun Journal of Semiconductors, 38 (2017) 113001.
- "Influence Of Strain On The Sensitivity Of Tin Sulphide Films" **Yashika Gupta**, P.Arun Materials Chemistry and Physics, 191 (2017) 86.
- "Influence Of Urbach Tail On The Refractive Index Of p-SnS Thin Films" **Yashika Gupta**, P.Arun Physics Status Solidi-C, 14 (2017) 1600207 .
- "Grain Size And Lattice Parameter's Influence On Band-Gap Of SnS Thin Nanocrystalline Films" **Yashika Gupta**, P.Arun, A.A. Naudi, M.V. Walz, E.A. Albanesi Thin Solid Films, 612 (2016) 310.
- "Suitability Of SnS Thin Films For Photovoltaic Application Due To The Existence Of Persistent Photocurrent" **Yashika Gupta**, P.Arun Physics Status Solidi-B, 3 (2016) 509.
- "Analysing The Diode With A Shunt Resistance In The Piecewise Model" **Yashika Gupta**, P.Arun Journal of Active and Passive Electronic Devices 14 (2019) 1.

ACADEMIC ARTICLES

- "A Comment on the Dependence of LED's Efficiency on Junction Ideality Factor" Anubhav Sethi, **Yashika Gupta**, P.Arun Physics Education UK, 53 (2018) 035024.
- "How A Diode Tames The Sun " **Yashika Gupta** Physics Education India, 33 (2016) 4.
- "First Step To Ellipsometry" **Yashika Gupta**, P.Arun International Journal of Physics, 3 (2015) 8.

- 3 additional papers under review
- 1 paper accepted for publication (waiting to be online)

Google Scholar Credentials

Citations : 86
h-index : 5
i10-index : 2



Tailoring the mechanical response of Ruddlesden Popper lead halide perovskites

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ABSTRACT

Two dimensional (2D) Ruddlesden Popper perovskites have been extensively studied for their exceptional optical and electronic characteristics while only a few studies have shed light on their mechanical properties. The existing literature mainly discusses the mechanical strength of single crystal perovskites, however a study of structure tunability of 2D perovskite thin films is still missing. In this study, we report the effect of number of inorganic layers 'n' on elastic modulus of 2D, quasi-2D perovskites and 3D perovskite thin films using nanoindentation technique. Our studies indicate the role of orientation of the inorganic layers in perovskite films in tailoring their mechanical response. The experimental results have been substantiated using first principle density functional theory (DFT) calculations. We also report other important mechanical parameters namely, shear modulus, bulk modulus, Poisson's ratio, Pugh's ratio, Vickers hardness, yield strength and the universal elastic anisotropic index using DFT simulations. Anisotropy is observed in the elastic modulus of the materials under study and has been discussed in detail in the manuscript. Understanding the mechanical behavior of 2D Ruddlesden Popper perovskites thin film in comparison with conventional 3D perovskite offers intriguing insights into the atomic layer dependent properties and paves the path for next generation mechanically durable and novel devices.

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1. Introduction

Metal halide organic-inorganic perovskites, having characteristic formula, ABX_3 , where $A = CH_3NH_3^+$ (MA), $HC(NH_2)_2^+$ (FA) etc; $B = Pb^{2+}$; $X = Cl^-$, Br^- , I^- , possess favorable properties like high absorption coefficient (10^4 – 10^5 cm⁻¹) [1,2], low exciton binding energy (10–60 meV) [3], tunable direct band-gap (2.3–1.5 eV) [4,5], long charge diffusion length ($> 10 \mu m$) [6,7] and defect tolerance [8]. These materials have revolutionized thin film technology, showing great potential in applications ranging from photovoltaics to light emitting devices to transistors to synaptic devices. However, poor stability of these perovskites towards ambient light, moisture and temperature raises a big question towards the commercialization of this material class. To remedy this situation, researchers have come up with a solution of "slicing" the conventional perovskite structures (ABX_3) into a 2D structure of the form $R_2A_{n-1}Pb_nX_{3n+1}$. This change in

