

Does chalcogenide have high photovoltaic potential?

However, unlike the halide perovskites, none of the chalcogenide candidates has shown any other primary indication of high photovoltaic potential, such as a high luminescence quantum yield that would suggest open-circuit voltage potential near the SQ limit.

Which chalcogenide materials are promising for photovoltaic applications?

On the basis of the result of screening study, they said that the promising chalcogenide materials are BaZrS_3 , BaZrSe_3 , SrZrSe_3 , SrHfS_3 and BaHfSe_3 , and Kuhar and co-workers published that BaZrS_3 , SrZrS_3 , SrHfS_3 , BaHfSe_3 , BaZrS_3 , CaZrS_3 and CaHfS_3 are the promising materials for the photovoltaic applications.

Are chalcogenide perovskite materials suitable for photovoltaic applications?

In this context, Perera et al. have synthesized the chalcogenide perovskite materials (BaZrS_3 and CaZrS_3) using high-temperature sulfurization method. Such fabricated $\text{BaZr}(\text{O}_{1-x}\text{S}_x)_3$ perovskites have shown the flexibility of bandgaps between 1.73 and 2.87 eV and, hence, excellent potential in photovoltaic applications.

Does chalcogen affect photovoltaic property of NFREAs?

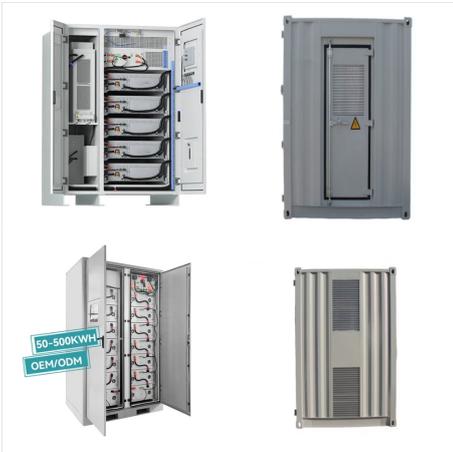
The chalcogen effect on the photovoltaic property of NFREAs was investigated. The champion power conversion efficiency 14.74% was achieved finally. Fused-ring electron acceptors (FREAs) are the current working horse for the top performing organic solar cells (OSCs).

Do nonfused ring electron acceptors based on chalcogen substituted side chains affect photovoltaic properties?

Nonfused-ring electron acceptors (NFREAs) based on chalcogen substituted side chains were developed. The chalcogen effect on the photovoltaic property of NFREAs was investigated. The champion power conversion efficiency 14.74% was achieved finally.

Does chalcogen substitution affect molecular geometry and electronic properties?

The chalcogen substitution effect on the molecular geometry and electronic properties was studied by density functional theory (DFT) at the B3LYP/6-31G (d,p) basis set (Fig. 2). All three NFREAs exhibited comparable torsional energies between the TT block and the steric TIP side chains (Fig. 2 a).



Title: Enhancing Chemical Stability and Photovoltaic Properties of Highly Efficient Nonfullerene Acceptors by Chalcogen Substitution: Insights from Quantum Chemical Calculations. Authors: Leandro Benatto, Since tellurium is a distinctive element among chalcogens, the basic features of Te compounds cannot be deduced straightforwardly from



As an emerging photovoltaic technology, organic photovoltaics (OPVs) present the unique merits of being flexible, semi-transparent, and compatible with large-scale printing. 1-3 Organic photovoltaic materials, especially non-fullerene acceptors (NFAs), contribute a lot to the progress of OPV owing to their readily tunable structures that can



Lead halide perovskites have emerged as promising photovoltaic (PV) materials owing to their superior optoelectronic properties. However, they suffer from poor stability and potential toxicity. Heavy cations with lone-pair electrons and mixed anions of chalcogens and halogens as a descriptor for simultaneous realization of defect tolerance



Chalcogenide perovskites are proposed for photovoltaic applications. The predicted band gaps of CaTiS_3 , BaZrS_3 , CaZrSe_3 , and CaHfSe_3 with the distorted perovskite structure are within the optimal range for making single-junction solar cells. The predicted optical absorption properties of these materials are superior compared with other high-efficiency solar a?)



