IMPACT OF QUATERNARY AMMONIUM GROUP POSITION IN SAMS ON THE PERFORMANCE OF PEROVSKITE SOLAR CELLS

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In recent years perovskite solar cells (PSCs) have emerged as a new and efficient way for green energy conversion. Extensive research has led said device performance to a remarkable 27%. However, interfacial engineering together with molecular and surface modifying strategies can further advance device performance. Incorporating self-assembled monolayers (SAMs) into PSC structure significantly increases both stability and device performance [1].

SAM architectures are typically defined by three key components: the functional group, the spacer, and the anchoring group. Molecules built following this principle can organize into a monolayer that promotes effective charge transport and further stabilizes the perovskite surface that is an essential factor for maintaining strong light absorption and overall exceptional device performance [2].

Years of sustained research have identified carbazole based SAMs containing phosphonic acid anchoring groups and alkyl chain spacers of varying length as particularly effective molecular structures [2]. In this work, phenylene groups were introduced into the structures in an attempt to reduce molecular aggregation and promote the formation of a more uniform monolayer. Additionally, ammonium salts were incorporated at different positions to improve the SAM/perovskite interface, an approach based on prior studies and theoretical insights expected to enhance overall device performance [3,4]. While this research is still ongoing, results should clarify whether ammonium functional groups and their position in the molecular structure have any positive effect on the performance of PSCs.

[1] L. Zhang et al., “Diverse perovskite solar cells: progress, challenges, and perspectives,” Advanced Materials, vol. 38, no. 1, p. e12221, Sep. 2025, doi: 10.1002/adma.202512221.

[2] Y. Yang et al., “Design and applications of hole-selective self-assembled monolayers for perovskite photovoltaics,” Chemical Engineering Journal, vol. 504, p. 158870, Dec. 2024, doi: 10.1016/j.cej.2024.158870.

[3] Z. Shi et al., “‘T-shaped’ carbazole alkylammonium cation passivation in perovskite solar cells,” ACS Energy Letters, vol. 9, no. 2, pp. 419–427, Jan. 2024, doi: 10.1021/acsenergylett.3c02357.

[4] H. Wu et al., “Tailored Lattice-Matched Carbazole Self-Assembled molecule for efficient and stable perovskite solar cells,” Journal of the American Chemical Society, vol. 147, no. 9, pp. 8004–8011, Feb. 2025, doi: 10.1021/jacs.5c00629.