Supplementary Materials: Investigation of Structural and Electronic Properties of $CH_3NH_3PbI_3$ Stabilized by Varying Concentrations of Poly(Methyl Methacrylate) (PMMA)

There was a good correlation between Grazing incidence X-ray diffraction (GIXRD) and surface photovoltage spectroscopy (SPV) since both give the similar order of information depth [1].GIXRD was used for determination of phase composition of perovskite film with the diffraction patterns from lattice planes perpendicular to perovskite film surface. On the other hand surface photo voltage spectroscopy (SPV) measures charge separation of photogenerated electrons and hole at the surface of perovskite film in which illumination induces changes in surface voltage. This implies that penetration depth of GIXRD and transport length of photogenerated charge carriers are of the order of hundreds of nm [2] Both SPV and PL measures electronic properties of perovskite layers and in this work both spectra was used to investigate the band gap of perovskite in the spectral regions slightly above the direct band gap. By combining SPV in the fixed capacitor arrangement with optical and structural techniques, it was possible to monitor the evolution of electrical, structural and optical properties of perovskite material, thereby establishing a correlation between them. SPV can give valuable information on the charge separation, exponential tail states (E_t), transport and recombination properties in perovskite layers. PL measurements were conducted to determine if photogenerated charge carriers could be efficiently extracted from $CH_3NH_3PbI_3$ film coated with PMMA and we found that changing concentration of PMMA had no influence on the band gap of $CH_3NH_3PbI_3$, probably due to insulating property of PMMA.

Figure S1 shows SPV spectra of $CH_3NH_3PbI_3$ on molybdenum substrate coated with 0 mg of PMMA in in 1 mL of butyl acetate after storage in air for 50 days. SPV spectra shows onset energy ($E_{g\text{-}on}$) at around 1.5 eV corresponding to band gap of $CH_3NH_3PbI_3$. However, another onset energy appeared between 2.3 and 2.4 eV corresponding to PbI_2 [3].This is also in agreement with PbI_2 peaks as detected with GIXRD in Figure 3.

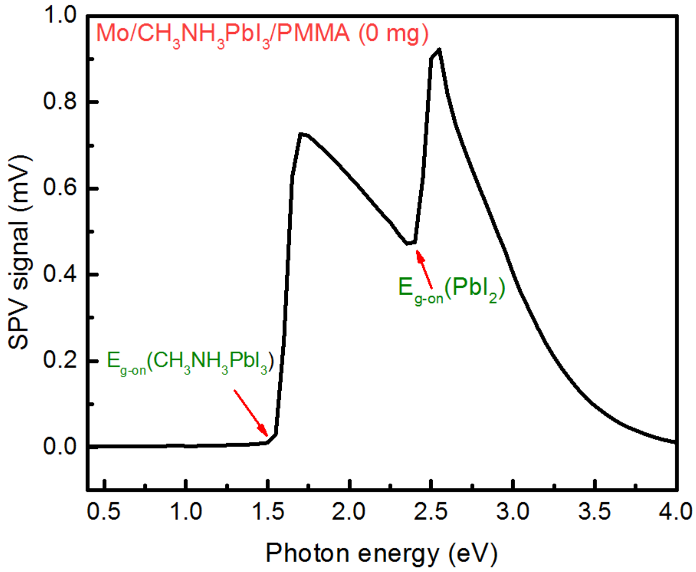

Figure S1. SPV spectra of perovskite on molybdenum substrate coated with 0 mg of PMMA in in 1 mL of butyl acetate.

Figure S2 shows GIXRD pattern for $CH_3NH_3PbI_3$ on molybdenum substrate coated with 0 mg of PMMA in 1 mL of butyl acetate after storage in air for 50 days. An impurity peak corresponding to PbI_2 peak is detected at 12.65°, 25.50°, 38.5° and 52.36° (blue arrows) corresponding to (001), (002), (003) and (004) planes of PbI_2 [3]. This impurity phase of PbI_2 is also detected by SPV (see Figure S2).

