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Interfacial Passivation Between $CsPbI_3$ and Hole Transport Layers: Experimental and Theoretical Insights

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Lead halide perovskites (LHPs) are promising materials for solar cells, offering outstanding optoelectronic properties, low-cost fabrication, and power conversion efficiencies. Among them, caesium lead triiodide ($CsPbI_3$) stands out for its superior thermal stability. However, it remains prone to phase instability, moisture sensitivity, surface defects, and interfacial recombination, which limit performance. Addressing these limitations requires effective interface engineering strategies to optimize charge transport, suppress non-radiative recombination, and enhance material stability. We investigated $CsPbI_3$ interfaces with hole transport layers (HTLs) and passivants using both computational and experimental approaches. Through Density Functional Theory (DFT) calculations we provided insights into interfacial adhesion and electronic structure modifications, which are critical for optimizing device design. Experimentally, we explored interface passivation using P3HT, OABr, and OAI to enhance interfacial quality and improve optoelectronic properties. We analyzed the interaction of $CsPbI_3$ with HTLs such as 2-PACz, PTAA, and Spiro-OMeTAD, as well as the passivant P3HT. Preliminary DFT results indicate that $CsPbI_3$ exhibits stronger interaction with Spiro-OMeTAD that is chosen as HTL in fabricated devices . Experimentally, we find that passivants such as OABr and OAI enhance photoluminescence, suggesting a reduction in non-radiative recombination, consistent with previous studies on similar perovskite compositions. This combined computational and experimental approach provides insights into interface engineering strategies for $CsPbI_3$ perovskite solar cells.

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