

Defects in the properties of solar materials

What are defects in solar cells based on perovskite-halides?

This Review describes what is known about the nature and impact of defects in solar cells based on perovskite-halides, with a focus on traps, recombination mechanisms, electrostatics, and defect conduction, which have an impact in both the bulk material and at the interfaces in devices.

How do point defects affect the performance of perovskite solar cells?

The performance of perovskite solar cells is significantly impacted by point defects, such as Schottky, Frenkel, interstitial vacancies, and substitutions. Interstitials (MA_i , Pb_i , I_i) exert a significant influence on carrier concentration and modify the band structure within the material.

What is defect physics in perovskite-halide semiconductors?

Understanding of defect physics in perovskite-halide semiconductors is essential to control the effects of structural and chemical defects on the performance of perovskite solar cells. Petrozza and Ball review the current knowledge of defects in these materials.

Do intrinsic material qualities affect solar cell activity?

This demonstrates the delicate interaction between intrinsic material qualities and solar cell activity, underlining the need for additional study to improve their efficiency and effectiveness in renewable energy applications. 3. 4.

Why do we need to study defects in Materials Engineering?

Additionally, it enhances accessibility to materials engineering processes and has the potential to improve material performance and reliability, leading to broader applications across industries. Similarly, investigate various mechanisms through which defects can be passivated.

Are perovskite solar cells limiting material properties?

Following the initial rise of power conversion efficiencies in perovskite solar cells, the understanding of the limiting material properties is catching up. An important area of focus for future effort is the understanding and control of defects, which have an impact on several aspects of device functionality.

Based on the first principles, the defect calculation plays an increasingly important role in understanding the material properties of solar cells and the bottleneck of device efficiency. At present, the calculation of defects based on the first principle mainly focuses on the formation energy and transition energy levels of defects.

In this study, tungsten di-sulphide (WS_2), one of the key transition-metal dichalcogenide (TMDC) materials, is used as solar cell absorber material with a suitable solar cell configuration and ...

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Such interactions can reduce coherence times, or act as a handle for engineering defect properties and defect-defect interactions. ... Investigation of the solar cell materials $\text{Cu}(\text{In,Ga})\text{Se}_2$ and $\text{Cu}_2\text{ZnSnS}_4$ with muon spin spectroscopy and density-functional calculations," J. Appl. Phys. 136, 055704

Identifying and quantifying defects in perovskite solar cells becomes inevitable to address these challenges and mitigate the deteriorating effects of these defects.

There is great interest in commercializing perovskite solar cells, however, the presence of defects and trap states hinder their performance. Here, recent developments in characterization ...

As an absorber in photovoltaic devices, Sb_2Se_3 has rapidly achieved impressive power conversion efficiencies despite the lack of fundamental knowledge about its electronic defects. Here, we present a deep level transient spectroscopy (DLTS) study of deep level defects in both bulk crystal and thin film device material. DLTS study of Bridgman-grown n-type bulk crystals ...

On the material level, perovskite films often feature abundant intrinsic defects, such as antisites, interstitials, and vacancies, as well as impurities and dangling bonds at ...

The power conversion efficiency of perovskite solar cells has been significantly improved in recent years. One of the key factors leading to this change is that the microstructure of the perovskite layer and its neighboring layers can be controlled. Grain size and grain boundaries, as basic components of perovskite film, have a significant impact on the device ...

Defects, including point defects, grain boundary defects, surface defects, and ion migration, are identified as key culprits behind performance degradation. By strategically ...

It is now widely recognized that surface and interfacial defects exhibit distinct behavior compared to bulk defects in metal halide perovskites. However, the transition from bulk to surface behavior and the spatial extent of the surface's influence are not well understood. To address this, we conducted first-principles calculations on iodine vacancies and interstitial ...

In this work, the extra Mg^{2+} incorporation is used to enhance the efficiency of CZTSSe solar cells for the first time. The extra Mg^{2+} incorporation can improve the crystallinity, reduce the harmful defects, and optimize the electrical properties of the CZTSSe thin films, which enhance the efficiency of solar cells to 9.00 % from 7.08 %. Therefore, the extra Mg^{2+} ...

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