Enhancing Efficiency and Stability in 2D/3D Hybrid Perovskite Solar Cells: A Simulation Study of N-I-P and P-I-N Architectures with Different Charge Transport Layers.

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Abstract:

Perovskite solar cells (PSCs) have achieved power conversion efficiencies (PCEs) exceeding 25% for single-junction devices, making them a promising low-cost photovoltaic technology. However, their long-term stability under environmental conditions remains a challenge to commercialization [1,2]. To address this, researchers have been studying 2D/3D hybrid perovskite structures, which combine the efficiency of 3D perovskites with the improved stability of 2D layers [3]. In our previous study, we used QuantumATK to investigate the intrinsic properties of the 2D/3D interface of ($BA_2FAPb_2I_7/FAPbI_3$) hybrid Perovskite, which showed optimal band alignment, facilitating efficient charge transfer, and enhanced light absorption.

However, optimizing device architectures and material selections remains critical to overcoming stability challenges and moving into commercialization. In this study, we investigate the performance and stability of the $FAPbI_3/BA_2FAPb_2I_7$ hybrid perovskite solar cell in both n–i–p and p–i–n device architectures using SCAPS-1D. We tested a combination of five electron transport layers (ETLs)—TiO_2, SnO_2, ZnO, IGZO, and In_2O_3:Zn—and five hole transport layers (HTLs)—Spiro-OMeTAD, CuSCN, NiOx, CuI, and PEDOT:PSS. This resulted in fifty different device configurations.

Our results show that the p–i–n structure performs better overall, achieving a higher open-circuit voltage, short-circuit current, and device efficiency, compared to the n–i–p structure. We further analysed the three best performing structures by varying absorber and ETL thickness, series and shunt resistance, and operating temperature. The obtained results from SCAPS-1D will be used in fabricating 2D/3D heterostructure perovskite solar cells (PSCs) for our future work.

References

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