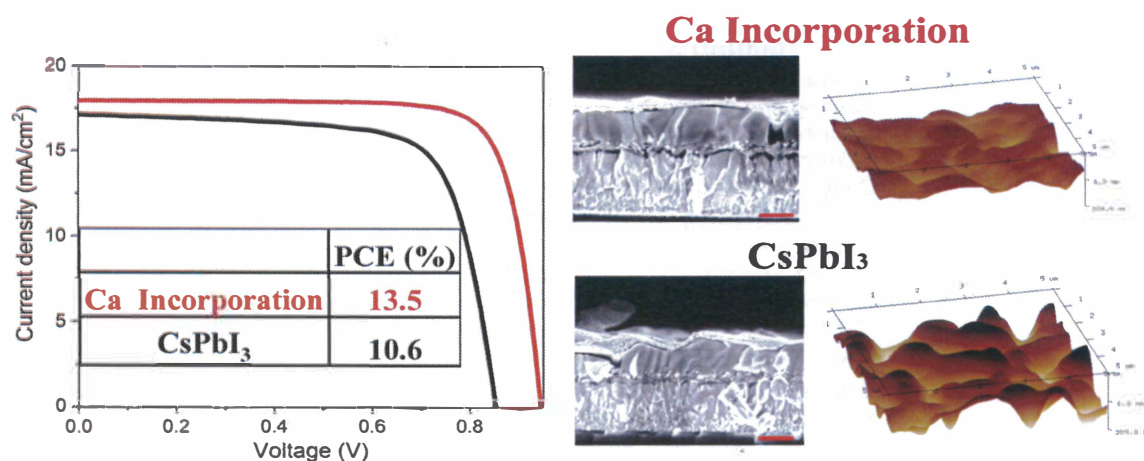


Enhanced Performance via Partial Lead Replacement by Calcium for CsPbI₃ Perovskite Solar Cell

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Cesium metal halides are potential light-harvesting materials as a top cell in multi-junction devices due to their suitable bandgap and good thermal stability. In particular, CsPbI₃ has a bandgap of 1.7eV which is suitable for perovskite/Si tandem. However, the desirable black phase for CsPbI₃ is not stable because Cs is too small to support the PbI₆ octahedra. Also, there is room for improvement in terms of cell performance. Herein, we partially replace Pb²⁺ with Ca²⁺ in the CsPbI₃ precursor producing multiple benefits. Firstly, more uniform films with larger grains are produced from CsPbI₃ with Ca²⁺, due to the reduction in the size of colloids in the precursor solution with Ca²⁺. This morphology improvement provides a better contact at the interface between perovskite and the hole transport layer. In addition, it is found that the surface of the film is modified by a formation of Ca rich oxide layer, providing a surface passivation effect. Finally, the incorporation of Ca increases the band gap, leading to increase in output voltage. The best CsPbI₃ solar cell using 5% Ca²⁺ substitution in the precursor achieves a stabilised efficiency of 13.3%, and maintains 85% of its initial efficiency over 2 months with encapsulation.



References

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