Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information for:

Electronic implications of organic nitrogen lone pairs in lead iodide perovskites

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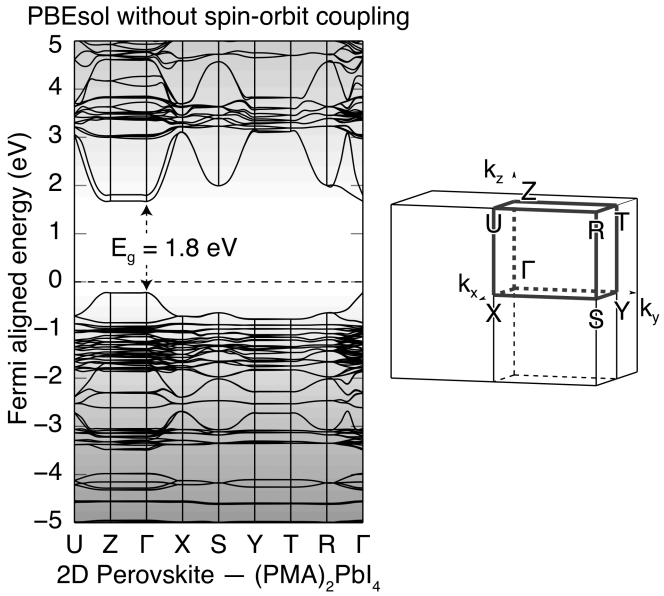

Figure S1 The calculated electronic band structure of $(PMA)_2PbI_4$, sampling the complete Brillouin zone.

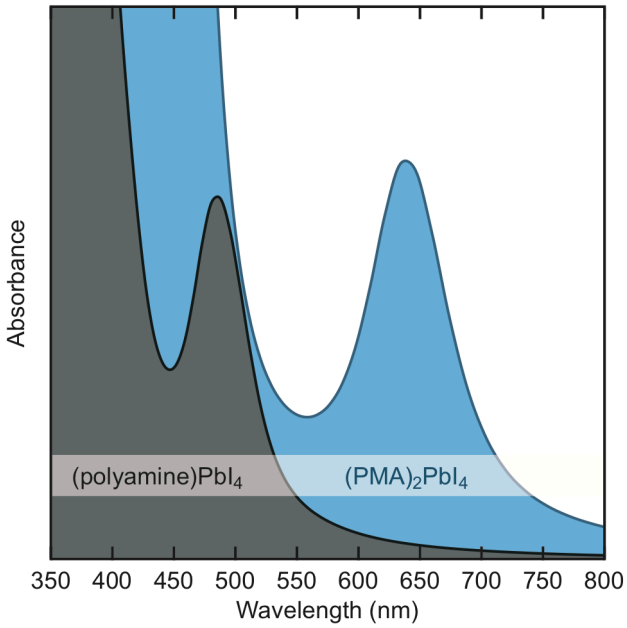

Figure S2 The calculated (PBEsol+SOC) optical absorption spectra of (polyamine)PbI_4 and $(PMA)_2PbI_4$. The absorption onset is blue-shifted by ~200nm owing to the increased band gap of the former. The contribution from N-states is not apparent in the optical spectra, but rather the significantly increased effective mass of holes.