

The Development of Halide Double Perovskites

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Solar cells are among the most promising renewable energy sources, capable of meeting the growing global energy demand while significantly reducing greenhouse gas emissions. Notably, solution-processed lead halide perovskites have garnered immense attention in photovoltaic applications, with an astonishing improvement in efficiency from 3.8% to around 27% over the past decade.¹ However, despite their rapid progress, these perovskite devices face a critical challenge—the toxicity of lead (Pb), which poses a significant barrier to their practical application.² Lead-free halide double perovskites (HDPs, $A_2BB'X_6$) have emerged as one of the most promising alternatives, offering attractive optical and electronic properties while addressing both the toxicity and stability concerns associated with lead halide perovskites (Fig. 1). HDPs exhibit a broad range of compositional possibilities and rich substitutional chemistry, making them intriguing candidates for various optoelectronic applications.³ However, their current performance remains inferior to lead halide perovskites, particularly in photovoltaics.⁴ One limitation is that HDPs typically possess large and/or indirect bandgaps, restricting their optical and optoelectronic performance in the visible and infrared regions. In this presentation, I will talk about our work on double perovskites, including the fabrication of the first planar double perovskite solar cell devices, strategies to modify the bandgap and optical properties of HDPs through metal doping/alloying and crystallization control,^{5,6} as well as a detailed atomic-level understanding of the alloying process.

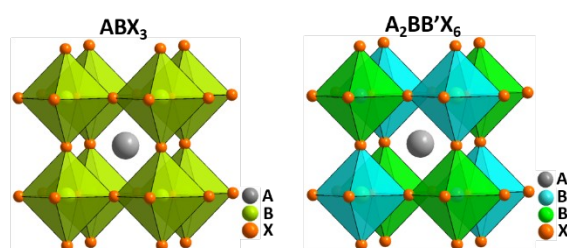


Fig. 1 Schematic diagram of the structure of common single perovskite ABX_3 (left) and double perovskite $A_2BB'X_6$ (right).

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References

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