Interfaces in Emerging Chalcogenide Based Solar Cells

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Program

&

Abstracts

Interfaces in Emerging Chalcogenide Based Solar Cells

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Foreword

All started for me back in 2023 when I joined the RenewPV community in Tallinn, Estonia during the 1st RenewPV conference. The very shorth beginning was like during other events, feeling little bit confused and like an intruder. Once I started to communicate with the participants, I said to myself that the choice of being there was an inspired idea and I jumped inside the RenewPV family without any fears.

The years till now were amazing, grace to new friends and to the funding opportunities via this Cost Action, years in which we received at NIMP wonderful researchers from different countries as well as participating to the events sponsored mainly by European Union. Part of the chalcogenide solar cells team from NIMP, took also advantage of this funding option participating to several STSMs and events.

This Joint WGs workshop "*Interfaces in Emerging Chalcogenide Based Solar Cells*" should be as best as the other RenewPV events, being confident due to interest from your side, either on-site or online participants and friends. Your contribution to this workshop is valuable to me and I really appreciate your warm feed-back when you get the invitation to join this reunion. *Thank you all in advance!*

I deeply acknowledge the support received from the NIMP directorate and from my laboratory mates, being all together also emotionally involved in organising this event. I acknowledge also the sponsors for being so kind to give financial assistance.

Concerning the program, as you see in the next pages, it contains attractive lectures, interactive sessions as well as ad-hoc developed best practices. In between, NetWorking in an ancient factory, while end of Friday considering and discussing the further steps of our collaboration during the visit in MIP laboratories.

In the end, I wish all of us, enjoyable and enlightening workshop! I hope this meeting will contribute to the development of new renewable energy concepts using non-toxic materials with low environmental impact and low greenhouse gas emissions, namely emerging inorganic chalcogenide thin-film PV technologies, and why not to meet (again) to the last big event which will be organized in the frame of CA21148.

Yours,

Aurelian

https://infim.ro/en/@galca/

Main responsible for local organization

p.s. Each section name has the online meeting hyperlink. The licence is only for 100 participants. If more, please accept my apologize and I hope that I will get the chance to make up to you other time. Thanks for your understanding.

Interfaces in Emerging Chalcogenide Based Solar Cells

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Thursday 23th April 2026
Bucharest time, Romania (EEST)

8:00-8.30	**Registration**		
Introductory session			
8.30-8.40	*Foreword*		**Nicolae Spalatu** (TALTECH, EST)
8.40-8.50	*Welcome*		**Lucian Pintilie** (NIMP, ROU)
8.50-9.00	*Event info/news*		**Aurelian Galca** (NIMP, ROU)
$Sb_2(S,Se)_3$ solar cell interfaces, Moderator: **Elisa Artegiani** (UNIVR, ITA)			
9.00-9.20	O01	*Electronic Structure of $Sb_2(S,Se)_3$ and Solar Cell Interfaces by Kelvin Probe and Photoelectron Yield Spectroscopy at Ambient Pressure*	**Marin Rusu** (HZB, DEU)
9.20-9.40	O02	*Atomic Layer Deposited SnO_x Interlayer for Interface Passivation in Co-Evaporated Sb_2Se_3 Solar Cells (online)*	**Hoang Van Quy** (VINUNI, VNM)
9.40-10.00	O03	*Interface-induced conformal growth of ultrathin Sb_2S_3 for high efficiency TiO_2-based photovoltaics*	**Hadeer Hussien** (TALTECH, EST)
10.00-10.30	Coffee Break & **Poster Session**		
$Sb_2(S,Se)_3$ absorber engineering & intrinsic properties, Moderator: **Natalia Maticiuc** (HZB, DEU)			
10.30-10.50	O04	*From Toxic to Sustainable: Low-Toxicity Solvent Strategies for High-Performance Sb_2S_3 Solar Cells*	**Lucia Leonat** (NIMP, ROU)
10.50-11.10	O05	*Solution-grown antimony sulfide selenide segmental absorber films for thin-film heterojunction solar cells*	**Natalia Kujawska** (P-LODZ, POL)
11.10-11.30	O06	*Intrinsic and Extrinsic Stability Factors in Sb_2S_{3-x} – based solar cells*	**Cristina Besleaga** (NIMP, ROU)
11.30-11.50	O07	*Decoupling growth kinetics and Sb_2S_3 absorber thickness via additive-assisted hydrothermal synthesis and post-growth etching (online)*	**Evgeniia Gilshtein** (DTU, DNK)
11.50-12.10	O08	*Environment-Induced Defect Dynamics in Sb_2Se_3 Thin Films for Emerging Chalcogenide Solar Cells*	**Gokhan Yilmaz** (MAKU, TUR)
12.10-12.30	O09	*Effect of TiO_2 Electron Transport Layer architecture on Spray Pyrolysis Deposited Sb_2S_3 Thin Films for Solar Cells*	**Rayene Merah** (U-Constantine, DZA)
12.30-12.50	O10	*Air annealing of the CdS layer to improve Sb_2Se_3 devices efficiency*	**Elisa Artegiani** (UNIVR, ITA)
12.50-14.20	Lunch & **Poster session**		
14.20-17.00	**Practical/interactive discussions***		**A.** *solution processed chalcogenides, HTLs, ETLs* **B.** *optoelectrical characterization and modelling* (including **DTLS** and **TSC**) **C.** *structural and compositional characterisation* (**FIB, TEM, SEM, XPS**) **D.** *First-principles calculations*
18.00-22.00	NetWorking in Fabrica (downtown Bucharest)		

Interfaces in Emerging Chalcogenide Based Solar Cells

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Friday 24th April 2026
Bucharest time, Romania (EEST)

Summary of interaction discussions (the day before) **Best practices**, Moderator: **Nicolae Spalatu** (TALTECH, EST)			
8.30-8.40	B01	*Solution processed chalcogenides*	**Natalia Kujawska** **Katharina Dehm**
8.40-8.50	B02	*Electrical measurements*	**Cristina Besleaga** **Elisa Artegiani**
8.50-9.00	B03	*Structural investigations*	**Aurelian Galca** **Cristian Radu**
9.00-9.20	B04	*Interfaces*	**Charif Tamin** **Abdessamad El Kanouny**
CdTe solar cells, moderator: **Charif Tamin** (INL, FRA)			
9.20-9.40	O11	*Sb_2Se_3 as an effective dopant for CdTe solar cells*	**Elisa Artegiani** (UNIVR, ITA)
9.40-10.00	O12	*The influence of the deposition working power on some physical properties of RF-sputtered cadmium telluride films for photovoltaic applications*	**Sorina Iftimie** (UNIBUC, ROU)
10.00-10.20	O13	*CdTe solar cells for tandem application with Silicon devices (online)*	**Mariyam Mukhtar** (UNIVR, ITA)
10.20-10.40	O14	*Effect of Large Bi-Exciton Binding Energy in Type II CdSe/CdTe QDs on Efficiency of MEG Solar Cells*	**Stanko Tomic** (VINCA, SRB)
10.40-11.00	Coffee Break & **Poster Session**		
Exotic and promising chalcogenides, Moderator: **Marin Rusu** (HZB, DEU)			
11.00-11.20	O15	*Selenium alloying in $BaZrS_3$ perovskite for efficient tuning of properties*	**Lorenza Romagnoli** (UNIROMA1, ITA)
11.20-11.40	O16	*First-Principles Determination of Pnictogen Chalcohalide Band Alignments for Improved Solar-Cell Applications*	**Cibran Lopez** (UPC, ESP)
11.40-12.00	O17	*TOPCon-Inspired Dielectric Tunnel Interfaces for Wide-Bandgap Se Solar Cells*	**Charif Tamin** (INL, FRA)
12.00-12.20	O18	*Tuning the Structural and Charge Transport Properties of GeS Thin Films*	**Audrius Drabavičius** (FTMC, LTU)
12.20-12.40	O19	*Interface Engineering of the c-TiO_2/SnS Junction for Enhanced Thin-Film Solar Cell Performance*	**Abdessamad El Kanouny** (U Hassan II, MAR)
12.40-14.10		Lunch & **Poster session**	
A Tale of a Magic Characterization Method & Moon of forehead, Moderator: **Sorina Iftimie** (UNIBUC, ROU)			
14.10-14.30	O20	*Hyperspectral photoluminescence mapping and analysis on chloride-activated chalcogenide CdSe thin films*	**Bohuslav Rezek** (CVUT, CZE)
14.30-14.50	O21	*Tuning the Optoelectronic Properties of Wide-Bandgap Cu_2ZnSnS_4 by Silver Substitution, Sodium and Lithium Co-Doping and Thermal Annealing*	**Messaoud Tamin** (UBE, FRA)
14.50-15.10	O22	*How the molybdenum process influences the growth of CZTS: A comparative study of different lab-grown and commercial molybdenum substrates*	**Alessandro Veneri** (UNIVR, ITA)
15.10-15.30		Closing remarks, impressions, perspectives and farewell	
15.30-17.30		**Visit of NIMP laboratories**	

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	Posters (during the coffee breaks and lunches in both days of the workshop)	
P01	*NiO_x nanoparticles as HTM in semi-transparent Sb_2S_3 solar cells*	**Alessandra Rocchina Palmieri** (TALTECH, EST)
P02	*Synthesis and Processing of Colloidal Nanocrystals for Sustainable Thin-Film Photovoltaic Devices*	**Katharina Dehm** (FAU, DEU)
P03	*Impact of hole transport layers on the performance of Sb_2S_3 solar cells*	**Viorica Stancu** (NIMP, ROU)
P04	*Influence of Post-deposition Annealing Temperature and Time on Sb_2S_3 films and Solar Cells grown by Ultrasonic Spray Pyrolysis*	**Robert Aleksander Liiv** (TALTECH, EST)
P05	*FIB-SEM tomography of structural, chemical and electronic properties of Sb_2Se_3 solar cell layer stacks*	**Jaroslav Kuliček** (CVUT, CZE)
P06	*Morphological and structural analysis of $Sb_2(S,Se)_3$ thin films based solar cells*	**Cristian Radu** (NIMP, ROU)
P07	*Development of Antimony Sulfide Selenization to From Antimony Sulfide Selenide Using Selenourea as a Selenium-Source*	**Jekaterina-Ketrin Rostsupkina** (TALTECH, EST)
P08	*Effect of the Annealing Atmosphere on the Properties of the $Cu_2ZnSn(S,Se)_4$ (CZTSSe) Thin Films and Their Photovoltaic Performance*	**Mehmet Ali Olgar** (OHU, TUR)
P09	*Influence of Annealing Temperature on the Properties of Cu_2ZnSnS_4 Thin Films Obtained via Ligand Exchange*	**Roman Golubovski** (UKIM, MKD)
P10	*Tunable Ag Incorporation in Electrodeposited Kesterite CZTS Thin Films for Photovoltaic Applications*	**Mohamed Yassine Zaki** (UM6P, MAR)
P11	*Optimization of Growth Parameters in Sol–Gel-Derived Bi_2S_3 Thin Films*	**Hamide Kavak** (CU, TUR)
P12	*The importance of XPS in the analysis of the dopants in solar cells*	**Amelia Bocirnea** (NIMP, ROU)
P13	*Advanced Characterization Techniques for Next-Generation Photovoltaic Technologies*	**Veton Haziri** (UBT, RKS)
P14	*Development of chalcogenide semiconductors for photovoltaic applications*	**Vladimir Dulev** (BAS, BGR)
P15	*Temporal Anomaly Evaluation and Feature Selection for Real-Time Health Monitoring of Solar Inverter Interfaces in Chalcogenide-Based PV Systems*	**Ibrahim Ozturk** (Osmaniye, TUR)
P16	*DFT study of diazonium-derived grafting on SnS surfaces*	**Avni Berisha** (UNI-P, RKS)
P17	*Biomass-Derived Activated Carbons as Sustainable Interfacial Materials for Energy Storage and Emerging Chalcogenide Photovoltaic Systems*	**Murat Yılmaz** (Osmaniye, TUR)

Electronic Structure of $Sb_2(S,Se)_3$ and Solar Cell Interfaces by Kelvin Probe and Photoelectron Yield Spectroscopy at Ambient Pressure

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Keywords: Chalcogenides, work function, surface photovoltage, ionization energy, band diagrams

$Sb_2(S,Se)_3$ has gained important attention in recent years as a promising material for application in photovoltaics (PV). Solar cell devices based on Sb_2Se_3 absorbers have already achieved power conversion efficiencies (PCEs) >10%, while according to Shockley-Queisser limit a theoretical PCE of ≈33% would be achievable. The essential difference between experimental and theoretical values are attributed, among others, to yet a lack of reliable optoelectronic data and non-optimized band alignments at interfaces. The development of the $Sb_2(S,Se)_3$ valence band maximum (VBM) and conduction band minimum (CBM) with the [S]/([S]+[Se]) atomic ratio is also still not completely clarified.

