

Supporting Information

Beneficial Effects of Tensile Strain on Charge Carrier Lifetime in Metal Halide Perovskites Containing Halogen Vacancies

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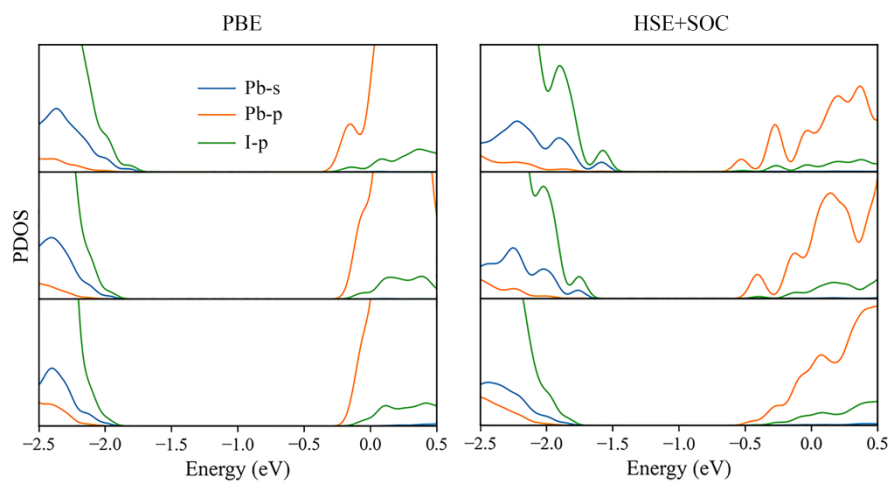


Figure S1. Projected density of states (PDOS) calculated using GGA-PBE and HSE+SOC calculations for **(top)** I_v , **(middle)** $I_v@2.5\%$, **(bottom)** $I_v@5\%$ systems, respectively.

Table S1. The calculated energy levels of VBM, trap, and CBM using PBE and HSE+SOC level of theory.

| | | Eg (eV) | |
|----------------------|------|---------|---------|
| | | PBE | HSE+SOC |
| I _v | VBM | 0.94 | 0.67 |
| | trap | 2.57 | 2.34 |
| | CBM | 2.75 | 2.59 |
| I _v @2.5% | VBM | 0.31 | 0.04 |
| | trap | 2.17 | 1.91 |
| | CBM | 2.21 | 2.05 |
| I _v @5% | VBM | -0.13 | -0.39 |
| | trap | 1.75 | 1.65 |
| | CBM | 1.78 | 1.73 |