dimensionality is brought by replacing or mixing the 'A' cation by a larger monovalent organic cation 'R' (Butylamine (BA), Phenylethylamine (PEA) etc.) giving perovskite a layered structure as shown in Fig. 1(a). These 2D perovskites also known as Ruddlesden Popper (RP) perovskites, are classified by the number of inorganic layers 'n' in between the large organic cation. Perovskite with $n = 1$ contains horizontal inorganic layers stacked vertically together by Van der Waal forces due to interaction between the organic cations of these layers, showing a complete two-dimensional behavior. As the number of layers increases, the structure goes from 2D to quasi-2D to finally a 3D structure (see Fig. 1(a)). These two-dimensional perovskites not only exhibit exceptional optoelectronic properties like 3D perovskites, they also hold the potential of great structural tunability arising due to its layered structure. The Van der Waal forces holding organic and inorganic layers together, opens great avenues for flexible applications like printed solar cells, foldable sensors, transistors and other wearable devices. Also, the relative ease and scalability of solution-based methods used in developing perovskite thin films and crystals provide an edge to these 2D Ruddlesden popper perovskites over other 2D materials (for example transition

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Materials Science inc. Nanomaterials & Polymers

A Novel Route for Fabrication of Stable CsPbI₃ Perovskite Thin Film by Thermal Evaporation

Yashika Gupta,^[a, b] Arun Palakkandy,^{*, [b]} Stepan V. Syrotyuk,^[c] Kuldeep Kumar,^[d] and Smriti Arora^[b]

Perovskite thin films hold promise as a potential candidate for high efficiency solar cells. In recent years, a wealth of results has been published on CsPbI₃ thin films. However, most of the literature reports that CsPbI₃ perovskite films are prone to aging where black colored CsPbI₃ films with cubic lattice change to yellow colored films with orthorhombic lattice upon exposure to ambient conditions. This poor stability presents

itself as a major challenge in utilization of CsPbI₃ for device applications. This manuscript presents an alternate route for fabricating stable CsPbI₃ thin films using thermal evaporation. Experimentally, our samples were found to be stable, visually and structurally, over a period of six months. Even annealing of the samples did not induce structural changes.

Introduction

In the past few years, perovskite materials have gathered attention from the scientific community owing to their interesting optical and electronic properties^[1] and also as potential candidates for high efficiency solar cells.^[2–4] These materials have a structural formula ABX₃, where A and B are cations of different sizes and X is an anion, generally a halide ion i.e. Cl, Br or I.^[5,6] Perovskites with this chemical formula are viewed as a layered structure of BX₃ in octahedral bondings trapping a heavy atom of A within the layer. The large, heavy atom contributes to an increase in the material's ability to absorb light.^[7] Also, the structure seems to ensure defect free structures unlike chalcogenide layered structures.^[8] Due to their high absorption coefficient, large diffusion length of the minority charge carriers and the suitable band gap, a record efficiency of ~22% has been achieved for perovskites (organic-inorganic hybrid) solar cells in a span of less than ten years of research.^[9] Despite such success, commercialization of these hybrid perovskite solar cells faces problems like their reaction with moisture, thermal instability etc.^[10,11] due to the organic cationic component.

To overcome this problem, Protesescu et al.^[8] developed an all-inorganic perovskite nano-crystal sample having the structural form CsPbX₃ by replacing the organic cation with Cs⁺. These inorganic perovskite solar cells, although were more stable, their efficiency remained much less than their organic counterparts.^[12,13] Thus, indicating the need for further study to understand the physics of the inorganic perovskites. Also, among these inorganic perovskite materials, CsPbI₃ remains the least popular despite having the most suitable band gap of ~1.7 eV for photo-voltaic applications.^[13] Literature points out that the main reason for its unpopularity is the conversion of its perovskite (cubic) phase into non-perovskite (orthorhombic) phase at room temperature.^[14–17] The orthorhombic CsPbI₃ lacks the suitable absorption coefficient and band-gap, making it unfit for use in photo-voltaic applications.^[14,15] However, there is a report by Frolova et al.^[13] where they have reported stable cubic phase at room temperature. There are recent works that have investigated the stability issues of perovskites.^[18–21] At this point the authors would like to point out that most of the literature talking about the aging of the CsPbI₃ thin films do so using their X-Ray Diffraction (XRD) results with few prominent peaks, rendering it impossible to do a lattice constant calculations from the XRD results.^[14,22–26] That is, most of these reports have just cross-referenced each other without giving any substantial proof of the formation of CsPbI₃ thin films. There is also a range of lattice constants reported in the literature for CsPbI₃ perovskite structure.^[13,23,27,28] These reports give the lattice parameters in the range 6.2 to 7.0 Å.