In the present work, for determination of the Fermi level and VBM positions, we employ the Kelvin probe (KP) and photoelectron yield spectroscopy (PYS) techniques under inert ambient, e.g., N_2 or Ar, at atmospheric pressure. [1] We determine in addition the charge carrier concentrations of materials. The development of the built-in voltage and related open circuit voltage (V_{oc}) is monitored from layer-by-layer surface photovoltage (SPV) measurements.

We investigate electronic properties of the $Sb_2(S,Se)_3$ thin film absorber as a function of [S]/([S]+[Se]) atomic ratio and the electronic structure of interfaces in solar cell devices such as ITO/ZnO/CdS/Sb_2Se_3/Mo/SLG, FTO/TiO_2/Sb_2S_3/P3HT/Au, FTO/TiO_2/$Sb_2(S,Se)_3$/P3HT/Au. We find that the VBM of the $Sb_2(S,Se)_3$ absorber changes monotonically from 5.09 eV to 5.60 eV when the material composition changes from Sb_2Se_3 to Sb_2S_3. By considering the $Sb_2(S,Se)_3$ bandgaps, we find the CBM to vary between 3.80–3.90 eV with the material composition. The conductivity type of $Sb_2(S,Se)_3$ changes from *p* to *n* at a sulfur concentration of about 80 at.%. For ITO/ZnO/CdS/Sb_2Se_3/Mo/SLG solar cells, we show the relevance of optimizing the band alignment at the CdS/Sb_2Se_3 interface. For FTO/TiO_2/$Sb_2(S,Se)_3$/P3HT/Au solar cell devices, the crucial importance of the P3HT/Au interface in developing a maximum V_{oc} is revealed from SPV measurements. For all solar cells, complete band diagrams are proposed, and the transport of current is discussed. The obtained data are of high relevance for modelling and development of $Sb_2(S,Se)_3$ PV devices with enhanced efficiencies.

[1] M. Rusu, T. Kodalle, L. Choubrac, N. Barreau, C. A. Kaufmann, R. Schlatmann, T. Unold, *ACS Appl. Mater. Interfaces* **13** (2021) 7745

Atomic Layer Deposited SnO_x Interlayer for Interface Passivation in Co-Evaporated Sb_2Se_3 Solar Cells

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Keywords: Sb_2Se_3 thin-film solar cells; atomic layer deposition (ALD); SnO_x interlayer; interface passivation; co-evaporation

To address the limited power conversion efficiency of co-evaporated Sb_2Se_3 solar cells, an ultrathin SnO_x interlayer was introduced between the Sb_2Se_3 absorber and CdS buffer layer via atomic layer deposition (ALD). The conformal ALD-grown SnO_x provided effective physical and chemical passivation at the heterointerface, significantly suppressing carrier recombination within grains and along grain boundaries. Moreover, the interlayer acted as a diffusion barrier, preventing Sb interdiffusion into the CdS layer. The uniform coverage of SnO_x also alleviated surface roughness of the co-evaporated Sb_2Se_3 absorber, leading to improved device uniformity and reduced variation in photovoltaic parameters. These results demonstrate that incorporating an ultrathin ALD- SnO_x interlayer is a simple and practical strategy to enhance the performance and reproducibility of Sb_2Se_3 thin-film solar cells.

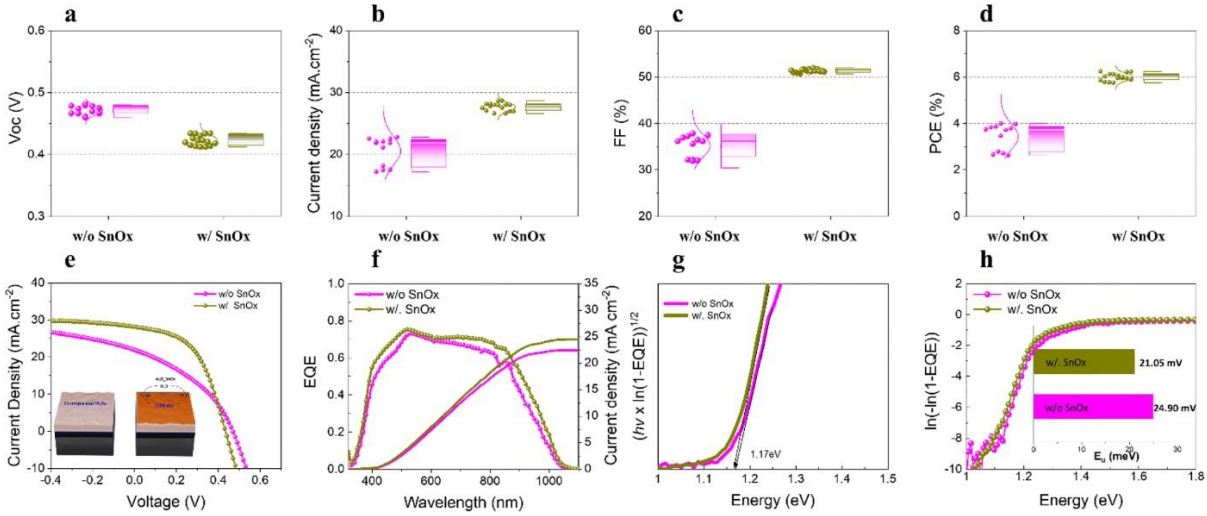

Figure 1: (a–d) Box plots of solar cell parameters for the tested devices. (e) Current density–voltage (J–V) curves of the highest-efficiency device within each group. (f) EQE spectrum of the best-performing device based on the standard AM 1.5G solar spectrum. (g) The bandgap calculated from EQE spectra. (h) Urbach energy values derived from EQE spectra for the control-Sb_2Se_3 and SnOx–Sb_2Se_3 solar cells, respective.

Interface-induced conformal growth of ultrathin Sb_2S_3 for high efficiency TiO_2-based photovoltaics

Hadeer Hussien[1*], Malle Krunks[1], Nicolae Spalatu[1], Atanas Katerski[1], Thanh Tai Nguyen[1], Bohuslav Rezek[2], Jaroslav Kuliček[2], Egor Ukraintsev[2], Ilona Oja Acik[1]

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Keywords: Ultrathin Sb2S3 films, interface engineering, ZnO interlayer

Antimony sulfide (Sb_2S_3) has emerged as a promising absorber material for photovoltaic applications. However, severe dewetting during crystallization remains a critical challenge for ultrathin Sb_2S_3 films, particularly on rough or textured substrates. During film deposition, Sb_2S_3 tends to accumulate in concave regions, and subsequent retraction upon annealing leads to poor surface coverage and film discontinuity. Moreover, in TiO_2-based device architectures, interfacial incompatibility between TiO_2 and Sb_2S_3 limits the open-circuit voltage (V_{OC}).

Surface modification of TiO_2 offers an effective route to mitigate dewetting and improve interfacial quality. Here, we introduce a nanostructured ZnO interlayer at the TiO_2/Sb_2S_3 interface via spray pyrolysis deposition from an ultra-low-concentration zinc acetate solution (5×10^{-4} M). Detailed investigation of the early-stage growth reveals that ZnO-modified TiO_2 suppresses film retraction and enhances interfacial adhesion, thereby promoting uniform nucleation and conformal growth of Sb_2S_3. As a result, nearly complete coverage of ultrathin (~100 nm) absorber layer is achieved on textured substrates. In contrast, Sb_2S_3 deposited on pristine TiO_2 tends to accumulate in concave areas, leading to pronounced film discontinuities. The ZnO interlayer further reduces surface roughness of the Sb_2S_3 film from 15 nm to 7.5 nm, improving interfacial contact with the hole transport layer.

Device analysis demonstrates that TiO_2-ZnO interlayer effectively suppresses trap-assisted recombination. Space-charge-limited current measurements indicate a reduction in trap density from
1.5×10^{16} cm^{-3} to 9.3×10^{15} cm^{-3}, contributing to enhanced open circuit voltage. The champion device achieves a power conversion efficiency (PCE) of 7.8% under AM 1.5G illumination, with a V_{OC} of 711 mV, a short-circuit current density (J_{SC}) of 18.4 mA cm^{-2}, and a fill factor of 60%, outperforming the reference device. Notably, the high current density obtained with an absorber thickness of only ~100 nm suggests efficient charge transport and extraction. This further supported by light-intensity-dependent measurements, where the ZnO modified device exhibits a J_{SC} light-intensity exponent of (0.99) much closer to unity than that of the reference device (0.88). To the best of our knowledge, this work represents the highest efficiency reported for TiO_2-based Sb_2S_3 solar cells with such an ultrathin absorber.

From Toxic to Sustainable: Low-Toxicity Solvent Strategies for High-Performance Sb_2S_3 Solar Cells

Lucia Nicoleta Leonat[1*], Viorica Stancu[1], Abdessamad El Kanouny[1], Sara Laafar[1], Andrei Gabriel Tomulescu[1], Cristina Besleaga[1], Aurelian Catalin Galca[1]

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Keywords: Antimony sulfide (Sb_2S_3), chalcogenide-based solar cells, green solvent engineering, DMF substitution, reduced-toxicity processing, eco-friendly fabrication

Antimony sulfide (Sb_2S_3) represents a compelling absorber for next-generation thin-film photovoltaics due to its suitable band gap, high absorption coefficient, earth-abundant constituents, and compatibility with low-temperature solution processing. Among molecular ink–based deposition routes, dimethylformamide (DMF) is conventionally employed as the primary solvent because it provides effective dissolution of $SbCl_3$ and thiourea, forming stable precursor complexes that enable uniform film growth. However, DMF is classified as a toxic solvent, raising significant environmental, health, and regulatory concerns that challenge the sustainability of large-scale Sb_2S_3 device manufacturing.

In this work, we address the solvent-related bottleneck in Sb2S3 thin-film fabrication by partially substituting DMF with less hazardous, environmentally benign alternatives in the preparation of precursor solutions. Importantly, the deposition parameters, interface engineering strategies, and post-deposition treatments were kept unchanged, allowing direct evaluation of each type of solvents system intrinsic impact on film formation and device performance. The modified solvent formulations preserved precursor solubility and enabled the formation of smooth, compact Sb_2S_3 layers with a specific, well-defined texture, favorable for charge transport across heterointerfaces.

When integrated into photovoltaic architectures, spin-coated Sb_2S_3 absorbers prepared with reduced-DMF formulations achieve power conversion efficiencies comparable to those obtained using films deposited by the widely adopted chemical bath deposition (CBD) method. These results demonstrate that environmentally safer solvent systems can be implemented without compromising optoelectronic performance or interfacial quality.

The present study provides a viable pathway toward greener processing of chalcogenide-based solar cells, highlighting that targeted solvent engineering can simultaneously reduce process toxicity and maintain device efficiency. This approach contributes to the broader objective of developing sustainable, low-impact fabrication routes for emerging thin-film photovoltaic technologies.

Solution-grown antimony sulfide selenide segmental absorber films for thin-film heterojunction solar cells

Natalia Kujawska[1,*], Katarzyna Znajdek[1], Padmanabhan Karunakaran Nair[2], Priyanka Bamola[2], Yareli Colín García[2], Asiel Neftalí Corpus Mendoza[2], Esteban Ojeda Durán[2]

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Keywords: antimony sulfide selenide layers, thin-film solar cells, emerging inorganic photovoltaics, chemical bath deposition technology

This study examined the fabrication and characterization of thin-film heterojunction solar cells based on antimony sulfide selenide $Sb_2(S,Se)_3$ segmental absorber layers deposited by chemical bath deposition (CBD). The device structure consisted of an FTO-coated glass substrate, a CdS window layer, a double (segmental) $Sb_2(S,Se)_3$ absorber layer, carbon electrodes and silver contacts.

