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

Supporting Information for

Electronic and optical properties of Janus Ga_2STe bilayer: A promising candidate for excitonic solar cell

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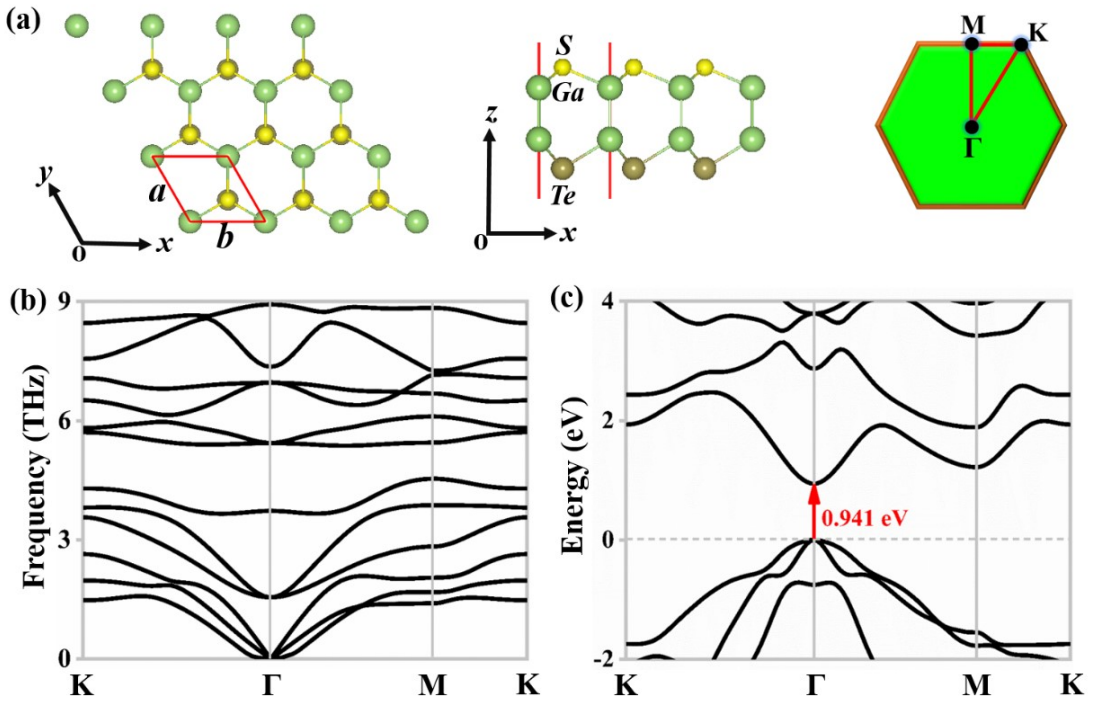

Fig. S1 (a) Top and side views of Janus Ga_2STe monolayer and high-symmetry directions of first Brillouin zone. Green, yellow, and brown spheres show the Ga, S, and Te atoms, respectively. (b)-(c) Phonon spectrum and band structure of Janus Ga_2STe monolayer at DTF-PBE level.

Table S1 The calculated lattice constant (*a*/*b*), bond lengths ($l_{S\text{-}Ga}$, $l_{Ga\text{-}Ga}$, $l_{Ga\text{-}Te}$), effective thickness (*h*) for Ga_2STe monolayer, and bandgap at PBE level. Length and energy units are Å and eV, respectively.

Name	*a*/*b*	$l_{S\text{-}Ga}$	$l_{Ga\text{-}Ga}$	$l_{Ga\text{-}Te}$	*h*	E_g
This work	3.881	2.438	2.455	2.628	4.789	0.941
Other work	3.899[1]	2.446[1]	2.468[1]	2.639[1]	4.802[1]	0.912[1]
	3.890[2]	2.470[2]	2.450[2]	2.640[2]		
	3.901[3]	2.471[3]	2.450[3]	2.642[3]		

Table S2 The calculated lattice constants *a*/*b* (Å), interlayer equilibrium distance d_0 (Å), blinding energies E_b (meV/Å^2), and bandgap E_g^{PBE} (eV) of eight high-symmetry stacking configurations for Janus Ga_2STe bilayer.