In light of this increasing importance of CsPbI₃ as a potential photo-voltaic candidate, it becomes important to address this lack of clarity about its structure and perovskite properties. Also, commercially it becomes important to find a method to obtain stable CsPbI₃ perovskites which does not age. Thus, in this manuscript we have tried to fill in these gaps about CsPbI₃ thin film's structural and optical properties, obtained by thermal evaporation technique. The formation of perovskite structure has been confirmed here by comparing

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Mitigating Reasons for the Poor Performance of n-CdS/p-SnS Solar Cells

Yashika Gupta, Chhaya Ravikant, and Arun Palakkandy*

In the present work, indium tin oxide (ITO)/n-CdS/p-SnS/Au structured solar cells are fabricated with best conversion efficiency of 0.005%. A detailed investigation is made into the cause of the poor conversion efficiency and the cause is narrowed down to defects in p-SnS which effect the junction and the neutral region of the cell. The junctions performance is quantified using the ideality factor which is found to be related to the band misalignment. The paper also investigates into literature and discusses efforts made to overcome the problems with this structure.

1. Introduction

Tin sulfide (SnS) promises to be one of the most suitable inorganic, nontoxic, readily available material suitable for photovoltaic application in thin film state.^[1–3] The structural, optical and electrical properties of SnS thin films such as grain size and orientation,^[1,4] conductivity,^[5,6] band-gap,^[7,8] etc. can be easily tuned by controlling the fabrication conditions. On top of this, Loferski et al.^[9] using theoretical simulations claim a possible conversion efficiency of 24% for SnS solar cells. The first ever solar cell using SnS was fabricated by Noguchi et al.^[10] in 1994 with a cadmium sulfide (CdS) window layer. Over the last two decades (1994–2016), conversion efficiencies ranging from 0.0025% to 0.29% have been reported for pristine CdS/SnS solar cells.^[10–13] This is far less than the Loferski's claim.^[9] However, recently researchers have reported efficiencies greater than 2.5% for CdS/SnS heterojunction solar cells by including

an extra Zn-based (mainly ZnO) buffer layer in the structure or inverting the cell geometry.^[14–17] Although the p-SnS solar cell performance has improved by adding the extra buffer layer, these results fail to comment upon the factors effecting the pristine CdS/SnS junction which leads to the need of a buffer layer.

This, hence implies serious gaps exist in our understanding of p-SnS based heterojunction solar cells which needs to be addressed in order to improve SnS based

solar cell's performance. A solar cell consists of three regions, namely a) the junction region, b) the neutral region, and finally c) the electrodes. A drop in performance of any one of the three regions would result in a substantial drop in the device performance. In our previous report,^[18] detailing our extensive study on p-SnS thin films properties as a function of film thickness, we had shown that the diffusion length of holes through the neutral region would play an important role in deciding the solar cell's conversion efficiency. Based on the results of that study, we claimed that a p-SnS active layer of 900 nm thickness would be best suited for solar cell application. The aim of this manuscript is to study the effect of SnS thin film properties on the heterojunction formed with CdS layer and to investigate the reasons for the poor efficiency reported to date for pristine n-CdS/p-SnS solar cells.