$X = N$, halogens, chalcogens. Over 32 000 systems in total. Convex hulls based on MP and OQMD: Quantification of instabilities is impossible based on one phase results only: Only cubic: Filippone et al. For PV devices, the strength of light absorption is an important parameter, because it determines the minimum thickness of the absorber



Enhancing the Chemical Stability and Photovoltaic Properties of Highly Efficient Nonfullerene Acceptors by Chalcogen Substitution: Insights from Quantum Chemical Calculations. Leandro Benatto * Leandro Benatto. Since tellurium is a distinctive element among chalcogens, the basic features of Te compounds cannot be deduced straightforwardly



of organic photovoltaic cells based PTB7:PC70BM .
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Chalcogenide photovoltaic (PV) materials such as CdTe[1,2] and Cu(In,Ga)Se₂ (CIGSe)[3a??5] have enabled remarkable progress in thin-film PV device performance, with each technology exceeding the 20% power conversion efficiency (PCE) barrier. However, two major concerns remain regarding these technologiesa??i.e., the negative environmental



Abstract: This thesis explores the structure and properties of silicon doped with chalcogens beyond the equilibrium solubility limit, with a focus on the potential presence of an impurity band and its relevance to photovoltaics.



We assess the viability for photovoltaic applications of proposed Pb-free perovskites with mixed chalcogen and halogen anions, $AB(\text{Ch},\text{X})_3$ ($A = \text{Cs}$ or Ba ; $B = \text{Sb}$ or Bi ; $\text{Ch} = \text{chalcogen}$; $X = \text{halogen}$), by examining critical issues such as the structural, electronic/optical properties, and stability through the combination of density-functional theory calculations and a?



$X = \text{N}$, halogens, chalcogens. Over 32 000 systems in total. Convex hulls based on MP and OQMD: Quantification of instabilities is impossible based on one phase results only: Only cubic: Filippone et al. For PV a?



criteria for PV materials: (1) utilization of cations with large atomic numbers and lone pairs as cations, (2) mixed chalcogen and halogen as anions, (3) optimal direct band gaps. There have been several reports on related materials for PV applications. Using first-principles calculations, mixed chalcogenide-halide perovskites (e.g., $\text{CH}_3\text{NH}_3\text{BiSe}_3$)



Chalcogens have fascinating historical significance. The study and use of chalcogens have played a significant role in the history of science and technology. From the discovery of oxygen by Joseph Priestley to the development of selenium photovoltaic cells, chalcogens have continuously pushed the boundaries of knowledge and innovation. Conclusion



Chalcogen effect on the photovoltaic performance of nonfused-ring small molecular electron acceptors for efficient organic solar cells
@article{Liu2024ChalcogenEO, title={Chalcogen effect on the photovoltaic performance of nonfused-ring small molecular electron acceptors for efficient organic solar cells}, author={Siyang Liu and Xiaowei Chen



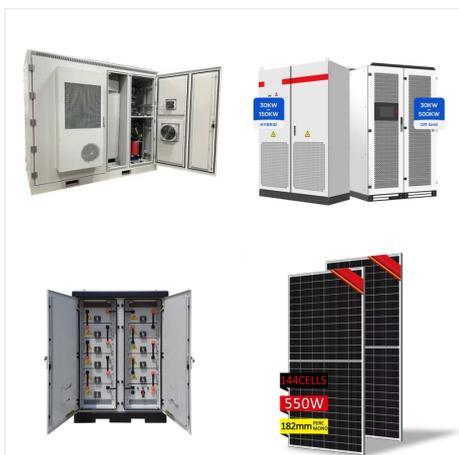
While further optimization of thin film fabrication and device engineering could offer more competitive photovoltaic performances, this unprecedented approach provides a proof-of a?



chalcogen atom p-orbitals and the I²-orbitals of the SMD as the chalcogen Z increases, while the relatively constant mPX HOMO energies are likely a result of the inability of the meta chalcogen substituents to I²-donate into the SMD backbone. Additionally, the lowest-lying FMOs among these SMDs of ca. a²?5.45 eV (HOMO) and a²?3.72 eV (lowest