The layered architecture and adjustable composition of $Sb_2(S,Se)_3$ make it possible to tune both optical absorption and charge carrier transport. The research investigated how variations in chemical deposition conditions influence device performance metrics such as electrical output and efficiency, testing second absorber layer deposition times of 30, 60, 75, and 90 minutes. The peak photovoltaic conversion efficiency of 4.36%, measured over a 0.302 cm^2 sample area, was achieved by the 30B variant, produced with a 30-minute second deposition step. Thermal post-processing was performed at 280°C over 30 minutes. The results obtained are presented in Table 1.

Table 1. Parameters at SUN in Temixco Morelos, Mexico - recalculated to STC (solar irradiation: 935-965 W/m^2 // temperature: 34 deg. C).

Solar cell code	Area (cm^2)	V (mV)	I (mA)	J (mA/cm^2)	FF (-)	Eff (%)
30B	0.302	456	5.44	19.19	0.501	4.36
30C	0.325	458	5.71	18.59	0.488	4.11
60B	0.367	448	6.71	18.50	0.458	3.72
60C	0.414	444	7.34	17.93	0.460	3.51
75B	0.338	437	5.90	16.80	0.450	3.24
75C	0.287	430	4.73	17.66	0.460	3.50
90B	0.345	432	6.10	17.99	0.451	3.47
90C	0.306	428	5.75	18.56	0.434	3.45

The research was carried out jointly by Lodz University of Technology (Poland) and IER-UNAM (Mexico).

Intrinsic and Extrinsic Stability Factors in Sb_2S_{3-x} – based solar cells

Cristina Besleaga*, Viorica Stancu, Abdessamad El Kanouny, Sara Laafar, Iulia Corina Ciobotaru, Amelia-Elena Bocirnea, Lucia Nicoleta Leonat, Claudiu-Alexandru Pescaru, Iosif-Daniel Simandan, Andrei Gabriel Tomulescu, George E. Stan, Ioana Pintilie, Aurelian Catalin Galca

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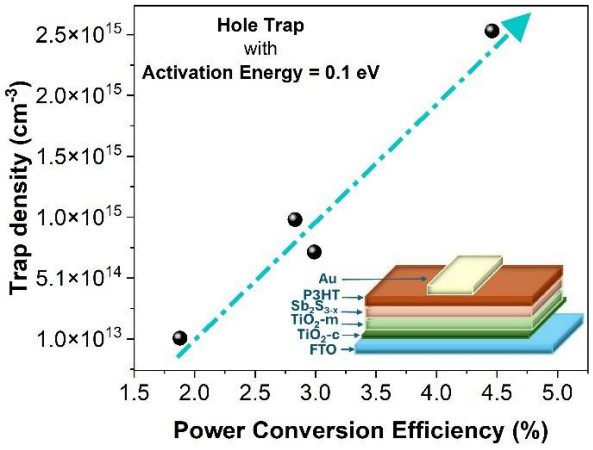
Keywords: solar cell, Sb2S3, DLTS, stability, humidity, temperature

The glass/FTO/TiO2/Sb2S3-x/P3HT/Au solar cells were investigated, with a focus on identifying the origin of performance degradation after exposure to high relative humidity and to mild heat stress. Analyzing the photovoltaic output and Deep-Level Transient Spectroscopy (DLTS) results, we probed the evolution of defect states after thermal exposure and after long-term storage of Sb2S3-x-based devices. The DLTS analysis revealed that shallow hole traps govern the stability of the Sb2S3-x cells. Significantly, it was shown that this shallow defect is not related to chlorine in the absorber, indicating an intrinsic origin. In the broader context of Sb2S3-x photovoltaics, this study underlines the paramount importance of defect engineering towards achieving more stable and efficient Sb2S3-x solar cells.



Reference: Besleaga C, Stancu V, El Kanouny A, et al (2026) Intrinsic and extrinsic stability factors in Sb2S3-x – based solar cells. Mater Des 264:115733. https://doi.org/10.1016/j.matdes.2026.115733

Decoupling growth kinetics and Sb_2S_3 absorber thickness via additive-assisted hydrothermal synthesis and post-growth etching

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Keywords: antimony sulfide, hydrothermal synthesis, absorber thickness

Hydrothermal synthesis offers a scalable route for the fabrication of antimony chalcogenide absorber layers for thin-film solar cells [1, 2]; however, precise control over film thickness and quality remains a key challenge. In this work, we investigate the role of thioacetamide (TA) as a sulfur-containing additive in modulating the growth kinetics of Sb_2S_3 films, and its implications for device performance.

We show that increasing TA concentration significantly enhances absorber growth, leading to thicker films compared to those obtained using sodium thiosulfate (STS) as S-precursor alone. This results in a clear thickness-dependent trade-off in device performance, where thinner films favor higher short-circuit current density (J_{SC}), while thicker films yield improved open-circuit voltage (V_{OC}). Adjusting precursor composition to maintain constant sulfur molarity only partially compensates for the TA-induced thickness increase, indicating that TA influences growth kinetics beyond simple sulfur supply. To decouple growth chemistry from final absorber thickness, we implement two complementary strategies: reduced hydrothermal growth time and post-growth hydrothermal etching, demonstrated earlier only for $Sb_2(S,Se)_3$ [3]. We demonstrate that etching provides a controllable route to tune absorber thickness while preserving the benefits of TA-assisted growth. Preliminary device results suggest that etched TA-grown films can achieve improved charge collection and fill factor (FF) compared to directly grown thin films, highlighting the importance of the growth pathway in determining device performance.

This study establishes additive-assisted growth combined with controlled etching as a versatile approach for engineering Sb_2S_3 absorber layers, and provides insights into the interplay between growth kinetics, film thickness, and photovoltaic performance.

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Environment-Induced Defect Dynamics in Sb_2Se_3 Thin Films for Emerging Chalcogenide Solar Cells

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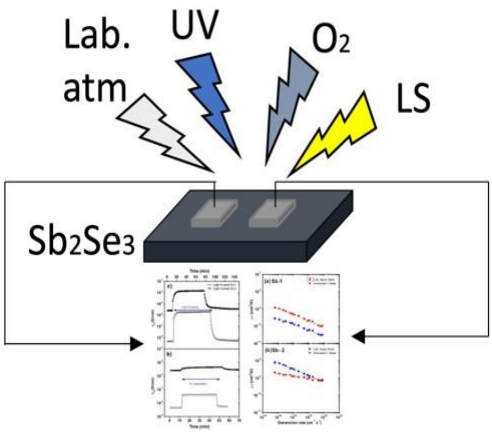

Keywords: Sb_2Se_3; Emerging chalcogenide solar cells; Magnetron sputtering; Defect dynamics; Environmental stability; Light soaking

In the pursuit of sustainable photovoltaic absorber materials, antimony selenide (Sb_2Se_3) has emerged as a promising candidate owing to its high optical absorption coefficient and favorable charge carrier mobility. Nevertheless, the long-term stability and defect-related electronic behavior of Sb_2Se_3 remain insufficiently understood. In this work, Sb_2Se_3 thin films were deposited by magnetron sputtering, followed by post-deposition annealing to induce a structural transition. The influence of different stress conditions on the electronic properties of the films was systematically investigated. The results demonstrate that atmospheric stress conditions significantly increase the dark conductivity (σ). This enhancement was found to be largely reversible upon vacuum treatment. For crystalline Sb_2Se_3 samples, UV aging produced a permanent modification in defect behavior, resulting in a decrease of the mobility–lifetime (μτ) product, whereas amorphous films exhibited predominantly reversible and transient responses. In addition, the μτ product increased during light-soaking experiments, indicating the activation of metastable defect states. Overall, these findings provide important insights into the environmental stress sensitivity and phase-dependent defect evolution of Sb_2Se_3 thin films, offering valuable guidance for improving the long-term stability and performance of Sb_2Se_3-based photovoltaic devices.

Effect of TiO_2 Electron Transport Layer architecture on Spray Pyrolysis Deposited Sb_2S_3 Thin Films for Solar Cells

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Keywords: Antimony sulfide, Thin-film solar cells, Vacuum spray pyrolysis, Semi-transparent PV

Antimony sulfide (Sb_2S_3) thin films were deposited by vacuum spray pyrolysis under a nitrogen atmosphere for solar cells using the Glass/FTO/TiO_2/Sb_2S_3/P3HT/Au superstrate configuration. This work explores the influence of TiO_2 underlayer architecture on the growth and optoelectronic properties of Sb_2S_3 absorber layers. Different TiO_2 substrate configurations were studied, including compact TiO_2 layers and hybrid compact–mesoporous TiO_2 structures, with different thicknesses, prepared under different deposition cycle conditions to optimize electron transport layer properties. X-ray diffraction (XRD) and Raman spectroscopy were used to examine crystallinity and vibrational properties. Optical transmittance measurements were performed to study light absorption behavior and determine optical bandgap energy. Current–voltage (I–V) characterization and external quantum efficiency (EQE) measurements were conducted to assess photovoltaic response. Scanning electron microscopy (SEM) was employed to investigate surface morphology and film microstructure. The results demonstrate that the configuration of the TiO_2 electron transport layer significantly influences Sb_2S_3 thin film growth, crystallinity, and charge transport behavior. Optimizing the TiO_2 underlayer enhances the properties of the absorber layer, which is essential for improving the efficiency of heterojunction solar cell devices.

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Air annealing of the CdS layer to improve Sb_2Se_3 devices efficiency

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Keywords: Sb_2Se_3, CdS

Sb_2Se_3 solar cells have been fabricated in a superstrate configuration with an FTO/TO/CdS/ Sb_2Se_3/Au structure. On commercial coated SnO_2:F/SnO_2 glass (NSG TEC 12D by NSG Pilkington), a 50-80 nm thick CdS layer is deposited by chemical bath, followed by a 400 nm thick Sb_2Se_3 layer deposited by thermal evaporation at a substrate temperature of 300 °C.
Recently, the CdS layer has been annealed in air at various temperatures and duration time to recrystallize and possibly incorporate oxygen; the optimization work has demonstrated that 400 °C for 30 min is the optimal treatment, increasing the efficiency of 1% of absolute value (Table I and Fig. 1).

Table I: average performance parameters of CdS/ Sb_2Se_3 devices, with and without CdS annealing.

	Voc (mV)	Jsc (mA/cm2)	FF (%)	Eff (%)
CdS/Sb2Se3	342 ±1	19.5 ± 0.8	53 ±1	3.6 ± 0.2
CdS 400 °C /Sb2Se3	337 ±1	26 ± 0.8	52 ±1	4.6 ± 0.2

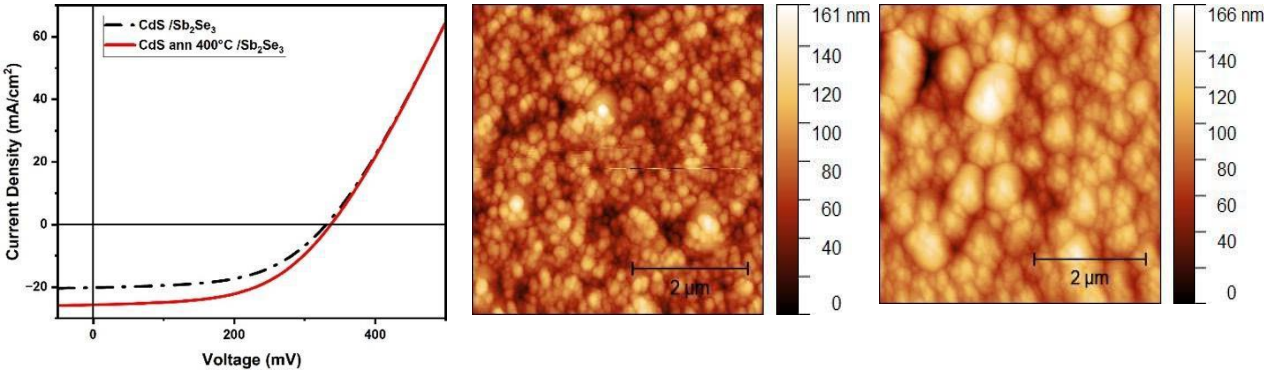

Fig. 1: Current-Voltage characteristic of CdS/ Sb_2Se_3 devices with and without CdS annealing (left) and AFM analysis of the CdS layer before (left) and after (right) annealing in air at 400 °C (right).

