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A machine learning approach to prediction of bandgap and optimum efficiency of perovskite solar cells based on SCAPS 1-D data simulation

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Abstract

Recent advances in perovskite solar cells (PSCs) have yielded power conversion efficiency (PCE) values exceeding 25.5% within a decade from their inception. Despite this rapid growth in PCE, one of the major drawbacks hindering large scale commercialization of PSCs is the toxicity of the lead (Pb) component in their composition [1]. Partially or wholly substituting Pb with other environmentally friendly metal elements offers a solution to circumvent this challenge. Due to the vast chemical landscape of perovskite materials, composition selection for mixed perovskites is still largely through tedious, costly and labour-intensive trial and error experiments [2].

In this contribution, solar cell capacitance simulator (SCAPS) was utilized to simulate a PSC device of methylammonium tin/lead iodide ($MASn_xPb_{1-x}I_3$). The simulated open voltage circuit (V_{OC}), fill factor (FF), current density (J_{SC}) and efficiency of the solar cell were optimized by varying input parameters of the perovskite absorber layer: thickness (200 – 1500 nm) and the bandgap (1.18 – 1.6 eV) corresponding to Sn_xPb_{1-x} composition. A set of supervised machine learning (ML) models were trained to predict the relative effect of varying the composition on the bandgap. Based on SCAPS simulated data, a second ML model was designed to predict the best possible PCE using the predicted bandgap and layer thickness values as input parameters. The results suggest that ML in conjunction with numerical SCAPS simulations can be an effective approach to accelerate discovery [3] of efficient, low cost and less toxic PSCs through narrowing down possible perovskite combinations to just a few permutations.

References

1.Parikh N. et al., Is machine learning redefining the perovskite solar cells?. Journal of Energy Chemistry. 2022, 66, p. 74-90.

2.Jebakumar, J. et al., Design and simulation of inorganic perovskite solar cell. Applied Nanoscience. 2022, 12(5), p. 1507-18.

3.Hasanzadeh Azar M. et al., SCAPS Empowered Machine Learning Modelling of Perovskite Solar Cells: Predictive Design of Active Layer and Hole Transport Materials. Photonics. 2023, 10(3), p. 271

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

Primary author: MASHAMBA, Dakalo Rollet (Tshwane University of Technology)

Co-authors: Prof. MSIMANGA, Mandla (Tshwane University of Technology); Dr KAPIMKENFACK, Abraham Dimitri (Tshwane Unioversity of Technology)

Presenter: MASHAMBA, Dakalo Rollet (Tshwane University of Technology)

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