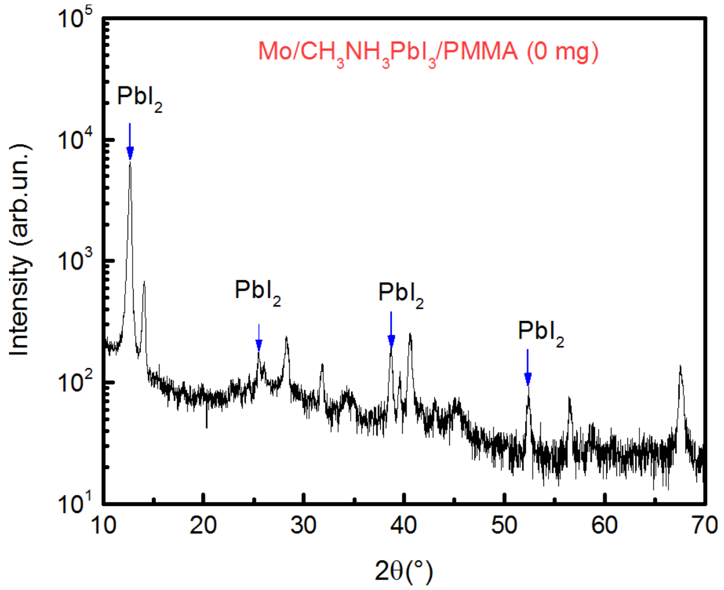

Figure S2. Grazing incidence X-ray diffraction (GIXRD) pattern for of $CH_3NH_3PbI_3$ on molybdenum substrate coated with 0 mg of PMMA in 1 ml of butyl acetate after storage in air for 50 days.

Figure S3 shows tauc gap obtained from SPV and PL spectrum for 40mg/mL of PMMA. The tauc gap from SPV is 1.59 eV and that from PL is 1.6 eV. The difference of 0.01 eV may be due to the difference in the nature of measurements employed by two methods. This is because PL is an optical absorption process while SPV is not an optical process. In the analysis of tauc plot, SPV signal was assumed to be proportional to absorption coefficient. This presumption was reasonable in the considered spectral range of measurement where the absorption length was larger than charge carrier diffusion/transport length and that there was no change of sign in the SPV signal so that modulated SPV signals could be considered as small signals.

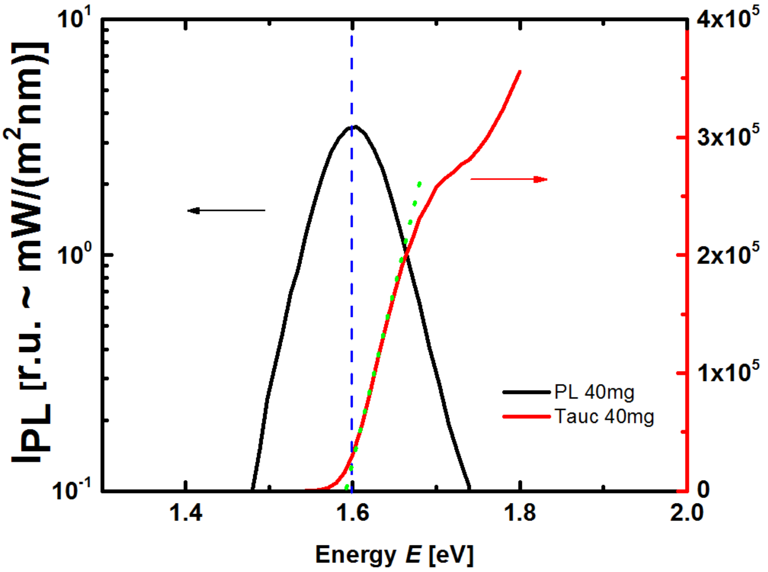

Figure S3. Tauc gap from SPV and PL spectrum for 40mg/mL of PMMA.

References

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