The efficiency improvement is given by a clear current gain. On the other hand, transmittance measurements done on the CdS layer before and after air annealing record a slight gain in transmission, which alone does not justify the increase in current. However, atomic force microscopy analysis of the CdS layer before and after annealing reveals an evident recrystallization of the layer, with a considerable enlargement of the grain size (Fig. 1. right).
A detailed analysis of the composition of CdS (bulk and surface) before and after annealing and its influence on the absorber growth and the operation of the devices will be presented.

Sb_2Se_3 as an effective dopant for CdTe solar cells

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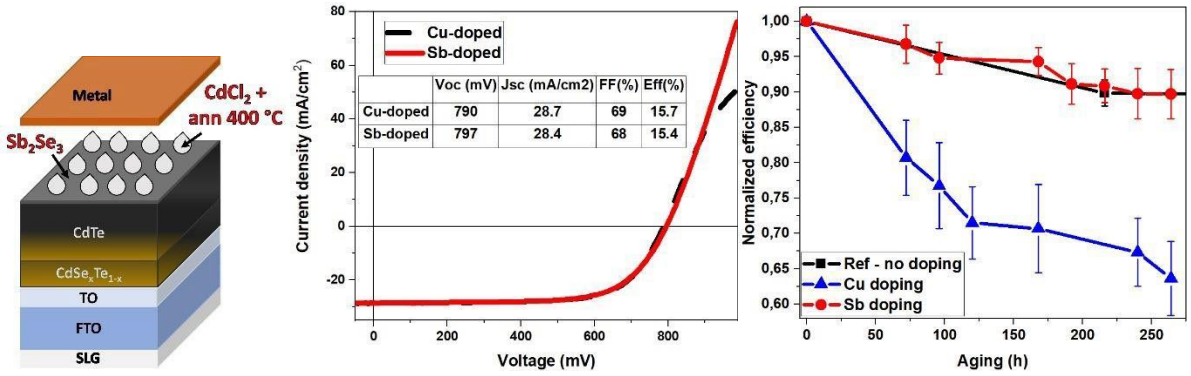
Keywords: CdTe, doping, Sb_2Se_3

Nowadays, the primary efforts in CdTe solar cell research aim to find an alternative to copper doping among the group V elements. In fact, Cu has limited solubility in the CdTe matrix, which prevents achieving higher open-circuit voltages (Voc), and it is also a fast diffuser, considered the main cause of device degradation.
In our lab, we have developed a novel method to dope CdSeTe/CdTe devices by depositing a thin Sb_2Se_3 layer on the top of the absorber. Sb is then driven inside the CdTe matrix by subsequent $CdCl_2$ treatment at 400 °C (Fig. 1 left). The choice of Sb_2Se_3 prevents the introduction of additional impurities and, moreover, reduces the Schottky barrier at the back contact.



	Voc (mV)	Jsc (mA/cm2)	FF(%)	Eff(%)
Cu-doped	790	28.7	69	15.7
Sb-doped	797	28.4	68	15.4

Fig. 1.: left: Schematic of the CdTe Sb-doping process; center: current density-voltage curves of the record Cu- and Sb-doped CdTe devices; right: graph reporting the performance degradation over time of Cu- and Sb-doped samples and the reference no-doped cells.

This method leads to effective CdTe doping, as demonstrated by CV-DLCP measurements, and to peak efficiencies very close to those obtained with Cu doping via the same low-temperature deposition process (Fig. 1 center). Also, with Sb_2Se_3, the back contact ohmicity of doped cells is improved compared to Cu-doped cells, and it does not require etching or a hole-transport layer during fabrication. Accelerated stability tests show remarkable stability for Sb_2Se_3-doped solar cells (Fig. 1 right). Sb-containing devices are so stable that their minimum degradation is equal to that of the undoped cells, suggesting that this is due solely to the lack of encapsulation. Furthermore, this simple post-deposition doping process has strong potential for application to any CdTe device fabricated by any deposition method.
This innovative use of Sb_2Se_3 as a back contact and dopant for CdTe was recently published by our group in the journal Progress in Photovoltaics: https://doi.org/10.1002/pip.70037.

The influence of the deposition working power on some physical properties of RF-sputtered cadmium telluride films for photovoltaic applications

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Keywords: cadmium telluride (CdTe) thin films, RF-magnetron sputtering, XRD, AFM, space-charge-limited conductivity

The photovoltaics industry based on thin films emerged as an alternative to bulk-silicon solar cells, and has the advantage of a relatively lower production cost. In this context, the cadmium telluride (CdTe) attracted important attention due to its advantages, such as a direct bandgap of approximately 1.45 eV at room temperature, high time-stability, and the possibility of growing samples by different physical and chemical techniques. A critical design feature of CdTe photovoltaic devices is the heterojunction formed with cadmium sulfide; the two components have a high match of their crystalline structure and band energy alignment.
This study proposes a comprehensive analysis of some physical properties of CdTe thin films grown by radio-frequency magnetron sputtering at four different working powers (70W, 80W, 90W, and 100 W), on p-type silicon substrates (100), while all the other deposition parameters remain constant. The structural features were discussed by X-ray diffraction characterization, and the morphological aspects were investigated using scanning electron microscopy and atomic force microscopy. The electrical measurements were performed on Ag/CdTe/Al “sandwich” structures, and consist of space-charge-limited conductivity evaluation. The electrical measurements enabled the identification of charge-transport mechanisms throughout the structure. The obtained results showed that a proper optimization of CdTe films may lead to a reduction of their volume, and a step forward can be taken toward the fabrication of ultra-thin photovoltaic structures.

CdTe solar cells for tandem application with Silicon devices

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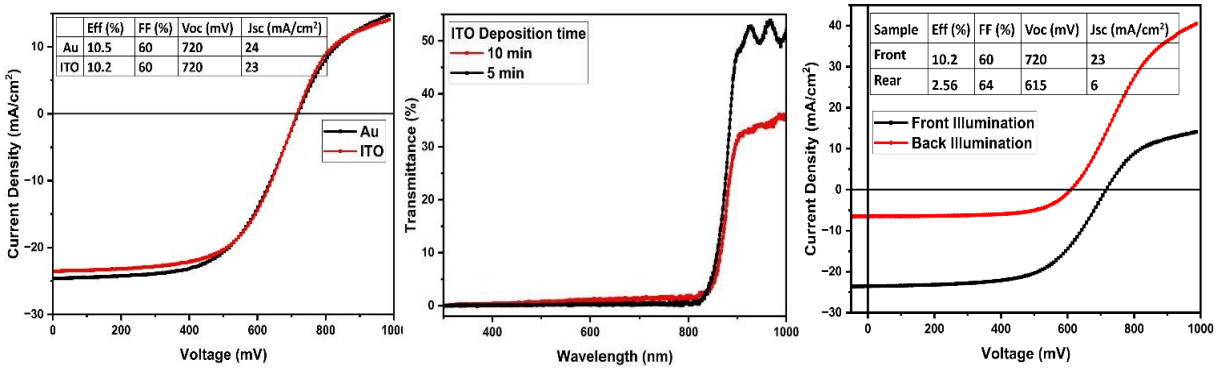
Keywords: Bifacial CdTe, CdTe/Si Tandem

CdTe is not only a simple binary alloy material but especially it has an extremely simple phase diagram that allows to fabricate thin films by a large variety of methods. Now, CdTe is the thin-film technology that sees the larger industrialization, with very good stability and very promising efficiencies (over 23%). To enable tandem CdTe-Si applications, the typical CdTe structure must be redesigned to be bifacial, and an optimization of the band gap value is required to maximize spectral synergy with the silicon bottom cell.
This work focuses on the fabrication and optimization of bifacial CdTe solar cells with RF sputtered Indium Tin Oxide (ITO) as a transparent back contact. We investigated the impact of copper layer thickness, optimized the Indium Tin Oxide (ITO) thickness, and compared the Indium Tin Oxide (ITO) with gold as back-contact materials. The optimized device, utilizing a 1 nm copper having thicker (10 minutes) ITO layer deposition, achieved a front-side efficiency of 10.2%, comparable to the 10.5% efficiency of standard opaque gold-contact devices.



Most importantly, the device showed full bifacial performance with a fill factor of 64% and an efficiency of 2.6% under rear illumination, it confirmed effective carrier extraction regardless of light direction. Thicker ITO layer (10-minute deposition) shows higher fill factors and current collection, resulting in 10.2% efficiency as compared to the 8.7% for the thinner layer (5-minute). The thinner layer of ITO shows better optical transmission (50% at 1000 nm vs. 35%) than the thicker layer. Although electrical losses in thinner layers currently offset these optical benefits, these results demonstrate that ITO can effectively function as a rear electrode to create a bifacial platform suitable for future tandem integration.

Effect of Large Bi-Exciton Binding Energy in Type II CdSe/CdTe QDs on Efficiency of MEG Solar Cells

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Keywords: Solar Cells, Quantum Dots, CdSe/CdTe

In conventional QDs, the multi-excitong generation (MEG) threshold depends mainly on the ratio between electron and hole effective masses. The core/shell QDs with type II band alignment offers extra degree of freedom in mediating the Coulomb interaction between charges. Preliminary experimental studies on CdSe/CdTe QDs have shown that type II QDs can exhibit giant attractive X-X interaction energies, in the order ~0.1 eV. This is a key development since it has been recognized that X-X attraction reduces the threshold for MEG by the amount of bi-excitong binding energy (Bxx). Theoretical predictions indicate that MEG has the potential to enhance the efficiency of the single gap material from 33% (Shockley-Queisser limit) to 42%, and a reduction in MEG threshold, via attractive Bxx, by as little as 0.1 eV could lead to 50% efficiency [1]. To assess faithfully the potential of Bxx on the efficiency, a theoretical methodology was established, based on an atomic symmetry adapted **k.p** Hamiltonian in combination with the full Configuration interaction method (CI), that incudes explicitly the effects steaming from the fermionic nature of carriers. In setting up the CI, particular attention was paid to accurate modeling of the dielectric constant variation through the structure as well as surface polarization effects on core/shell and QD/colloid interfaces, that were predicted using ab initio time-dependent density functional theory [2,3,4]. By changing the CdSe/CdTe QD core size and shell thickness we have concluded that: (i) the Bxx binding can only be predicted with full CI Hamiltonian ie with the effect of correlations oposite to previus studies [5,6]; (ii) CI predicts Bxx binding as big as 70 meV with for structures with 0.5 nm thick shell; (iii) by changing the value of the dielectric constant of colloid material from 1 to 2 the variation in the Bxx binding energy is as big as 100 meV; (iv) for proper estimate of the Bxx inclusion of correlations and surface polarization effects are necessary while effect of self-polarization is negligible. We provide the explanation, for contra intuitive appearance of the bound Bxx with inclusions of shells in terms of stronger reduction in the Columbic repulsion among holes in the Bxx then reduction of the e-h attraction. Based on the Aufbau principle and Hund rule, it is consequence of 4 fold degeneracy of h-ground state imposed by symmetry of the structure.

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Selenium alloying in $BaZrS_3$ perovskite for efficient tuning of properties

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Keywords: Chalcogenide perovskites, solid solutions, selenium, structural characterization.