Name	AA_1	AA_2	AA_3	AA_4	AB_1	AB_2	AB_3	AB_4
a/*b*	3.923	3.926	3.922	3.923	3.927	3.923	3.923	3.926
d_0	3.983	3.736	3. 937	4.055	3.704	3.990	3. 879	3.424
E_b	−13.77	−14.40	−14.07	−13.15	−14.66	−13.76	−14.22	−14.76
E_g^{PBE}	0.533	0.563	1.070	0.979	0.562	0.532	0.977	1.066

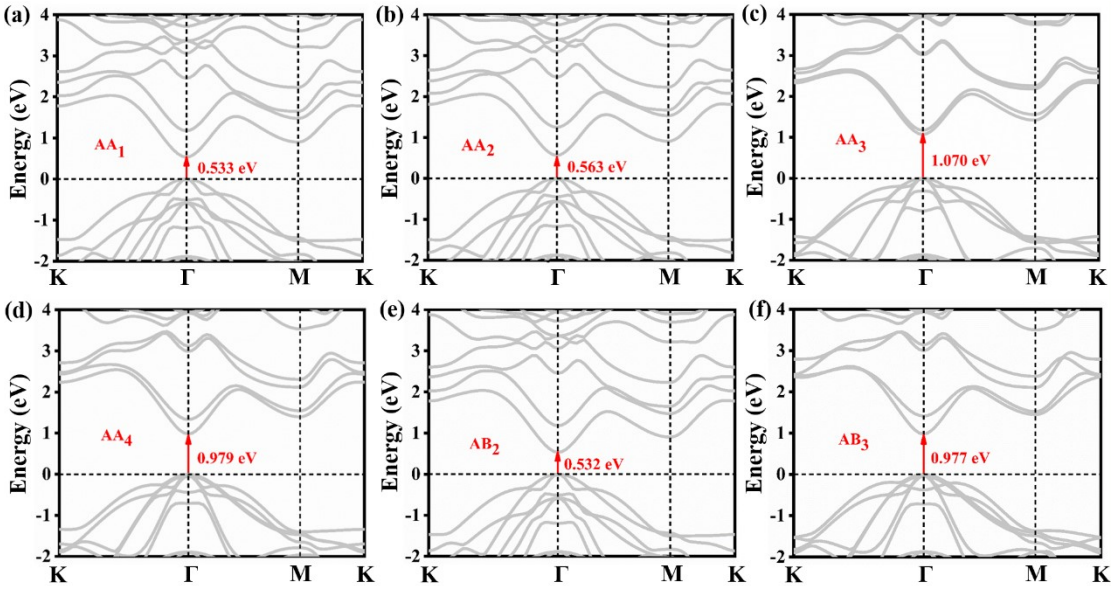

Fig. S2 Band structures of Ga_2STe bilayers with different stacking configurations at the

DFT-PBE level: (a) AA_1, (b) AA_2, (c) AA_3, (d) AA_4, (e) AB_2, (f) AB_3.

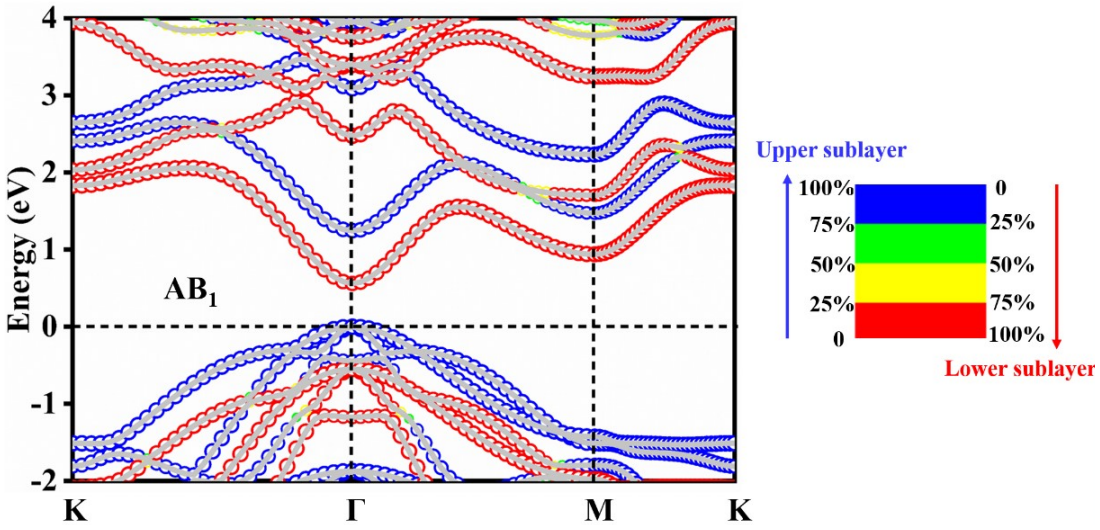

Fig. S3 Projected band structure of Ga_2STe bilayer with AB_1 stacking configuration.

