Title: Performance optimization and machine learning-guided parameter sensitivity analysis of lead-free $KGeCl_3$ perovskite solar cells

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Abastact: This study gives a realistic insight into the effectiveness of lead-free Ge-based perovskite solar cells (PSCs) using $KGeCl_3$ as the absorber layer in combination with four different electron transport layers (ETLs), including WS_2, ZnSe, $PC_{60}BM$, and SnS_2, with copper iron tin sulfide (CFTS) serving as the hole transport layer (HTL). Initially, key material parameters such as layer thickness, donor density (N_D), acceptor density (N_A), defect density (N_t), interface defect densities (IL1 & IL2), series resistance (R_s), shunt resistance (R_{sh}), operating temperature (K), and back contact work function (eV) are varied using a SCAPS-1D simulator to optimize device performance. Between the four cell configurations, the FTO/CFTS/$KGeCl_3$/WS_2/Au structure has achieved the highest performance with a power conversion efficiency (PCE) of 21.39%, short-circuit current density (J_{SC}) of 39.526 mA cm^{-2}, fill factor (FF) of 76.56%, and open-circuit voltage (V_{OC}) of 0.706 V at a simulated temperature of 300 K. Other configurations using ZnSe, $PC_{60}BM$, and SnS_2 as ETLs showed PCE values of 21.38%, 21.05%, and 20.43%, respectively. Furthermore, an integrated machine learning framework with four supervised learning methods, *i.e.*, Random Forest, XGBoost, CatBoost, and Decision Tree, has been utilized to effectively evaluate the importance of material features. Out of the algorithms, CatBoost has the highest performance with R^2 and accuracy values of 0.984 and 99.344%, respectively.

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