In the last few years, chalcogenide perovskites, of which $BaZrS_3$ is the most important representative, have established themselves among the most promising emerging chalcogenide materials for photovoltaic applications, thanks to their high absorption coefficients and band gap values, the latter being 1.8 – 1.9 eV for $BaZrS_3$, in the optimal range in particular for tandem applications as top cell. However, strategies to lower the band gap to the ideal value of 1.34 eV, in order to make these materials good candidates for single-junction solar cells, are actively sought. For example, it has been predicted theoretically that alloying of $BaZrS_3$ with other elements may lead to a reduction of its band gap and, in this sense, substitution of Ti for Zr has been tried experimentally, showing effective band gap reduction upon addition of 10% Ti, while phase segregation occurs for higher Ti concentrations[1]. On the other hand, computational works have also suggested that substitution of Se for S should lead to a reduction in band gap value of $BaZrS_3$, nevertheless experimental reports in this sense are, to the best of our knowledge, absent. For this reason, there is plenty of room for investigation aimed at assessing the effectiveness of this approach for band gap reduction along with the structural characteristics of Se-alloyed $BaZrS_3$.
In this work, we therefore describe the synthesis of a series of solid solutions of general formula $BaZrS_{3-x}Se_x$, which were prepared following a strategy similar to a recently developed one for $BaZrS_3$, $BaHfS_3$ and their solid solutions[2], characterized by the use of relatively mild conditions (500 °C for 16 hours), the method for their purification from excess S and Se and the characterization of the prepared materials by means of powder X-ray diffraction, energy dispersive X-ray spectroscopy, diffuse reflectance UV-visible spectroscopy and Raman spectroscopy. Results of these analyses reveal substitution of Se for S with retention of perovskite structure up to a Se concentration of 21.4%, while formation of phases different from the perovskite one takes place at higher Se concentrations. Moreover, a slight reduction in band gap value is observed upon Se incorporation in $BaZrS_3$, as well as a change in the lattice parameters and a modification of Raman spectra with increasing Se content. These effects, although their complete rationalization still has to be performed and will probably require the aid of theoretical calculations, confirm Se-alloying as a practical way to tune the opto-electronic and structural properties of $BaZrS_3$. Moreover, this study extends the scope of the new synthetic method developed by our group.

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First-Principles Determination of Pnictogen Chalcohalide Band Alignments for Improved Solar-Cell Applications

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Keywords: *ab initio* modelling, interfaces,

Pnictogen chalcohalides with the general formula MChX (M = Bi, Sb; Ch = S, Se; X = I, Br) have emerged as promising photovoltaic absorber materials due to their favorable synthesis conditions and strong optoelectronic properties [1]. Despite this potential, experimentally reported power conversion efficiencies remain below 10% [2], well short of the Shockley-Queisser limit of 32%.

Efficient charge separation in photovoltaic and photocatalytic devices critically depends on the proper alignment of electron and hole transport layers [3]. However, the absolute positions of the valence band maximum and conduction band minimum in MChX compounds remain poorly constrained. To address this gap, we perform a systematic first-principles investigation of MChX surface energetics and electronic structure. Our results show that the [010] and [011] surfaces are consistently the most energetically favorable, while surface orientation can induce variations in band-edge positions of up to 0.8 eV.

These findings provide a microscopic explanation for the experimentally observed variability in band alignments across MChX-based devices. More broadly, our work establishes a predictive framework for rational interface engineering, enabling the informed selection of electron and hole transport layers to enhance both photovoltaic efficiency and photocatalytic performance.

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TOPCon-Inspired Dielectric Tunnel Interfaces for Wide-Bandgap Se Solar Cells

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Keywords: Selenium (Se); Ultrathin dielectrics, Band alignment; Interface passivation

Selenium (Se) is a promising absorber material for emerging photovoltaic (PV) technologies due to its wide bandgap (~1.9 eV), high absorption in the visible range, and compatibility with low-temperature processing, which makes it well-suited for indoor PV applications and top cells in tandem architectures.

The performance Se solar cells are strongly influenced by the quasi-one-dimensional (quasi-1D) structure of the absorber chains and the quality of the interfaces with the electron transport layer (ETL) and the hole transport layer (HTL). In standard device architectures, the ETL is typically made of TiO_2, which forms a direct TiO_2/Se heterointerface with a cliff-like conduction band offset (CBO). This cliff-like CBO tends to facilitate interfacial recombination's in the presence of defects, resulting suboptimal efficiency. Recent record-breaking performances have been achieve using alternative ETL based on ZnMgO. These ETL introduce a spike-like CBO at the ETL/Se heterointerfaces, leading to reported efficiency > 10% and open-circuit voltage (V_{oc}) > 1 V. These results highlight the critical role of interface band alignment for high-efficiency Se solar cells.

Inspired by tunnel oxide passivated contact (TOPCon) architectures developed for high-efficiency crystalline silicon (c-Si) solar cells, we propose an alternative interface engineering strategy for TiO_2/Se using dielectric tunnel interfaces. Various ultrathin dielectric interlayers were applied between the TiO_2 and Se to modify the interface and facilitate charge transport via quantum tunneling. Device prototypes, including opaque and semi-transparent single-junction Se solar cells, as well as Se/c-Si tandems, have been fabricated. Initial results show improved performance compared to reference cells without dielectric interlayers.

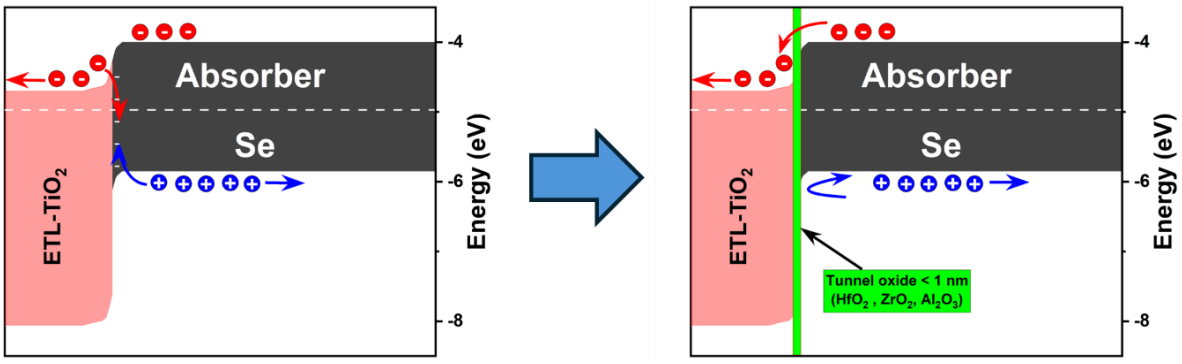

Figure (Left) Conventional TiO_2/Se junction with cliff-like CBO. (Right) Dielectric-passivated tunnel interface with improved band alignment.

Tuning the Structural and Charge Transport Properties of GeS Thin Films

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Keywords: Chalcogenides, Thin-Films, Germanium Sulfide

Layered germanium monosulfide (GeS) has recently emerged as a highly promising, Earth-abundant, and low-toxicity semiconductor for next-generation optoelectronic applications. Despite its attractive direct bandgap and high environmental stability, depositing continuous, highly oriented polycrystalline films on a large scale has remained a significant challenge. This work details the controlled synthesis of large-area polycrystalline GeS thin films using a scalable rapid thermal evaporation (RTE) method and explores how structural engineering - specifically through post-deposition sulfurization and boron doping - affects the material's fundamental properties and charge carrier dynamics.

To achieve controlled crystal growth and preferential layer orientation, a two-step deposition process was developed. This involved the initial deposition of an amorphous film at temperatures below 350°C, followed by thermal annealing to ensure complete crystallization. The structural, morphological, and optical properties of pristine, sulfurized, and boron-doped GeS films were then systematically investigated utilizing X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Raman spectroscopy, and Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES). XRD analysis confirmed that the synthesized films exhibited a pure GeS phase with a dominant (100) orientation, which is a key characteristic signature of its layered structure.

Crucially, morphological and compositional characterizations revealed that the sulfurization process successfully shifted the film composition from a sulfur-poor to a sulfur-rich state. This sulfur-rich environment significantly decreased the concentration of deep-level sulfur vacancies by increasing their formation energy, thereby promoting stronger p-type conductivity. Furthermore, the successful introduction of boron provided additional p-type doping, unlocking further tunability of the material's optoelectronic properties.

To gain deeper insight into the optoelectrical behavior of engineered films, transient photocurrent and time-delayed collection field (TDCF) measurements were employed to study charge carrier dynamics. The polycrystalline GeS exhibited notably long charge carrier lifetimes, which are highly advantageous for photosensitive materials. However, these extended lifetimes were accompanied by a rapid decrease in mobility on a sub-microsecond timescale - a phenomenon attributed to carrier trapping and the presence of potential barriers inherent to the polycrystalline structure.

Ultimately, comprehensive material characterization demonstrates that the structural and electrical properties of GeS thin films can be highly tailored through specialized two-step deposition, sulfurization, and boron doping techniques. While these optimized films proved highly effective when integrated into lateral visible-light photodetector architectures, the fundamental insights gained regarding their defect engineering and charge carrier dynamics highlight the broader, foundational potential of GeS across a wide variety of scalable optoelectronic devices.

Interface Engineering of the TiO_2/SnS Junction for Enhanced Thin-Film Solar Cell Performance

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Keywords: SnS; TiO_2, molecular ink; thin-film solar cells; ETL engineering

Tin monosulfide (SnS) is an attractive absorber material for thin-film photovoltaics due to its earth abundance, low toxicity, chemical stability, and suitable optoelectronic properties, including a band gap of ~1.3 eV and a high absorption coefficient. Despite these advantages, the efficiency of solution-processed SnS solar cells remains limited, largely because of challenges in controlling crystallinity, morphology, and charge-transport pathways. Preferential grain orientation along the
[010] direction is frequently observed and significantly affects carrier transport.

In this work, we investigate how electron transport layer (ETL) interface engineering influences the growth behavior of SnS thin films derived from a molecular-ink $SnCl_2$–thiourea precursor and deposited by spin coating, followed by rapid thermal annealing at 375 °C under nitrogen atmosphere. Three ETL configurations were examined: compact TiO_2, compact TiO_2 combined with mesoporous TiO_2, and compact TiO_2 modified with a CdS interlayer. Structural and morphological analyses (XRD, Raman spectroscopy, SEM, and TEM) show that the ETL-SnS interface plays a crucial role in nucleation, grain growth, crystallization, and surface morphology. Incorporating a mesoporous TiO_2 layer improved SnS crystallinity and interfacial contact, resulting in more efficient charge extraction and reduced recombination losses.

As a result, device performance increased from ~2% with compact TiO_2 alone to ~3% with the combined compact/mesoporous TiO_2 configuration under AM1.5G illumination. These findings emphasize the importance of ETL interface engineering for advancing molecular-ink-processed SnS hybrid photovoltaic devices.

Hyperspectral photoluminescence mapping and analysis on chloride-activated chalcogenide CdSe thin films

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Keywords: chalcogenide solar cells, microscopy, photoluminescence, opto-electronic properties

Defects and not the band structure now set the upper limits for chalcogenide-based solar cells, including CdSe and Se-enriched Cd(Se,Te) layer stacks. Even the photoluminescence (PL) of pristine CdSe films and single crystals remains disputed. There are conflicting assignments of near-band-edge and sub-gap bands and how temperature, carrier injection, and microstructure couple to radiative pathways. Moreover, chloride activation rewrites the defect landscape, it was found as a route to device-grade material quality and hPCE over 20% [1]. Here we show that hyperspectral confocal micro-photoluminescence (PL) imaging represents an essential tool for analyzing and understanding structural and optoelectronic properties of CdSe thin films with $CdCl_2$ activation [2]. CdSe samples were prepared on TEC12D glass by thermal evaporation, treated by $CdCl_2$ and annealed. The comprehensive hyperspectral data were recorded through 100x objective lens (NA/0.9) across the 10 x 10 um^2 areas by using a confocal Raman/PL microscope (WITec alpha300 RAS) coupled with a quasi-tunable white laser source (NTK Photonics) with excitation wavelength set to 520 nm, laser power set to 130 µW. The obtained data cube was analyzed by several methods. The band-edge−filtered PL intensity mapping resolved the polycrystalline CdSe texture. Emission was strongest on grains and suppressed along boundaries, with variations within larger grains. The PL peak position shifts between 713-723 nm were the most pronounced along grain edges, revealing the microstructure-correlated local heterogeneity due to electrostatic potential fluctuations and/or disorder-related band-tail effects at the grain boundaries. The map of PL line width (FWHM), which was narrower in interior of large CdSe grains and broader at the grain edges and in small grains, corroborated the view of inhomogeneous disorder and local field fluctuations in the edge-rich microstructure regions. Further insight was gained by principal component analysis of the hyperspectral PL data using two component spectra. The component with a strong infrared tail (>850 nm, related to defect emission) dominated at the grain boundaries whereas the component with stronger band-edge PL emission dominated grain interiors. The CdSe photoluminescence characteristics can thus provide guidance for future materials research towards higher chalcogenide solar cell efficiencies. This work was supported by COST Action ReNewPV CA21148, supported by COST (European Cooperation in Science and Technology) and the MEYS project CZ.02.01.01/00/22_008/0004617 (EcoStor).

