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Supplementary Information

Enhanced Photocurrent in Heterostructures Formed between $CH_3NH_3PbI_3$ Perovskite Films and Graphdiyne†

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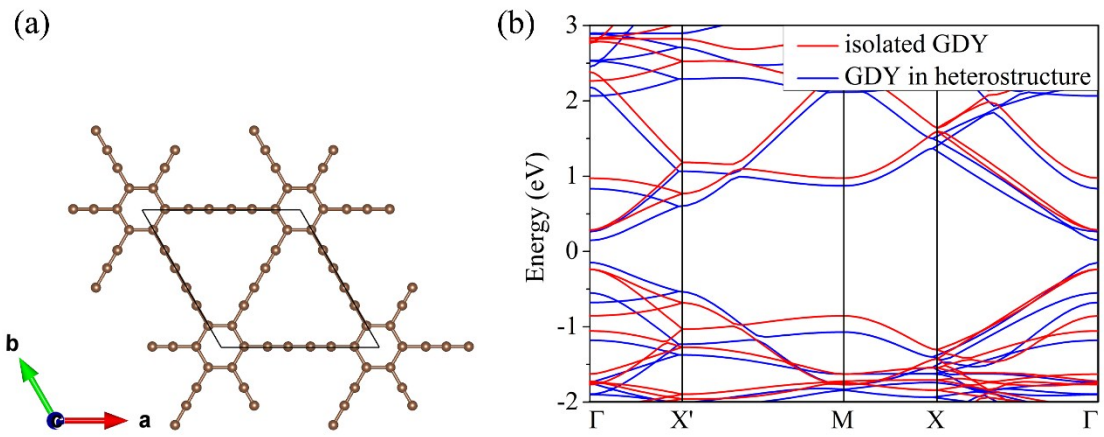

Fig. S1 (a) Optimized stable primitive cell structure of GDY; (b) Band structures of isolated GDY and GDY in heterostructure correspond to the 1x$\sqrt{3}$ GDY supercell constructed by $\vec{a}+\vec{b}$ and $\vec{a}-\vec{b}$ of the primitive cell.

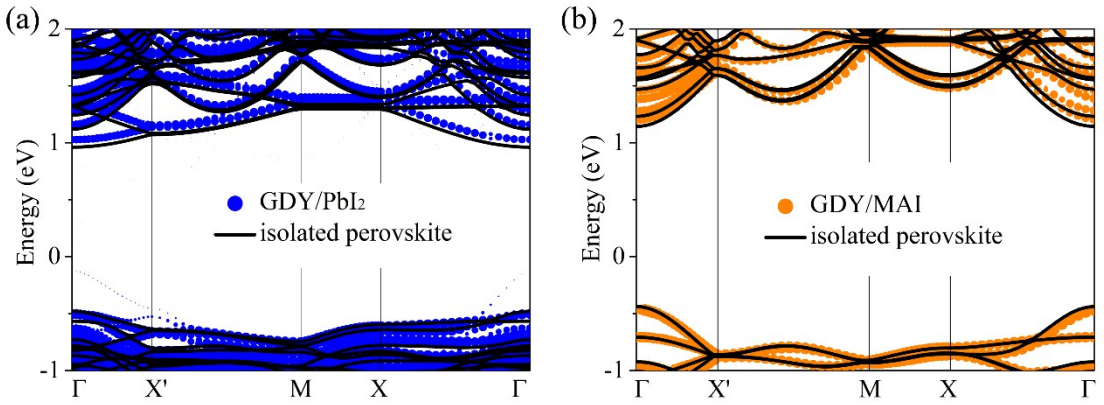

Fig. S2 Projected band structure of perovskite slab in the GDY/PbI_2 (a) and the GDY/MAI (b) heterostructures compared to isolated perovskite slab. The size of the symbol indicates the contribution weight.

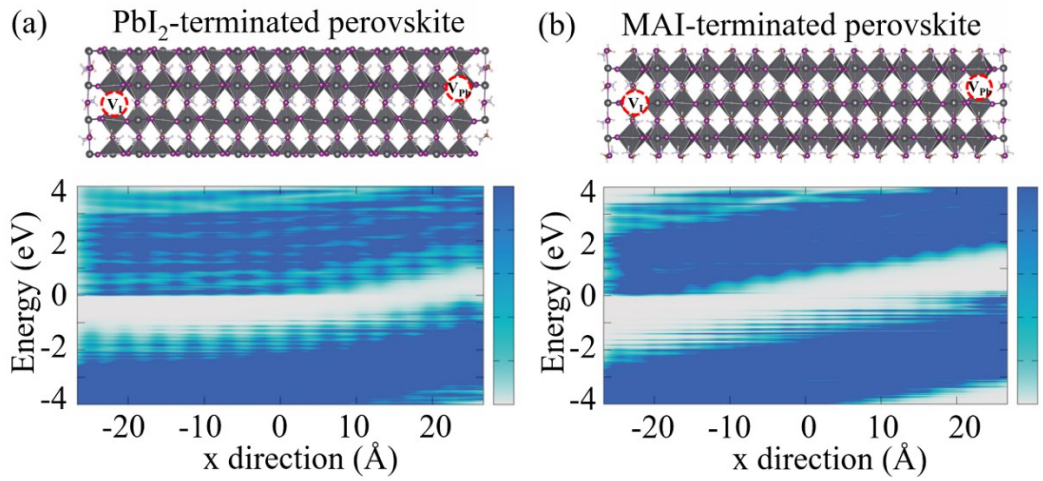

Fig. S3 (a) The structure of p-n heterojunction (top panel) and the LDOS in transport direction (bottom panel) of PbI_2-terminated surface; (b) The structure of p-n heterojunction (top panel) and the LDOS in transport direction (bottom panel) of MAI-terminated surface.

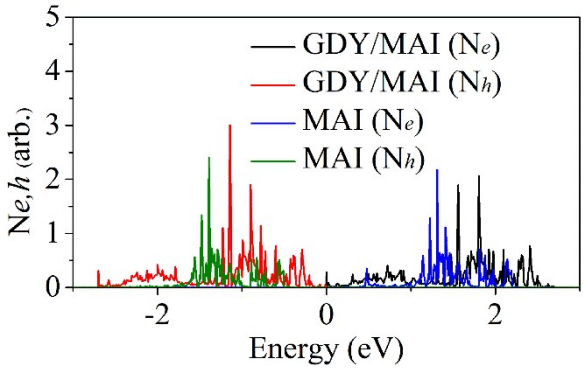

Fig. S4 The number of photogenerated electrons and holes on the energy level E in the MAI-terminated system.