2. Solar Cell Fabrication

Thin films of CdS and SnS were fabricated in our lab on indium tin oxide (ITO) substrate by thermal evaporation using a Hind Hivac (12AUD) coating unit, in vacuum better than 10^{-5} Torr. The layers were fabricated one after another as per the schematics shown in **Figure 1**. The window layer, CdS films grown on the etched ITO layer of 150 nm. The etching was done to prepare ITO as the front transparent electrode of the solar cell. CdS thin film grown at room temperature is invariably n-type.^[19] On this CdS layer, p-SnS active layer was grown. The thickness of CdS layer was controlled during evaporation using a digital quartz monitor (and subsequently verified with Dektek surface profilometry) at 365 nm in this study. CdS layer thickness was selected on the basis of literature on n-CdS/p-SnS heterojunction solar cells having same geometry as the present work.^[12,13,20] To study the behavior of n-CdS/p-SnS structure as a function of p-SnS film thickness, p-SnS layers of different thicknesses were fabricated on top of the CdS films. Since SnS films take-up p-type conductivity when grown on heated substrate,^[12] the ITO/n-CdS were kept at 180 °C. The nature of film conductivity were verified by hot-probe method. Finally, a gold electrode was grown on the p-SnS surface using

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Zener Behaviour of p-SnS/ZnO and p-SnS/ZnS Heterojunctions

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Abstract

p-SnS absorbing layers were grown by thermal evaporation on layers of various Zinc compounds, like ZnO and ZnS. This present work reports the J-V characteristics of thus obtained p-SnS/ZnO and p-SnS/ZnS heterojunctions. The pn junctions of these structures did not show any photovoltaic activity, however a zener like behaviour was observed in the 3rd quadrant of their J-V characteristics. Our analysis of the diodes suggest that the reverse breakdown or zener voltage obtained from the dark J-V characteristics can be used to estimate the energy band diagram of the junction and in turn the band-alignment at the junction. This makes it an easy alternative to X-ray Photoelectron Spectroscopy method usually used.

1. Introduction

Tin Sulfide (SnS) is an earth abundant, less toxic semiconductor material which has attracted a great deal of attention as an absorber layer in solar cells [1, 2]. However, until now only $\approx 5\%$ efficiency [3] has been achieved for p-SnS based solar cells. Researchers are still searching for a suitable window layer to form a better heterojunction with p-SnS absorber layer to improve its conversion efficiency. While investigating the nature of junction that SnS forms with accompanying window layers and their role in conversion efficiency, we observed a zener like behaviour. Lan et al [4] too have reported a zener like behaviour of Silicon-Tungsten disulfide (p-Si/WS₂) heterojunction. Their work aroused considerable interest in researchers of material science. Considering that SnS too is a IV-VI group semiconductor material with layered structure like WS₂, we have analysed the heterojunction's zener behaviour (formed with different complimentary layers such as ZnS and ZnO) along the method suggested

by Lan group. In this manuscript, we list the results of our analysis and confirm Lan et al's observation.

2. Experimental

Heterojunction diodes of p-SnS/ZnO and p-SnS/ZnS were fabricated on ITO substrates. In these heterojunctions, ZnO and ZnS work as n-type window layers. ZnO and ZnS layers of 400 nm thickness were grown on ITO substrate using spin coating and thermal evaporation techniques, respectively. On these window layers, p-SnS absorber layer of thickness 1000 nm (for ZnO/p-SnS) and 740 nm (for ZnS/p-SnS) was grown by thermal evaporation. Thermal evaporation was done using Hind High Vac (12A4D) thermal evaporation coating unit at vacuum better than $\approx 4 \times 10^{-5}$ Torr. Deposition of the ZnS was done by evaporating ZnS powder with substrate maintained at room temperature while the SnS layer was done using SnS powder, with the substrate maintained at 180°C. It should also be mentioned here that p-type conductivity in SnS thin films is obtained when SnS is evaporated on substrates maintained at 150 – 250°C [5, 6]. In our study, we consistently got p-type conductivity for 180°C and hence for our study substrate temperature was maintained

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Optimization of SnS active layer thickness for solar cell application

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Abstract: This work presents a comparative study of n-SnS and p-SnS active layers for increased solar cell efficiency. Tin sulphide thin films of various thicknesses having p-type and n-type conductivity were fabricated by thermal evaporation. Both type of films had the same (113) orientation of the crystal planes with a constant tensile strain of ~ 0.003 and ~ 0.011 , respectively. The persistent photocurrent was observed in all n-SnS and p-SnS samples with the current's time decay constant decreasing with increasing film thickness. Hole mobility of thicker p-SnS films was found to be greater than the electron mobility in n-SnS samples, with mobility (both hole and electron) showing an increasing trend with film thickness. The optimum absorber layer thickness for both p- and n-SnS layers should have a high value of diffusion length for a given absorption coefficient and band-gap.

