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Improving film quality of a bismuth perovskite variant by investigating the role of organic cation into the film morphology

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Lead halide perovskites have been dominantly playing the champion role in perovskite photovoltaics. However, lead toxicity and device instability are among the main challenges in this research area. To address these issues, bismuth (III) has been explored as an alternative of lead (II) to obtain lead-free halide perovskite variants with a chemical formula of A3Bi2I9. One of the prominent limitations for this class of material is their film quality regarding film coverage and control of morphology, which limits the capability of Bi-Based lead-free components as an efficient light-absorbing layer for photovoltaic application. In this work, we demonstrate that the organic cation with a long alkyl chain plays a beneficial role in improving film quality of the bismuth based perovskite variant. To this end, we introduce phenethylammonium (PEA) cations to achieve $(PEA)_3Bi_2I_9$ as a new class of bismuth halide material to achieve a film with considerably high coverage upon the substrate, Figure 1 (a) and (b). Single-crystals of the $(PEA)_3Bi_2I_9$ have been synthesized and analysed for this new material which reveals at room temperature, $(PEA)_3Bi_2I_9$ has a monoclinic crystal system with space group of P21/n with a zero dimensional characteristic Figure 1(c) with isolated $Bi_2I_9^{3-}$ octahedrals, Figure 1 (d). Using UV-Vis measurement indicates band gap of 2.23 eV, Figure 1 (e). Thin film of mesoporous structure devices containing $(PEA)_3Bi_2I_9$ as the active layer confirm the supremacy of this material over $MA_3Bi_2I_9$ by showing better proof of contents for the final photovoltaic results depicted in Figure 1 (f) and summarized in Table 1.

Table I. Various device parameters of best performing devices with $MA_3Bi_2I_9$ and $(PEA)_3Bi_2I_9$ perovskites as active layer in FTO/ C-TiO_2/ Perovskite/ P3HT/ Au structure

Active Layer	J_{sc}(mA/cm^2)	V_{oc} (V)	FF	PCE(%)
$MA_3Bi_2I_9$	0.406	0.515	0.44	0.092
$(PEA)_3Bi_2I_9$	0.814	0.614	0.46	0.230

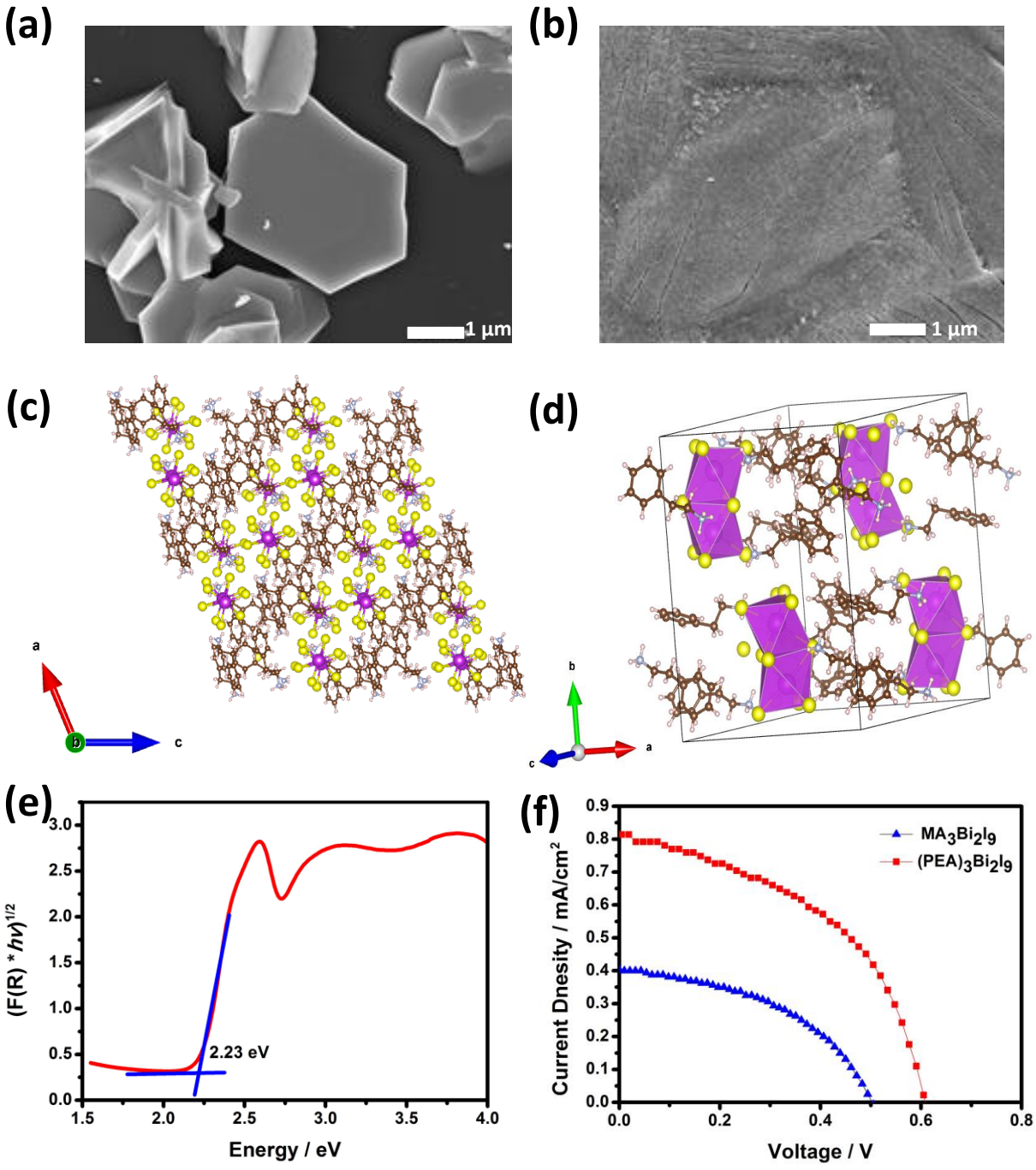

Figure 1. SEM images of (a) $MA_3Bi_2I_9$, (b) $(PEA)_3Bi_2I_9$ on FTO, (c) Three dimensional and (d)local structure of the Crystal structure of $Bi_2I_9^{3-}$, octahedrons and organic $C_8H_{12}N^+$ $(PEA)^+$ cation, (e) Energy band gap of $(PEA)_3Bi_2I_9$, $(PEA)_3Bi_2Br_9$ and $(PEA)_4Bi_2Cl_{10}$ film on FTO using the transmission-mode ultraviolet-visible, (f) J–V curve of the best performing devices with $MA_3Bi_2I_9$ and $(PEA)_3Bi_2I_9$ as the active layer