Optimizing $FAPbI_3$ Perovskite Solar Cells *via* Defect Passivation: The Role of DFT Simulations

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$FAPbI_3$ perovskite has recently garnered significant attention as a promising material for the active layer in solar cells due to its lower cost and superior durability compared to silicon-based solar cell devices. Despite these advantages, the power conversion efficiency (PCE) of pristine $FAPbI_3$, currently around 24.26%, must be improved to surpass the PCE of approximately 25% achieved by Si-based devices. To enhance the performance of $FAPbI_3$, various engineering strategies have been proposed. Among these, iodine defect passivation during the synthesis of FAPbI3 has emerged as the most effective strategy, with numerous studies demonstrating enhanced PCE through this approach. However, despite the success of defect passivation in improving perovskite performance, understanding the precise behavior and origin of defect passivation mechanisms remains challenging when relying solely on experimental methods. To address this gap, density functional theory (DFT) simulations are instrumental. These studies employ DFT to explore the $FAPbI_3$ perovskite system through various innovative approaches. These include investigating pseudo-halide interactions within $FAPbI_3$ and examining the passivation effects of larger organic molecules, such as those containing phosphorous groups or benzoquinone-related structures. Our research confirmed the impact of non-bonding interactions between additional additives and the $FAPbI_3$ structure, as well as their binding tendencies and electronic characteristics. The DFT simulations provided valuable insights into the electronic features and stability of these passivated structures, contributing to a deeper understanding of the defect passivation process.