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| **Abstract:** |  |
| Cesium lead iodide bromide (CsPbIBr2) perovskite solar cells (PSCs) have improved stability compared to other perovskite compositions. However, they still face significant challenges due to their poor photovoltaic performance parameters, which limit the devices’ power conversion efficiencies (PCEs). This study proposes a novel device design to tailor the potential of CsPbIBr2 PSCs by improving their optoelectronic properties. An advanced 3D multiphysics approach was rigorously used to investigate the optics and electrical properties of the proposed CsPbIBr2 PSCs. This approach combines finite-difference time-domain (FDTD) and finite element method (FEM) techniques with the particle swarm optimization (PSO) algorithm. The outcome from the adapted numerical approach is in good agreement with the experimental results. The optimized CsPbIBr2 PSC demonstrates a promising power conversion efficiency (PCE) of over 16.4%, associated VOC of 1.53 V, FF of 80.6%, and JSC of 13.4 mA cm2. Therefore, the potential of CsPbIBr2 perovskites could be further explored with continued research and development in material science and device physics. | |