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Study of the Interactions Between Carbazole-Based Quaternary Ammonium Salts and Lead-Based Perovskite.

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Perovskite solar cells (PSCs) have undergone a remarkable increase in power conversion efficiency, rising from 3.8% to 27% within a relatively short period [1;2]. However, limited operational stability remains a major obstacle to their widespread commercialization. Surface defect passivation has therefore become an important strategy for improving both device performance and long-term stability [3;4]. Despite numerous reported approaches, the mechanisms governing the effectiveness of different passivating agents are still not fully understood.

In this work, we systematically investigated quaternary ammonium and thiouronium organic salts as surface passivating agents for triple-cation PSCs and compare their behavior with the commercially available sulfonium-based salt DMPESI. A combination of steady-state photoluminescence (PL), time-resolved photoluminescence (trPL), X-ray photoelectron spectroscopy (XPS), liquid-state nuclear magnetic resonance (NMR), and photovoltaic device measurements were used to evaluate organic–perovskite interactions and their influence on device properties.

The results demonstrated that different characterization techniques probe distinct aspects of the passivation process. While several surface treatments enhance radiative recombination, as indicated by PL and trPL measurements, these improvements do not necessarily translate into enhanced photovoltaic performance. Among the investigated compounds, only the iodide-containing quaternary ammonium salt CzEAI produces a clear improvement in device performance, consistent with the interactions observed by XPS.

These findings highlight the complex relationship between molecular interactions, defect passivation, and photovoltaic performance, emphasizing the importance of combining complementary characterization techniques when evaluating surface passivation strategies for PSCs.

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