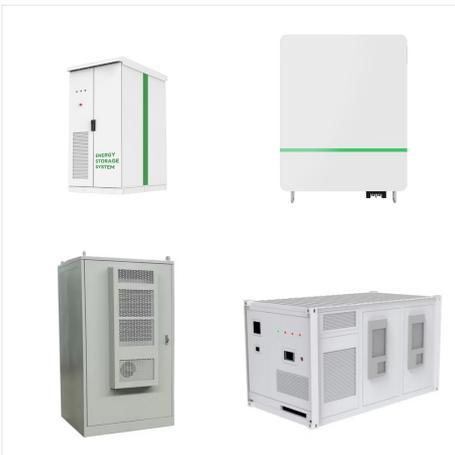
to chalcogen-mediated interactions, such as chalcogen (Ch)^a?^d? interactions [29a²?31] or d²?^a?hole chalcogen bonding (CB) between a polarized Ch atom and a d²? system or a Lewis base



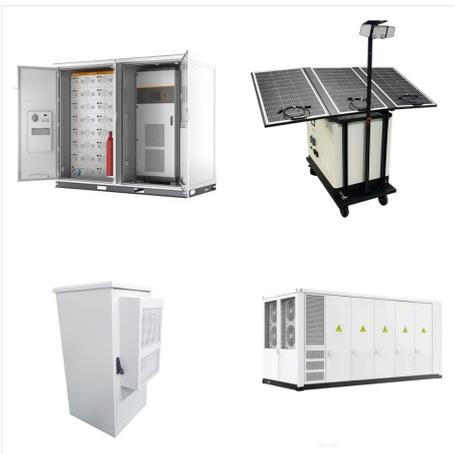
DOI: 10.1002/advs.202405622 Corpus ID: 270960883; From Chalcogen Bonding to Sa²?¹? Interactions in Hybrid Perovskite Photovoltaics @article{Luo2024FromCB, title={From Chalcogen Bonding to Sa²?¹? Interactions in Hybrid Perovskite Photovoltaics}, author={Weifan Luo and SunJu Kim and Nikolaos Lempesis and Lena Merten and Ekaterina Kneschaurek and Mathias a?



Applications across materials science, biology, pharmaceutical science and environmental topics highlight to readers the impact of chalcogen chemistry in many aspects of research. Edited by international leaders in the field, Chalcogen Chemistry brings together contributions from acclaimed researchers around the world. This book is ideal for



photovoltaic devices. Cadmium Telluride belonging to the II-VI group is widely used material for CdS/CdTe heterojunction photovoltaic devices. It is due to the fact that CdTe have intermediate energy band gap, reasonable conversion efficiency, stability and low cost [5-7]. The increasing interest in solar absorption has



The study focuses on the optoelectronic properties of chalcogenide perovskites and perovskite-based chalcogenide as possibilities for future photovoltaic applications. In 2015, a class of unconventional semiconductors, Chalcogenide perovskites, remained projected as possible solar cell materials. The MAPbI₃ hybrid lead iodide perovskite has been considered the best a?]



We assess the viability for photovoltaic applications of proposed Pb-free perovskites with mixed chalcogen and halogen anions, $AB(\text{Ch},\text{X})_3$ (A = Cs or Ba; B = Sb or Bi; Ch = chalcogen; X = halogen)



This thesis explores the structure and properties of silicon doped with chalcogens beyond the equilibrium solubility limit, with a focus on the potential presence of an impurity band and its relevance to photovoltaics. The investigations that we report here shed new light on the electronic role of sulfur dopants in particular, and also provide new evidence of a semiconductor-to-metal



Photovoltaic devices based on evaporated LaYS 3 thin films have been reported, but no photocurrent was observed. Problems for other chalcogen perovskites or with specific deposition methods. This



The effect of chalcogen atoms on the overall photovoltaic property was systematically investigated. Among three NRFEAs, the moderate S_a??a??a??S interactions in TTS-4F molecules guaranteed the high crystallinity and enabled an optimal blend morphology, facilitating the charge separation and transport. As a result, TTS-4F based devices achieved



The fill factor (FF) of organic photovoltaic (OPV) devices has proven difficult to optimize by synthetic modification of the active layer materials. In this contribution, a series of small-molecule donors (SMDs) incorporating chalcogen atoms of increasing atomic number (Z), namely oxygen, sulfur, and selenium, into the side chains are



Computational predictions indicated a steady form of the mixed chalcogen-halogen perovskite, which merited photovoltaic advancement [67]. The Summarized data for device performance of Perovskite-based Chalcohalide photoabsorbers has been displayed in Table 6.



Molecular level understanding of chalcogen atom effect on chalcogen-based polymers through electrostatic potential, non-covalent interactions, excited state behaviours, and radial distribution