Defect Engineering of Perovskites for Next-Generation Optoelectronics

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Metal-halide perovskites have emerged as a highly promising material for next-generation optoelectronic devices such as light-emitting diodes (LEDs) and solar cells. Over the past decade, device performance has improved significantly; however, internal defects remain a critical challenge for practical application. Defects in perovskites can result in quenching of charge carriers via non-radiative recombination channels, leading to degraded optoelectronic performance. In addition, defect migration gives rise to peculiar electronic and optical behavior of devices such as current-voltage hysteresis and luminance overshooting, which severely impact the stability of the perovskite optoelectronic devices accelerating their degradation. To address these challenges, various defect passivation strategies have been proposed.

In this talk, we discuss approaches for defect passivation in metal-halide perovskites, involving organic chemical reagents and low-dimensional perovskites, as well as the incorporation of perovskite polytypes such as a corner-sharing 6H phase to achieve coherent intervention at halide position effectively screening halide defect formation. Our results demonstrate that these defect engineering strategies enhance both the optoelectronic characteristics and the stability of LEDs and solar cells. Furthermore, we highlight the detrimental impact of shallow-level defects, particularly the iodide vacancy (V_I^+), which has conventionally been regarded as benign. We believe that our findings pave the way for the employment of perovskite polytypes in practice to achieve high-performing perovskite optoelectronic devices, while also elucidating the necessity of engineering shallow-level defects.

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Reference

[1] H. Kim *et al.*, *Nature Communications*, **15**, 5632 (2024)
[2] H. Kim *et al.*, *Nature Communications*, **11**, 3378 (2020)
[3] H. Kim *et al.*, *Advanced Energy Materials*, 2200837 (2022)
[4] H. Kim *et al.*, *Advanced Functional Materials*, **30**, 1910620 (2020)