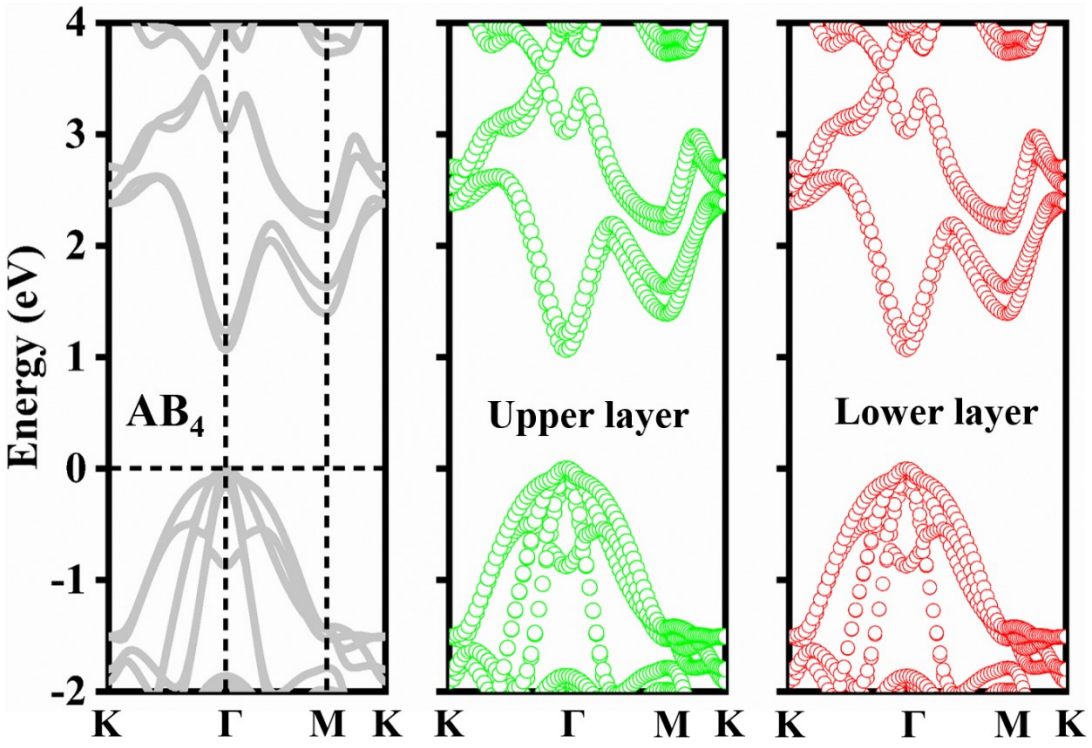

Fig. S4 Band structure of Ga_2STe bilayer with AB_4 stacking configuration and the contribution of constituent layer. The contribution of constituent layer to every energy band is equivalent.