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Tuning the Optoelectronic Properties of Wide-Bandgap Cu_2ZnSnS_4 by Silver Substitution, Sodium and Lithium Co-Doping and Thermal Annealing

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Keywords: Kesterite , Solution-processed, Wide bade gap, indoor photovoltaics, Ag alloying

Cu_2ZnSnS_4 (CZTS) kesterite is a promising absorber material for next-generation photovoltaic (PV) technologies, especially for indoor applications. These quaternary chalcogenides offer tunable optoelectronic properties, an earth-abundant elemental composition, low cost, and high chemical stability. However, the intrinsic bandgap of CZTS (≈1.5 eV) is suboptimal for indoor PV applications, which require a wider bandgap in the range of 1.65-1.9 eV. Alloying strategies based on cation substitution offer a flexible approach for engineering the structural, morphological, and optoelectronic properties. In particular, combining Ag alloying with alkaline metal incorporation enables effective tuning of these properties, offering a promising approach for bandgap widening and absorber optimization.

In this study, Ag-alloyed $(Ag_xCu_{(1-x)})_2ZnSnS_4$ (ACZTS) thin films were fabricated on Mo-coated soda-lime glass (SLG/SiO_2/Mo) substrates using a chemical solution processing route. Molecular precursor solutions were prepared from metal salts and thiourea dissolved in 2-methoxyethanol. The films were deposited by spin coating, followed by drying. After ACZTS film deposition, Na-Li was incorporated by spin-coating an alkali precursor solution onto the absorber, followed by drying. The films were then heat treated under an argon atmosphere with solid sulfur at temperatures ranging from 600 to 660 °C to promote crystallization. A CdS buffer layer was then deposited by chemical bath deposition as an electron transport layer (ETL). Transparent conductive oxide (TCO) layers of ZnO/ITO were deposited by sputtering, followed by rapid thermal annealing (RTA). Finally, Ag-based front contact grids were deposited by electron-beam evaporation to complete the device structure.

The impact of Ag alloying and Na-Li incorporations, as well as the effect of varying heat-treatment temperatures, on the structural, morphological, and optoelectronic properties. Structural, morphological, and chemical analyses (XRD, Raman, and SEM/EDS) together with optical measurements (UV-Vis diffuse reflectance spectroscopy) and current-voltage characteristics revealed enhanced grain growth, improved cation stoichiometry, a widened bandgap (>1.5 eV), confirmed Ag incorporation, and kesterite crystal structure. The heat treatment temperature was found to strongly influence crystallinity, as well as grain morphology. Na-Li incorporation significantly improved the solar cells efficiency.

These results highlight ACZTS as a promising wide-bandgap absorber for indoor photovoltaic applications. Ag alloying and Na-Li codoping provide complementary ways to adjust the bandgap and crystal structure and enhance absorber quality and device performance.

How the molybdenum process influences the growth of CZTS:

A comparative study of different lab-grown and commercial molybdenum substrates

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Keywords: CZTSSe, molybdenum, sputtering, pressure

In the pursuit of high-efficiency CZTSSe solar cells, the choice of substrate is widely recognized as a key factor, as it strongly influences the photoconversion efficiency.
In this work, we present a systematic comparative study focused on evaluating the differences between laboratory-sputtered molybdenum and commercially available Mo/glass substrates. We investigate how the efficiency of CZTSSe solar cells is affected when fabricated on sputtered molybdenum deposited at two different temperatures (200 °C and 400 °C, hereby after Mo200 and Mo400, respectively), and on commercial molybdenum/glass substrates (Mo-C). The distinct microstructure and morphology of the substrates lead to higher sheet resistance in the sputtered samples (Mo-C < Mo200 < Mo400), resulting in reduced device efficiency. Additionally, different inert gas pressures (400, 550 and 700 mbar) were applied during the selenization step, so to find the optimal CZTSSe recrystallization conditions on all the substrates and prevent the peeling-off of the absorber. The choice of the substrate is also found to affect the cation reorganization during the selenization step, as shown in the XPS data (**Figure 1**), with particular regards on the mobility of tin and zinc.
The best result was obtained with 700 mbar, with the devices grown on Mo-C showing superior photovoltaic performance (best cell efficiency: 10.20%) compared to sputtered counterparts (Mo200 best 8.43%, Mo400 best 6.99%) (**Figure 2**).

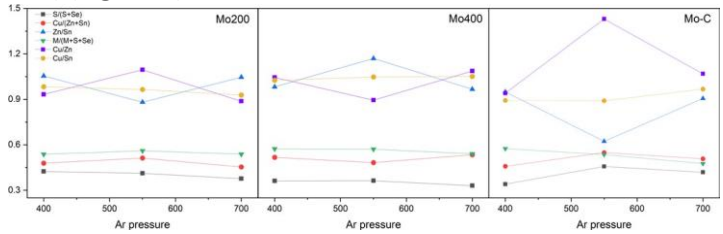

Figure 1. Element ratios from XPS analysis of all samples

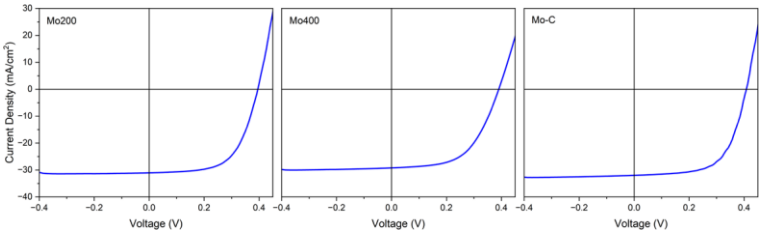

Figure 2. J-V curve of CZTSSe solar cells selenized at 700 mbar

NiO_x nanoparticles as HTM in semi-transparent Sb_2S_3 solar cells

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Keywords: Hole transport layer, Sb_2S_3 solar cells, NiO_x nanoparticles, NiO_x thin film, Inorganic solar cells

Sb_2S_3 is attractive for semi-transparent photovoltaics due to its ~1.7 eV bandgap, high absorption coefficient, and chemical stability. Sb_2S_3 solar cells employ organic HTMs such as P3HT and Spiro-OMeTAD; the highest reported efficiencies for devices using these HTMs are ~7-8%. However, commercialization is hindered by hygroscopicity, high cost, complex processing, and limited operational stability. Therefore, inorganic p-type HTMs- particularly NiO_x, which offers a wide bandgap, high optical transmittance, excellent chemical stability, and tunable energy levels- are increasingly pursued to enable more stable Sb_2S_3 devices. In this study, the semi-transparent Sb_2S_3 solar cells employing NiO_x nanoparticles as the hole-transport material (HTM) were fabricated by optimizing nanoparticle preparation and device fabrication parameters. NiO_x powders were synthesized by chemical precipitation and annealed at controlled temperatures in the range of 270-700°C; XRD, FTIR, XPS, and UV–Vis analyses showed that annealing at higher temperature above 500°C improves crystallinity and reduces organic/precursor residues, identifying 500°C as the optimal compromise between annealing temperature and structural/optical quality. Devices with a stacked thin-film architecture (glass/FTO/TiO_2/Sb_2S_3/NiO_x/Au) were created, revealing that the choice of dispersant and the hole-transport layer (HTL) thickness govern film uniformity and, in turn, device performance. Compared with devices without NiO_x, the inclusion of the HTM increased performance metrics: V_{OC} goes from 0.42 to 0.47 V, J_{SC} from 10.87 to 11.48 mA/cm², FF from 42.0% to 45.12%, and PCE from 1.7% to 2.16%. Annealing of glass/FTO/TiO_2/Sb_2S_3/NiO_x stack after deposition of the NiO_x HTM at temperatures of 160-180°C and 225°C for 15 minutes in air was also examined, indicating the most favourable post-deposition conditions of the solar cell stack were found to be 180°C for 15 min as the PCE increases to 2.8%. Finally, studies on NiO_x ink filtration indicated a slower degradation for unfiltered inks, plausibly due to a higher surface packing density that limits moisture ingress, while increasing the overall performance and achieving a PCE of 3%, without compromising device semi-transparency. Overall, the results elucidate process-structure-property relationships that enable a balance between efficiency and transparency, positioning NiO_x as a viable HTM for stable, architecturally integrable Sb_2S_3-based photovoltaics to obtain fully inorganic solar cells.

Synthesis and Processing of Colloidal Nanocrystals for Sustainable Thin-Film Photovoltaic Devices

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Keywords: nanocrystals, ternary chalcogenides, thin-film devices

Identifying novel chalcogenide materials is essential for advancing the sustainability of photovoltaic (PV) technologies and developing next-generation renewable energy concepts. Colloidal inorganic semiconductor nanocrystals (NCs) offer a versatile platform to explore alternative absorber materials for PV applications. These materials are solution-processable and provide exceptional tunability: their band can be controlled via quantum confinement, and the energy level alignment can be modulated through surface ligand selection. Although Pb- and Cd-based materials such as PbS and CdTe have been extensively studied, the transition toward less toxic and more sustainable alternatives remains a crucial challenge.

Herein, we present two promising ternary chalcogenide materials characterized by comparably low toxicity and composed of relatively earth-abundant elements. First, we investigate the tunability and optimization of $CuInS_2$ NCs during wet-chemical synthesis as well as through post-synthetic processing, to enable their integration into thin-film PV devices. We identify key limitations of synthetic pathways associated with the necessary replacement of long-chain organic ligands with shorter and/or more conductive alternatives and introduce strategies to mitigate these challenges.

Further, we present initial results on the incorporation of emerging ternary chalcogenides such as $BaZrS_3$ NCs into thin-film device architectures, highlighting the potential of these alternative absorbing materials.

Addressing material development as well as practical strategies for advancing solution-processable chalcogenide nanomaterials toward thin-film device structures in the presented work underlines the potential of these novel absorber materials for next-generation PV concepts.

Impact of hole transport layers on the performance of Sb_2S_3 solar cells

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Keywords: inorganic solar cell, ETL contribution, PCE

The performance of antimony trisulfide (Sb_2S_3) solar cells is strongly influenced by the properties of the electron transport layer (ETL), which governs electron extraction and interfacial recombination. In this work, we investigate the effect of TiO_2-based ETL thickness on the photovoltaic performance of Sb_2S_3 solar cells. The Sb_2S_3 absorber layer was prepared by chemical bath deposition using $SbCl_3$ and $SC(NH_2)_2$ precursors in N,N-dimethylformamide (DMF). Using an FTO/TiO_2/Sb_2S_3/P3HT device architecture, solar cells with optimized thin compact and mesoporous TiO_2 layers achieved a power conversion efficiency of approximately 5%. Structural, morphological, and optical properties were analyzed by X-ray diffraction, scanning electron microscopy, and Raman spectroscopy, while photovoltaic performance was evaluated from current–voltage characteristics. These results demonstrate that TiO_2 ETL optimization significantly enhances charge collection and suppresses recombination losses, highlighting the crucial role of ETL engineering in efficient Sb_2S_3-based photovoltaic devices.