Key words: thin film; chalcogenides; optical properties

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1. Introduction

For a material to be a potential candidate as an active layer in a solar cell, it should not only have an optimum bandgap and high absorption coefficient in visible range for maximum quantum yield, but it should also allow for the easy flow of charge carriers without recombination across the neutral length of the active layer (i.e. a large diffusion length). While most of the works focus on band-gap and the absorption coefficient, there are very few reports in the literature that compare materials on the basis of their diffusion length in the active layer^[1], with no comment on tin sulphide (SnS). SnS is rapidly emerging as a popular inorganic thin film candidate for alternative solar cell material. Tin sulphide (SnS) is an earth-abundant, cost-effective material having high absorption coefficient ($\approx 10^4 \text{ cm}^{-1}$) and band-gap varying from 1.1–2.1 eV^[2, 5] for films ranging from polycrystalline to nanocrystalline. Also, a blue shift in band-gap values due to quantum confinement in SnS nano-crystalline thin films is widely observed. SnS thin films are also interesting since they can exist with p-type or n-type conductivity, depending on the presence of tin or sulphur-vacancies respectively^[6, 9]. While much of the focus has been dedicated to p-SnS thin films^[10, 12], there are only few reports on n-type SnS thin film solar cells^[13, 14].

Hence, it would be interesting to not only compare the band-gap, the absorption coefficient of p-SnS with n-SnS, but also investigate the difference in diffusion length in the two types of films. In our previous paper^[15], we had investigated just the persistent photocurrent due to recombination-generation (RG) centers/traps present in p-SnS thin films and its suitability for improving charge carrier lifetime. In this manuscript, we will carry the work forward and compare the optical and transport properties (such as mobility) of n-SnS and p-SnS thin films and comment on the optimum active layer thickness, based on diffusion length, for solar cell applications.

2. Experimental

Thin films of SnS were fabricated on glass substrates ($3 \times 3 \text{ cm}^2$) kept at room temperature by thermal evaporation technique using a Hind High Vac 12A4D vacuum coating unit. The evaporation was done in a vacuum of 540×10^{-5} Pascal ($\approx 4 \times 10^{-5}$ Torr) at a constant rate of 2 nm/s. Films of varying thicknesses (d) were obtained by varying the duration of deposition. Hot probe measurement was done to detect the type of conductivity in the films, one extreme of the film was locally heated at 80 °C while the second extreme remained at room temperature. Probes were kept at two different extremes (hot and cold) to measure the direction of current, in other words polarity. For fabricating 'n-type' SnS films, pellets of SnS were used while SnS₂ starting material was used for fabricating 'p-type' SnS films. Both starting materials were provided by Himedia (Mumbai). While fabricating the samples, the source and the substrate were maintained at a distance of 12 cm from each other (for both n- and p-SnS films). Details as to why the film's nature of conductivity depends on the starting material and fabrication technique would be given in the section below. The thickness of the films was measured using Dektak Surface Profiler (150) by moving the stylus of the instrument across the edge of the film. Structural and morphological properties of the films were studied at room temperature using a Bruker D8 X-ray Diffractometer and a field-emission scanning electron microscope (FEI-Quanta 200F) respectively. The Raman spectra of the films under study were obtained using Renishaw InVia Raman microscope with Ar²⁺ laser in reflection mode. Calibration of the instrument was done using a standard silicon wafer. Photoconductivity studies of the films were carried out using the SMU-01 source meter of Marine (India) and a Tungsten lamp was used as the light source. Two contacts were made on the film surface using silver paste and a constant bias of 10 V

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