# Supporting Information for

# Theoretical Screening of Lead-Free Hybrid Organic–Inorganic Halide Double Perovskites for Solar Cells

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**Table S1.** Benchmarked functional test, including the GGA-level PBE, PBEsol and PW91 and the hybrid-level PBE0 and HSE06 with and without the SOC effect on calculating the band gaps of traditional $FAPbI_3$.

| Functional | w/o SOC | w/ SOC |
|---|---|---|
| PBE | **1.53 eV** | 0.47 eV |
| PBEsol | 1.37 eV | 0.30 eV |
| PW91 | **1.42 eV** | 0.34 eV |
| HSE06 | 2.00 eV | 0.93 eV |
| PBE0 | 2.61 eV | **1.53 eV** |
| Exp. [Ref.] | 1.47eV | |

Ref. F. Ma, J. Li, W. Li, N. Lin, L. Wang and J. Qiao, *Chem. Sci.*, 2017, 8, 800-805

**Table S2.** Comparisons of the band gaps of 11 stable OIHDPs under the PBE and PBE0+SOC functional.

| OIHDPs | PBE | PBE0+SOC |
|---|---|---|
| $FA_2AuAuF_6$ | 1.12 eV | 1.77 eV |
| $MA_2AuSbCl_6$ | 1.36 eV | 2.14 eV |
| $MA_2AgSbI_6$ | 1.43 eV | 2.10 eV |
| $MA_2AuSbI_6$ | 1.54 eV | 2.03 eV |
| $FA_2AgAuBr_6$ | 0.17 eV | 1.20 eV |
| $MA_2AgAuF_6$ | 0.25 eV | 0.24 eV |
| $MA_2AgAuI_6$ | 0.34 eV | 0.99 eV |
| $MA_2AgAuBr_6$ | 0.35 eV | 1.23 eV |
| $FA_2AgAuF_6$ | 0.43 eV | 0.90 eV |
| $MA_2AgAuCl_6$ | 0.44 eV | 1.45 eV |
| $FA_2AgAuCl_6$ | 0.53 eV | 1.84 eV |