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Influence of Post-deposition Annealing Temperature and Time on Sb_2S_3 films and Solar Cells grown by Ultrasonic Spray Pyrolysis

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Keywords: Sb_2S_3 Solar cell, annealing temperature, annealing time, ultrasonic spray pyrolysis

Antimony sulfide (Sb_2S_3) emerges as a promising absorber layer material in photovoltaic technologies owing to its direct bandgap of 1.7 eV, absorbtion coefficint of 10^4 - 10^5 cm^{-1} in visible light and its capacity for growth at low temperatures, around 300°C. While various deposition techniques exist, including Chemical Bath Deposition (CBD), this study employs Ultrasonic Spray Pyrolysis (USP) due to its superior speed and scalability. Films produced by these methods typically exhibit amorphous characteristics and low crystalline quality, necessitating post-deposition annealing. This research investigates the effects of annealing time and temperature on the structural and electrical properties of Sb_2S_3 films, as well as their performance in solar cells.
In this work, thin films of Sb_2S_3 were synthesized using USP and subsequently annealed at temperatures ranging from 270 °C to 420 °C to identify the optimal annealing temperature. Structural characterization through X-ray diffraction (XRD) and Raman spectroscopy confirmed the presence of orthorhombic crystalline peaks for Sb_2S_3, albeit without significant trends in crystallinity. Electrical study revealed that this temperature also yielded the highest short-circuit current density (J_{SC}) and power conversion efficiency (*PCE*) of 14.5 mA/cm² and 5.71%, respectively. Subsequent trials examined the influence of varying annealing times (6, 12, and 18 minutes) on film characteristics. Consistent with earlier results, XRD and Raman analyses reiterated the presence of standard Sb_2S_3 peaks. However, a reduction in absorber thickness was observed, decreasing from approximately 93 nm to 74 nm as the annealing time extended from 12 to 18 minutes. Electrical assessments indicated optimal performance at 12 minutes, correlating with a *PCE* of 6.12%, J_{SC} of 14.8 mA/cm², and a fill factor (*FF*) of 60%. Importantly, a significant increase in open-circuit voltage (V_{OC}) was noted, rising from 710 mV to 734 mV as the annealing time increased from 6 to 18 minutes.
The overall enhancement in V_{OC} with extended annealing time suggests improvements in the TiO_2/Sb_2S_3 junction quality. Conversely, the observed decline in J_{SC} may be attributed to sublimation of the absorber layer. The reductions in both absorber thickness and grain size leads to diminished device performance under prolonged annealing conditions which additionaly shows a treadeoff between J_{SC} and V_{OC}. Our findings show a pathway for optimizing Sb_2S_3 solar cell parameters through post-deposition annealing treatments, contributing to the advancement of solution-processed photovoltaics.

FIB-SEM tomography of structural, chemical and electronic properties of Sb_2Se_3 solar cell layer stacks

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Keywords: Sb_2Se_3 solar cells, opto-electronic properties, plasma FIB, SEM-EDS, Thin Films

Sb_2Se_3 is an earth-abundant, low-toxicity semiconductor with an optimal 1–1.2 eV band gap and high absorption coefficient, enabling efficient light harvesting in sub-micrometer films [1]. Its quasi one dimensional structure promotes anisotropic charge transport and reduces grain boundary recombination, making it highly promising for photovoltaics. Carrier transport in n-i-p Sb_2Se_3 solar cells shows pronounced thickness dependence, where absorber thickness of ~550 nm was shown optimal for photocarrier extraction. The absorber thickness is thus directly linked to overall device efficiency [2]. Our recent work has shown that ultrathin (~400 nm) Sb_2Se_3 absorbers can indeed outperform thicker layers, especially with post-annealing in air, which further enhanced efficiency by increasing carrier concentration, suppressing deep defects, and improving both Voc and fill factor [3]. It was attributed mainly to oxygen-assisted defect passivation.

Here, we present a preparation method and analysis of structural, chemical and electronic properties across solar cell interfaces by employing highly efficient and smooth plasma FIB etching combined with correlative UHR FE-SEM system (Tescan Amber X). We applied simultaneous high resolution secondary electron and EDS analysis at the layer stack cross-section, further corroborated by fast plasma FIB-SEM tomography for 3D reconstruction. We demonstrate how this methodology can provide prompt and more detailed investigation of the ETL/buffer/absorber interface in the thin film Sb_2Se_3 solar cells as function of the absorber thickness and post-annealing treatment. By correlation with the recently reported effects on solar cell performance [3], it enables us deeper insight into the structural, chemical and electronic mechanisms that govern carrier extraction for the design of Sb_2Se_3 solar cell with improved efficiency. This work was supported by COST Action ReNewPV CA21148, supported by COST (European Cooperation in Science and Technology) and the MEYS project CZ.02.01.01/00/22_008/0004617 (EcoStor).

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Morphological and structural analysis of $Sb_2(S,Se)_3$ thin films based solar cells

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Keywords: antimony sulfide, antimony selenide, solar cells, transmission electron microscopy

Chalcogenide-based thin-film solar cells, particularly those utilizing antimony sulfide (Sb_2S_3) and antimony selenide (Sb_2Se_3), have garnered significant attention due to their tunable bandgaps, high absorption coefficients, and potential for low-cost, scalable manufacturing.

The optoelectronic performance of multilayer solar cells is fundamentally dictated by the structural quality of the individual thin films and the integrity of their interfaces. For $Sb_2(S,Se)_3$devices specifically, growing columnar grains with a preferred crystallographic orientation is critical for enabling efficient charge carrier transport. Consequently, Transmission Electron Microscopy (TEM) serves as an indispensable characterization technique, providing unparalleled insights into the nanoscale morphology, crystal structure, and interfacial quality of these devices.

The $Sb_2(S,Se)_3$ thin films were synthesized via close-space sublimation (CSS) on FTO-coated glass. Complete solar cell devices were fabricated with a standard architecture of FTO/TiO_2/$Sb_2(S,Se)_3$. To preserve the structural integrity of the interfaces, cross-sectional lamellae were prepared using a Focused Ion Beam (FIB) scanning electron microscope. The nanoscale characterization was performed using a spherical aberration-corrected JEOL ARM 200F operating at 200kV. Structural analysis was conducted via High-Resolution TEM (HRTEM) assisted by Fourier Transform analysis techniques and Selected Area Electron Diffraction (SAED). Chemical compositions were mapped using High-Angle Annular Dark-Field Scanning TEM (HAADF-STEM) coupled with Energy-Dispersive X-ray Spectroscopy (EDS).

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Development of Antimony Sulfide Selenization to From Antimony Sulfide-Selenide Using Selenourea as a Selenium-Source

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Keywords: Antimony Sulfide-Selenide, Antimony-Chalcogenide, Ultrasonic Spray Pyrolysis, Thin Films

Antimony sulfide-selenide ($Sb_2(S,Se)_3$) is a promising absorber material in next-generation photovoltaic devices due to its tunable band gap of 1.1-1.7 eV, high absorption coefficient > 10^5 cm^{-1} and possibility to integrate in semi-transparent device architectures. The highest solar cell efficiencies > 11% have been reported for $Sb_2(S,Se)_3$ material [1].
This study focused on developing a wet-chemical selenization process for antimony sulfide (Sb_2S_3) to obtain an $Sb_2(S,Se)_3$ absorber layer through the partial exchange of sulfur with selenium.
The research included several stages. In the first stage, selenourea and triphenylphosphine selenide (Ph_3P=Se) were tested and compared as selenium sources using Sb_2S_3 powder. The results demonstrated that both compounds are suitable selenium sources, as XRD and UV-Vis analyses confirmed the formation of $Sb_2(S_x,Se_{1-x})_3$ with a band gap of approximately 1.2-1.3 eV after a 22 h reaction. However, Ph_3P=Se requires higher processing temperatures. Based on these experiments, selenourea was identified as the most suitable selenium source. In the second stage, selenourea was applied to Sb_2S_3 thin films deposited by ultrasonic spray pyrolysis in order to determine the optimal processing parameters for thin film samples. The results showed that increasing the Se-bath process time from 1 h to 22 h decreased the band gap of the formed material from 1.7 eV to 1.3 eV, whereas the Eg of Sb_2S_3 was 1.7 eV and the Eg of Sb_2Se_3 was 1.3 eV. XRD and Raman studies confirmed the formation of the mixture of Sb_2S_3 and Sb_2Se_3 phases after processing time of 4 h, and the Sb_2Se_3 formation after processing times longer than 6 h. Finally, after optimizing the selenization conditions for thin films, a solar cell device (glass/FTO/TiO_2/$Sb_2(S_x,Se_{1-x})_3$/P3HT/Au) was fabricated and its performance was evaluated. The results of this study demonstrate the possibility of employing a sulfur-selenium exchange process via wet-chemical post-deposition treatment for the fabrication of $Sb_2(S_x,Se_{1-x})_3$ absorber layer.

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Effect of the Annealing Atmosphere on the Properties of the $Cu_2ZnSn(S,Se)_4$ (CZTSSe) Thin Films and Their Photovoltaic Performance

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Keywords: CZTSSe, Annealing atmosphere, Sputtering, Rapid Thermal Processing (RTP)

The $Cu_2ZnSn(S,Se)_4$ (CZTSSe) thin films have attracted significant attention as promising absorber materials for thin-film solar cells. Their direct and tunable band gap (1.0-1.5 eV), high absorption coefficient (>10^4 cm^{-1}), and composition based on earth-abundant and environmentally friendly elements make them an attractive alternative to conventional materials such as CIGS and CdTe [1,2]. However, the structural and optoelectronic properties of CZTSSe are highly sensitive to processing conditions, particularly the annealing step, which plays a crucial role in determining film quality and device performance.

In this study, CZTSSe thin films with a thickness of approximately 1 µm were deposited by magnetron sputtering and subsequently annealed at 525 °C using Rapid Thermal Processing (RTP). The annealing was carried out under four different environments: without chalcogen, sulfur, selenium, and sulfur + selenium atmospheres. The effects of the annealing environment on the structural, compositional, optical, electrical, and photovoltaic properties of the films were systematically examined. Energy-dispersive X-ray spectroscopy (EDX) results showed that the S/(S+Se) atomic ratio strongly depends on the annealing atmosphere, varying between 0.12 and 0.84. X-ray diffraction (XRD) analysis revealed a shift in the main diffraction peak from 27.42° to 28.32° (2θ), indicating compositional and structural changes. In agreement with these findings, Raman spectroscopy measurements showed that the dominant vibrational band shifted from 330 cm^{-1} to 191 cm^{-1} depending on the annealing conditions. The optical band gap was found to be tunable between 1.04 and 1.32 eV. Electrical measurements further demonstrated a significant variation in carrier concentration, ranging from 10^{18} to 10^{20} cm^{-3}. Finally, SCAPS-1D simulations were performed using the experimentally obtained parameters to evaluate the photovoltaic potential of the absorber layers, and the most promising configuration was identified.

Overall, the results clearly show that the annealing environment is a key factor in tailoring the material properties and optimizing CZTSSe thin films for photovoltaic applications.

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Influence of Annealing Temperature on the Properties of Cu_2ZnSnS_4 Thin Films Obtained via Ligand Exchange

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Keywords: Nanocrystals, Cu_2ZnSnS_4 (CZTS), Ligand exchange, Kesterite structure, Thin films, Annealing temperature, Optical properties, Electrical resistivity

Cu_2ZnSnS_4 (CZTS) is a semiconductor material with an optimal direct band gap, low specific resistivity, and a high absorption coefficient. Therefore, it is considered a promising candidate for low-cost photovoltaic applications with minimal environmental impact. The synthesis of Cu_2ZnSnS_4 nanocrystals was carried out using butylamine at room temperature, resulting in a stable ink. The nanocrystals were separated from the solution by decantation, with isopropanol used as the solvent.

In this study, the properties of Cu_2ZnSnS_4 thin films obtained via ligand exchange are investigated. Thin films of Cu_2ZnSnS_4 (CZTS) were prepared by the drop-casting method on soda-lime glass substrates. The resulting films exhibited a kesterite crystal structure, with an average grain size of 2 nm after annealing at 200 °C. The grain size increased to 10 nm when the films were annealed at 400 °C.

Band gap values of 1.48 eV for films annealed at 200 °C and 1.34 eV for films annealed at 400 °C were determined from UV–Vis spectra. The electrical resistivity of the films annealed at 200 °C was 5000 Ω·cm, while that of the films annealed at 400 °C was 2.5 Ω·cm.

