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Computational Discovery of Halide-Tuned Double Perovskites for Sub-1 eV Thermophotovoltaic Materials

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The search for novel semiconductors with sub-1 eV bandgaps is critical for efficient infrared photon-to-electricity conversion from high-temperature thermal emitters in thermophotovoltaic (TPV) systems. Double perovskites with the general formula $A_2B'B''X_6$ offer exceptional chemical tunability, making them attractive for targeted infrared bandgap engineering. For TPV devices operating with emitter temperatures in the 1100 - 1500 K range, the optimal bandgap lies between 0.6–0.75 eV, enabling spectral matching while minimizing thermalization losses.

Experimental studies of lead-free halide double perovskites report bandgaps in the ~1.8–1.9 eV range, well above the TPV-optimal window. These materials also exhibit relatively low mobilities compared to lead-halide perovskites; for example, $\text{Cs}_2\text{AgBiBr}_6$ thin films have a lower bound of $\sim 1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, while single crystals can reach $\sim 11.8 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. Given that both optimal bandgap positioning and balanced carrier transport are intrinsic design criteria for high-efficiency TPV converters, we conducted a computational screening of candidate double perovskites. Using density functional theory (VASP), Boltzmann transport modeling with AMSET, and structural data from the Materials Project API, we screened $\text{Cs}_2\text{CuSbCl}_6$, Cs_2SnBr_6 , and $\text{Cs}_2\text{CuSbBr}_6$. The computed bandgaps closely matched literature values, validating our approach and indicating that $\text{Cs}_2\text{CuSbBr}_6$ is the most promising candidate. High-throughput calculations were then performed to systematically vary the halide composition in the $\text{Cs}_2\text{CuSb}(\text{Br}_x\text{I}_{6-x})$ series.

Fully iodide-substituted $\text{Cs}_2\text{CuSbI}_6$ exhibits a direct bandgap of 0.683 eV, squarely within the TPV-efficient range. The evolution of bandgap with halide substitution, the temperature-dependent transport properties for the full halide series at $n_h = 10^{16} \text{ cm}^{-3}$, and the carrier mobilities calculated via AMSET will be demonstrated. While factors such as Auger recombination and phase stability are essential for practical implementation, this study will provide an initial screening for the batch of candidate materials that deserve future experimental investigations.

Authors: Mr HAMER, Caiden (Duke Kunshan University); WANG, Xiawa (Duke Kunshan University)

Co-authors: Dr HUSSAIN, Ghulam (Duke Kunshan University); Ms ZHANG, Man (Duke Kunshan University)

Presenter: WANG, Xiawa (Duke Kunshan University)

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