



Contribution ID: 18

Type: not specified

Numerical Modeling and Optimization of CaZrS₃ chalcogenide Perovskite Solar Cell by Using SCAPS-1D with theoretical efficiency approaching 20%

Wednesday, 16 November 2022 11:30 (30 minutes)

1. Introduction

Chalcogenide perovskites ABX₃ (A=Alkaline earth metals; B=Transition metals; X=S or Se) have recently been studied, but they still need to be rigorously tested under various conditions. Several experimental studies on these materials have been conducted [1] [2]. Zr-based chalcogenide perovskites (AZrS₃, where A is an alkaline earth metal such as Ca, Sr, or Ba) have a d-orbital character, whereas the 4d states are less localized than the 3d states, resulting in a high absorption coefficient and a low effective mass of the charge carriers in these compounds [3].

In this study, a device simulation of CaZrS₃ material is reported for the first time, which makes this new study interesting, using the one-dimensional solar cell capacitance simulator SCAPS-1D. Therefore, we tried to propose low cost Electron Transport Materials ETMs (TiO₂, ZnO, and SnO₂). The influence of thickness, doping concentration (NA), and the working temperature on the device performance were studied.

1. Results

As a result, we have found that for CaZrS₃ the most preferment structure is found to be: Au/NiO_x/CaZrS₃ (Absorber)/ZnO/FTO with a maximum PCE of 19.36%, V_{OC} of 1.79 V, J_{SC} of 16.13 mA/cm² and FF of 89.85%.

1. References

- [1] Shaili H 2021 Synthesis of the Sn-based CaSnS₃ chalcogenide perovskite thin film as a highly stable photoabsorber for optoelectronic applications J. Alloys Compd. 9
- [2] Zitouni H, Tahiri N, El Bounagui O and Ez-Zahraouy H 2020 Electronic, optical and transport properties of perovskite BaZrS₃ compound doped with Se for photovoltaic applications Chem. Phys. 538 110923
- [3] Kumar M, Singh A, Gill D and Bhattacharya S 2021 Optoelectronic Properties of Chalcogenide Perovskites by Many-Body Perturbation Theory J. Phys. Chem. Lett. 12 5301-7

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Session Classification: Partner

Track Classification: Partner