Tunable Ag Incorporation in Electrodeposited Kesterite CZTS Thin Films for Photovoltaic Applications

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Keywords: Kesterite thin films; $(Cu,Ag)_2ZnSnS_4$; Electrodeposition; Thin-film solar cells

$(Cu,Ag)_2ZnSnS_4$ thin films were prepared through a cost-effective aqueous electrodeposition route followed by high-temperature sulfurization, aiming to obtain earth-abundant absorber materials for thin-film photovoltaics. The films were deposited in a three-electrode configuration, where the Cu/Ag ratio was systematically adjusted to control the degree of Ag incorporation in the kesterite lattice. Target compositions corresponding to 0, 25, 50, and 100% Ag substitution were investigated, covering the compositional range from Cu_2ZnSnS_4 (CZTS) to Ag_2ZnSns_4 (AZTS). All depositions were performed potentiostatically at −1.15 V vs Ag/AgCl on FTO-coated glass substrates. Subsequent sulfurization was performed at 550 °C in a tubular furnace under a sulfur-rich atmosphere, with samples enclosed in a graphite box to promote crystallization and grain growth. The influence of Ag incorporation on phase formation, composition, morphology, and optical properties was investigated using X-ray diffraction, Raman spectroscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and UV–Vis spectroscopy. Structural analyses confirmed the formation of kesterite-type phases, with systematic shifts in diffraction and Raman peaks indicating progressive substitution of Cu by Ag. Morphological observations revealed improved grain development and film densification after sulfurization, while compositional analysis revealed a progressive increase in Ag content accompanied by a corresponding decrease in Cu concentration, reaching complete substitution at the highest Ag level. UV–Vis measurements showed strong absorption in the visible range, and the optical band gap increased with increasing Ag content, reaching the highest value for the fully substituted AZTS film. These results demonstrate the viability of controlled Ag alloying in electrodeposited CZTS absorbers and highlight the combined role of compositional tuning and process optimization in tailoring structural and optical properties for photovoltaic applications.

Optimization of Growth Parameters in Sol–Gel-Derived Bi_2S_3 Thin Films

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Keywords: Chalcogenides, Bismuth Sulfide, Spin Coating, Thin Film

Bismuth-based chalcogenides have emerged attention as promising solution-processable semiconductors for next-generation optoelectronic applications due to their non-toxic, low-cost, air-stable, and environmentally friendly constituents. Among them, bismuth sulfide (Bi_2S_3) is a metal chalcogenide semiconductor with significant potential owing to its favorable optical and electronic properties. Despite this potential, only a limited number of studies have reported the fabrication of *n-type* Bi_2S_3 thin films using low-cost sol–gel techniques, in contrast to more expensive deposition methods.

In this work, Bi_2S_3 thin films were successfully deposited using a sol–gel spin-coating method, which enables the fabrication of large-area and uniform thin films in a cost-effective manner. Key growth parameters, including bath temperature, precursor concentration, film thickness, and post-deposition annealing temperature, were systematically optimized to obtain well-adherent and high-quality Bi_2S_3 thin films. The influence of film thickness and annealing temperature on the structural, morphological, optical, and electrical properties was thoroughly investigated.

Structural analysis confirmed that the prepared Bi_2S_3 thin films possess a polycrystalline orthorhombic phase. Optical studies revealed a direct band gap in the range of 1.56–1.58 eV, with a high absorption coefficient on the order of 10^5 cm^{-1}. These results demonstrate that sol–gel-processed Bi_2S_3 thin films are promising candidates for optoelectronic devices, including solar cells.

The importance of XPS in the analysis of the dopants in solar cells

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Keywords: absorber layers, doping, XPS, bonds

The solar cells field is already competitive and the next generation devices are dependent upon the successful doping of the absorber layer with both anions and cations. While the effects of the doping process can be clear in photovoltaic characteristics and electrical measurements, as well as bulk techniques (eg. XRD, SEM+EDX, Raman Spectroscopy, Ellipsometry), the doping process can be improved by using XPS in the development of the doping recipe.
One already knows the performance of the solar cells is determined by the stability of the surface of the absorber. Being sensitive to both surface chemistry and elemental identification, it can identify the unwanted contaminants with precision up to 0.1%. The contamination level gives information on the film stability. By using Ar^+ sputtering for depth profiling, XPS can determine if the doping and the main absorber are homogeneous. A rough stoichiometry can also be extracted from XPS measurements.

Advanced Characterization Techniques for Next-Generation Photovoltaic Technologies

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Keywords: Photovoltaic technologies; Renewable energy; Advanced characterization techniques; Solar cell efficiency; Thin-film solar cells

The rapid development of photovoltaic (PV) technologies is central to the global transition toward sustainable and renewable energy systems. Continuous improvements in device efficiency, stability, and scalability rely heavily on advanced characterization techniques that provide detailed insights into the structural, optical, electrical, and chemical properties of PV materials and devices. This work presents a comprehensive overview of state-of-the-art characterization methodologies applied to emerging and established photovoltaic technologies, including crystalline silicon, thin-film, and perovskite-based solar cells. Advanced techniques such as time-resolved photoluminescence, impedance spectroscopy, synchrotron-based analysis, scanning probe microscopy, and operando measurements are highlighted for their ability to probe charge carrier dynamics, defect states, interfacial phenomena, and degradation mechanisms at multiple length and time scales. The integration of these advanced characterization approaches enables a deeper understanding of performance-limiting processes and long-term reliability issues in photovoltaic devices. The results demonstrate how correlating multi-technique data can guide material optimization, device engineering, and predictive modeling, ultimately contributing to the development of high-efficiency, durable, and commercially viable photovoltaic systems.

Development of chalcogenide semiconductors for photovoltaic applications

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Keywords: chalcogenide, SnS, hole transport

Tin sulfide (SnS) thin films have emerged as promising absorber materials for next-generation chalcogenide semiconductor photovoltaics due to their earth-abundant constituents, non-toxicity, suitable direct band gap (1.3–1.5 eV), and high optical absorption coefficient (>10^4 cm^{-1}). In this work, we report the synthesis, structural optimization, and optoelectronic characterization of SnS thin films aimed at advancing their application in low-cost and sustainable solar cell technologies. SnS films were deposited using scalable physical vapor-based techniques, followed by post-deposition thermal annealing to control phase purity.

Optical measurements demonstrated strong absorption across the visible spectrum with tunable band gaps depending on the annealing conditions. Hall effect and conductivity analyses indicated p-type behavior with improved carrier mobility after sulfurization treatments. Prototype heterojunction devices incorporating optimized SnS absorber layers exhibited enhanced open-circuit voltage and short-circuit current density compared to untreated films.

In the measurements of SnS samples on glass substrates with ITO, a work function value of 4.7 eV was obtained. The data from the surface measurements with Kelvin Probe show an inhomogeneity in the readings in the range of less than 1%.

We decided to use MoO_3 as a hole transport layer in a photovoltaic structure as it is widely used for this purpose in perovskite solar cells. Measurements performed on thin-film structures ITO/SnS/MoO_3/Ag allow us to determine the height of the energy barriers at the oxide-semiconductor contact between the layers in the structure and the location of the Fermi level of the studied SnS material. The measurements show diode curves with a rectification factor of over 100 and a breakdown voltage of about 1.9 V.

The results highlight the critical role of compositional control, defect engineering, and interface optimization in improving the performance of SnS-based chalcogenide semiconductors. This study contributes to the development of cost-effective photovoltaic materials and provides insight into pathways for increasing power conversion efficiency in tin sulfide solar cells.

Temporal Anomaly Evaluation and Feature Selection for Real-Time Health Monitoring of Solar Inverter Interfaces in Chalcogenide-Based PV Systems

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Keywords: Anomaly detection, early fault prediction, photovoltaic, temporal, time series

Background: As emerging inorganic chalcogenide thin-film PV technologies move from lab-scale cells to field-deployed modules, the stability of the heterojunction interfaces (HTL/Absorber/ETL) under thermal and electrical stress becomes a critical factor for long-term deployment. While material science focuses on the chemistry of these interfaces, operational reliability depends on the early detection of "soft" thermal anomalies that signal interface degradation or contact resistance increases.

Methodology: In this work, we propose a high-sensitivity diagnostic framework using a PCA-based feature selection and the Proximity-Aware Time Series Anomaly Evaluation (PATE) metric. Unlike conventional threshold-based systems, our approach comparatively analyzes three distinct feature sets: heatsink-supported, temperature-supported, and DC-feature-supported. We utilized real-field data collected at minute-level resolution to model the relationship between electrical variables and thermal behavior, specifically examining the Pearson correlation between DC variables and heat dissipation—a proxy for interface and contact health.

Key Results: Our analysis of six months of field data shows that single-sensor approaches are insufficient for detecting slowly developing thermal shifts. By integrating DC-based electrical variables, we achieved strong correlations (up to 0.94) and a PATE sensitivity score of 0.78. Crucially, the model identified a "pre-alarm" anomaly region occurring 30 to 60 minutes prior to critical failure.

Conclusion: This data-driven modeling approach provides a robust tool for WG2 and WG4 researchers to evaluate the "real-world" durability of emerging chalcogenide solar cells. By identifying temporal sensitivities in the electrical-to-thermal interface of the system, we can better predict the impact of interface chemistry on long-term device performance and greenhouse gas emission reduction goals.

The comprehensive findings of this research have been synthesized into a full-length manuscript, which is currently finalized and prepared for submission to IEEE Access (a Q1-ranked journal), reflecting the high technical standards and novelty of the methodology.

DFT study of diazonium-derived grafting on SnS surfaces

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Keywords: SnS, diazonium chemistry, covalent bonding, density functional theory (DFT), chalcogenide solar cells, surface states, band gap

The chemical bonding between organic grafting layers and chalcogenide surfaces is a key factor controlling interface stability and electronic properties in SnS-based solar cells. In this work, density functional theory (DFT) calculations are used to investigate the nature of the bond formed between diazonium-derived phenyl groups and SnS surfaces [1].

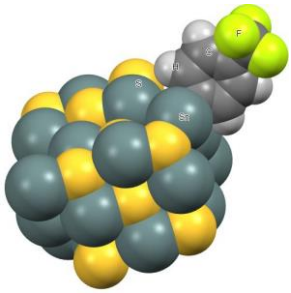

Figure 1. SnS cluster model used to represent the SnS surface in the DFT calculations, showing the atomic arrangement of Sn and S atoms and the grafting site for diazonium-derived trifluoromethyl-substituted phenyl groups.

A SnS cluster model (Figure 1) is employed to represent the surface, allowing a detailed analysis of local bonding and charge transfer. Phenyl groups with electron-withdrawing (−I) and electron-donating (+I) substituents are grafted onto the SnS cluster, and their bonding configurations and electronic effects are compared. The results show that covalent Sn–C bonds are formed, leading to stable surface functionalization and effective passivation of under-coordinated surface atoms. The inductive character of the grafted phenyl groups is found to influence charge redistribution at the interface and the position of surface-related electronic states. The results provide a simple atomistic understanding of how diazonium-based grafting modifies SnS surfaces and offer guidelines for tuning interfaces in chalcogenide solar cells through molecular design.

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Biomass-Derived Activated Carbons as Sustainable Interfacial Materials for Energy Storage and Emerging Chalcogenide Photovoltaic Systems

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Keywords: Biomass-derived activated carbon, Interfacial engineering, Chalcogenide solar cells, Supercapacitors, Sustainable energy storage systems

Interface engineering plays a decisive role not only in emerging chalcogenide-based solar cells but also in the development of integrated renewable energy systems combining photovoltaic (PV) conversion with efficient energy storage. In this context, sustainable, low-toxicity, and high-surface-area carbon materials offer promising opportunities as multifunctional interfacial and charge-transport components.

This study presents a literature-based analysis of biomass-derived activated carbons (ACs) as sustainable materials for energy storage devices—particularly supercapacitors—and discusses their potential relevance to interfacial engineering in emerging chalcogenide PV technologies. Activated carbons synthesized from agricultural residues (e.g., tea waste, olive seed, peanut shell) exhibit high specific surface area (>1500 $m^2\ g^{-1}$), hierarchical porosity, tunable surface functionalities, and excellent electrical conductivity after controlled activation. These features enable efficient charge storage through electric double-layer capacitance (EDLC) and pseudocapacitive contributions, achieving specific capacitances exceeding 250–350 $F\ g^{-1}$ in aqueous and organic electrolytes.

Recent studies highlight that carbon-based interlayers and selective contacts can improve charge extraction, suppress interfacial recombination, and enhance energy-level alignment in chalcogenide solar cells such as Cu2ZnSnS4 (CZTS) and Sb2Se3 absorbers. Biomass-derived carbons, due to their tunable surface chemistry and low environmental footprint, may serve as sustainable hole-transport interlayers, buffer layers, or conductive scaffolds in next-generation PV–supercapacitor hybrid systems.

By bridging materials processing (WG3), modelling of charge transport (WG2), and advanced characterization (WG5), this contribution emphasizes the potential of bio-based porous carbons in coupling chalcogenide PV devices with high-performance supercapacitors. Such integrated, low-carbon energy solutions support the RENEW-PV objective of developing environmentally benign, high-efficiency renewable energy technologies.