Supporting Information

Enhancing Perovskite Solar Cells Performance through PbI_2 In-Situ Passivation by One-Step Process: Experimental Insights and Simulations.

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2.1 Martials.

Methylamine (40 wt% in methanol, Sigma Aldrich), hydroiodic acid (HI, 57 wt% water, Avantor VWR), lead iodide (PbI2) (99%, Sigma Aldrich), N-N dimethylformamide (DMF, anhydrous, 99.8%, Sigma Aldrich), diethyl ether (DEE, ≥99.5%, GC, Sigma Aldrich), isopropanol (IPA, anhydrous, 99.5%, Sigma Aldrich), acetone and ethanol (99%, Sigma Aldrich) were used as received without any further purification.

2.2 Fabrication and Characterization of $MAPbI_3$ film.

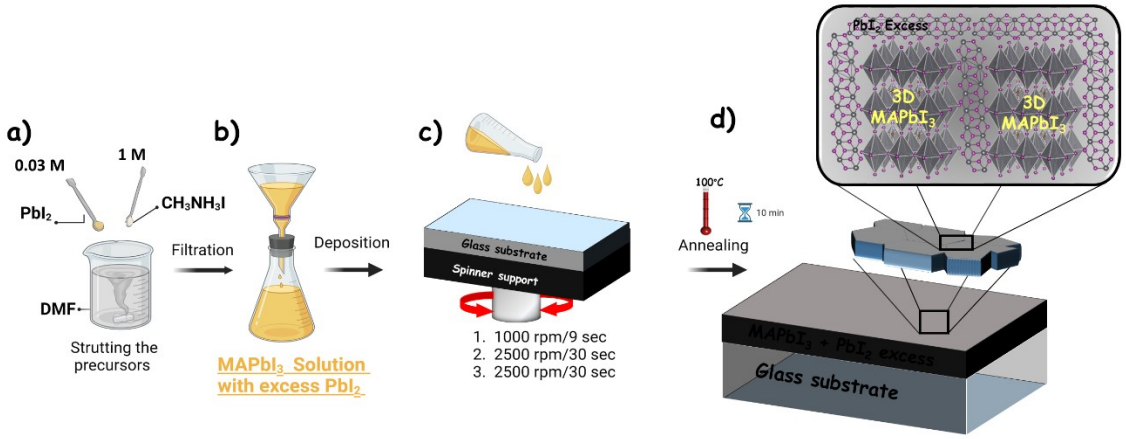

Figure S1. Overview schematics of $MAPbI_3$ film fabrication procedures. a) Strutting the perovskite precursors: 0.03M of PbI_2 quantity is three times higher than 1M of CH_3NH_3I. (b) Filtration of the $MAPbI_3$ solution to avoid grains that are not solubilized with DMF. (c) spin-coated the solution and annealing the sample at 100°C for 10 minutes. (d) Schematics of excess in PbI_2 and its distribution on GBs of the perovskite with an illustration structure of $MAPbI_3$ and PbI_2.

Similar to the approach outlined by Tauc, we utilize a linear fit for the fundamental peak. Furthermore, a linear fit is employed as an abscissa for the slope below the fundamental absorption. The intersection of these two fitting lines provides an estimation of the band gap energy, as illustrated in **Figure S2.**

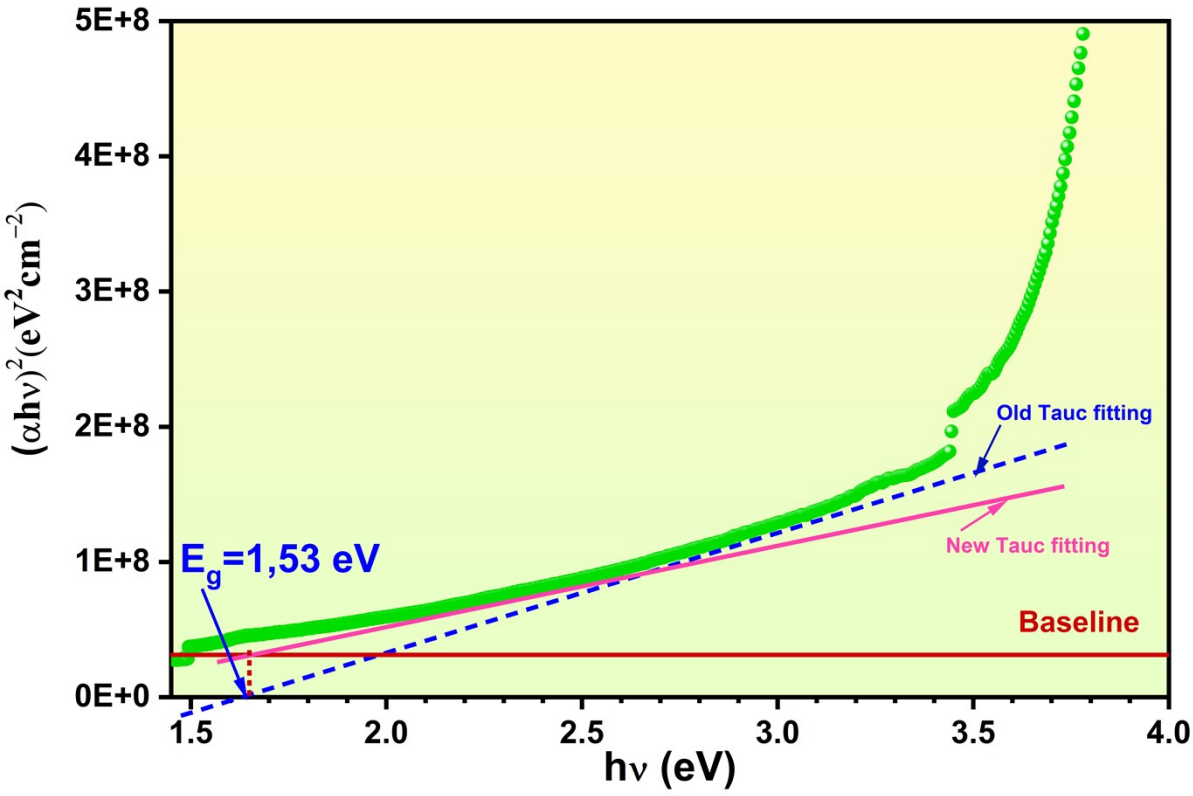

Figure S2. The determination of the E_g using a new approach.