Supporting Information

Interfacial electronic and vacancy defect engineering coupling of Z-scheme $CsSnBr_3/SnS_2$ heterostructure for photovoltaic performance: a hybrid DFT study

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Supporting Figures

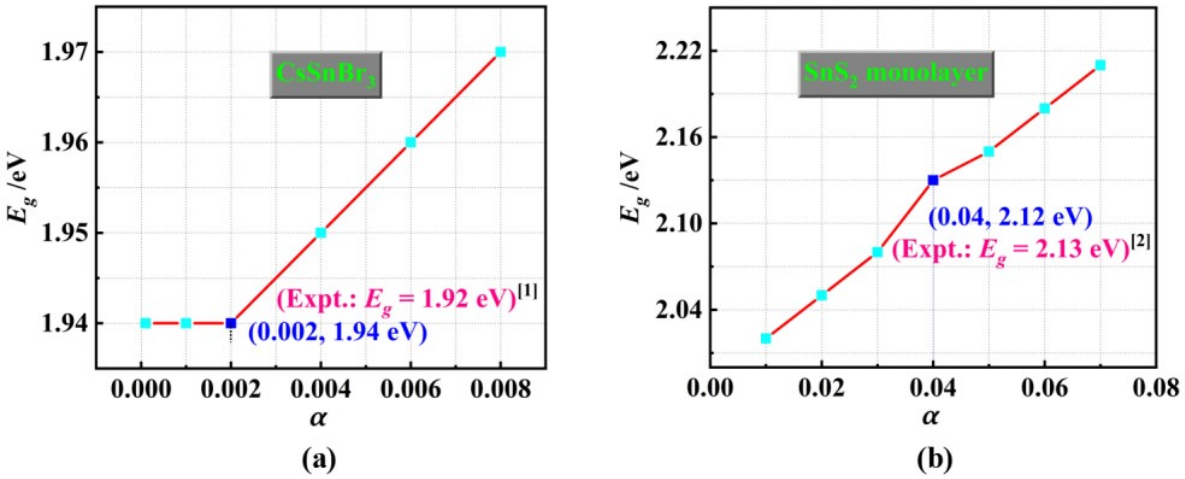

Fig. S1. The calculated band gap concerning different α parameters: (a) $CsSnBr_3$ and (b) SnS_2 monolayer.

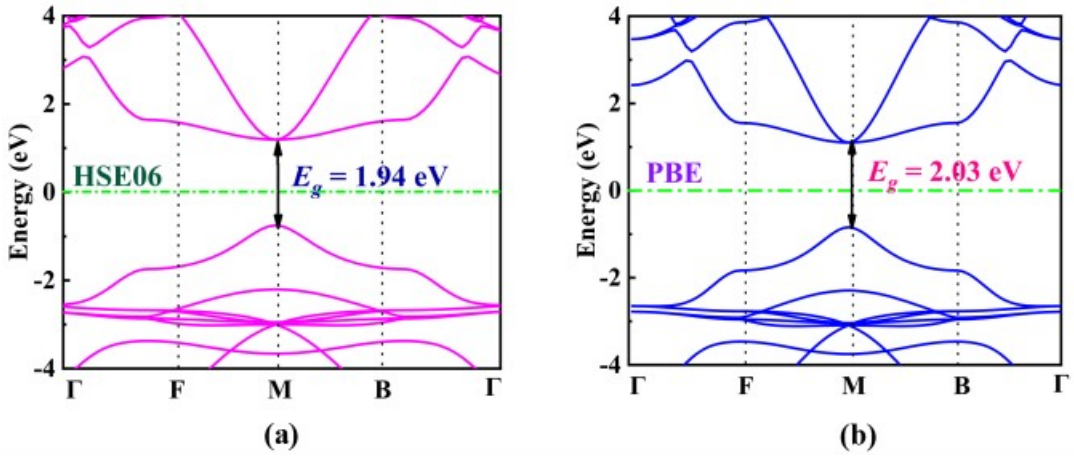

Fig. S2. Calculated energy band structure of $CsSnBr_3$ bulk using HSE06 and GGA-PBE method, respectively.

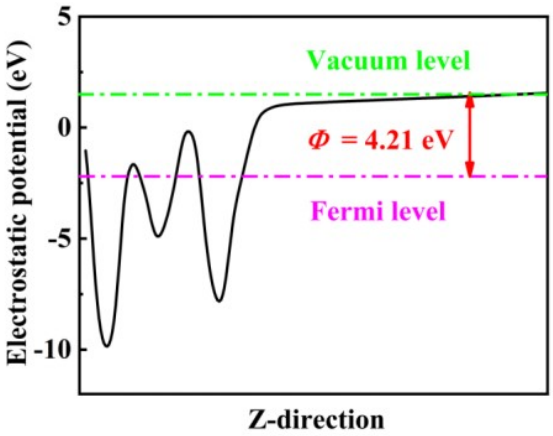

Fig. S3. Calculated work function of V_{Br}-$CsSnBr_3$ (001) surface.

References

[1] B.H. Li, R.Y. Long, Y. Xia and Q.X. Mi. *Angew Chem*. 2018, **130**, 13338-13342.

[2] S.K. Arora, D.H. Patel and M.K. *Res. Technol*. 1993, **28**, 623-627.