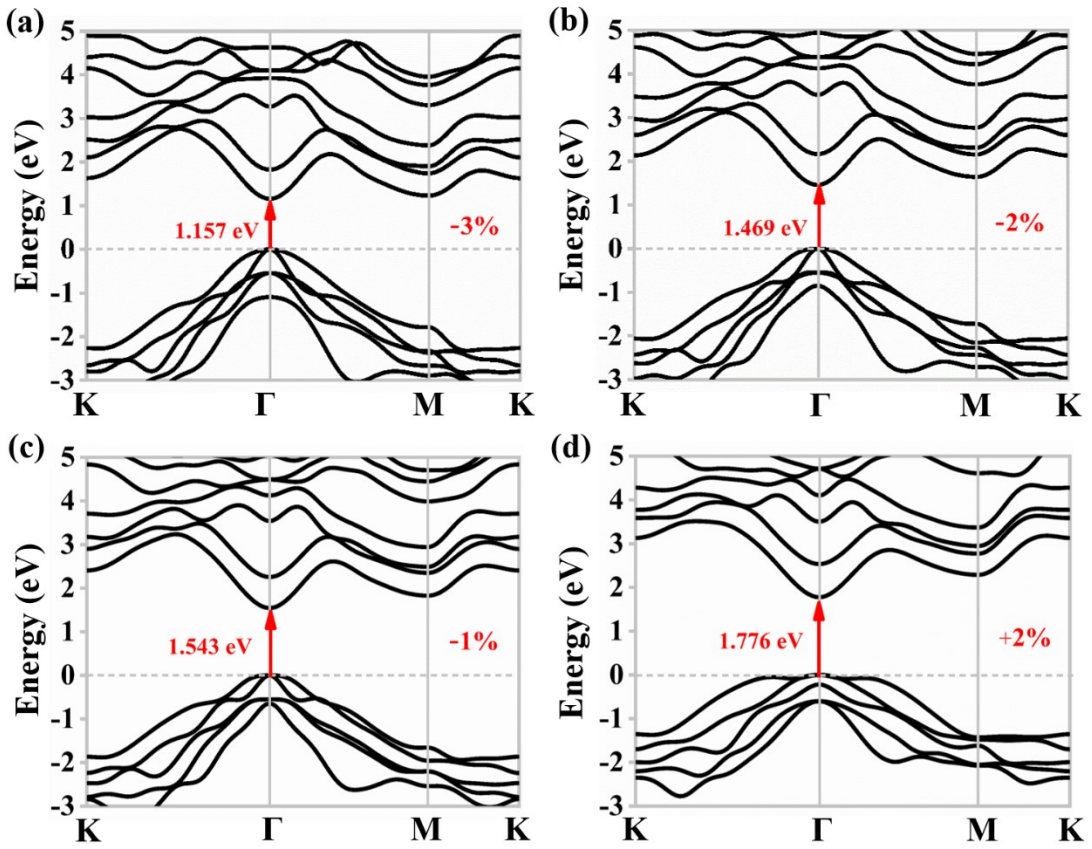

Fig. S5 Quasi-particle band structures of Ga_2STe bilayers with AB_1 configuration at G_0W_0 level under different biaxial strains: (a) −3%, (b) −2%, (c) −1%, (d) +2%.

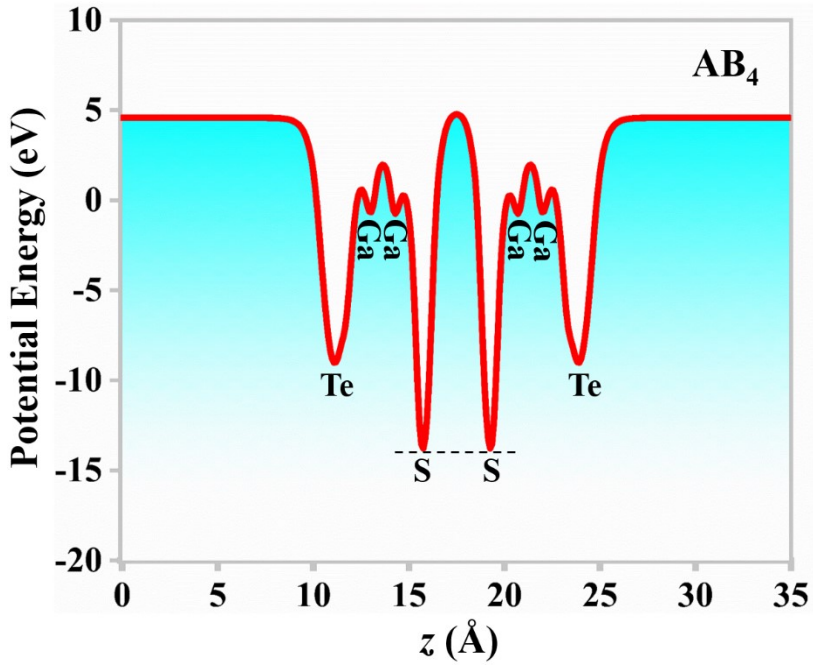

Fig. S6 Plane averaged electrostatic potential profiles across the interface of the AB_4

Ga_2STe bilayer.

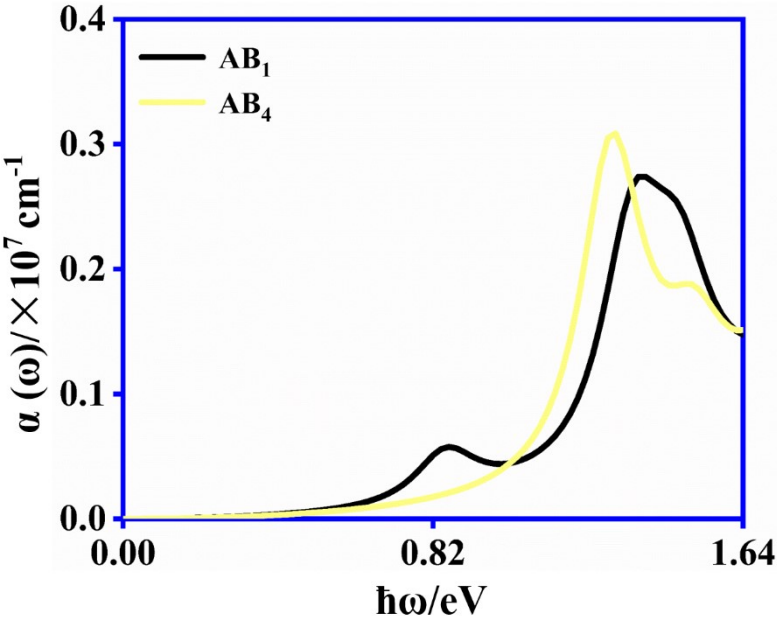

Fig. S7 Light absorption coefficient $\alpha(\omega)$ of Ga_2STe bilayers with AB_1 and AB_4 configurations as a function of photon energy ($\hbar\omega$).

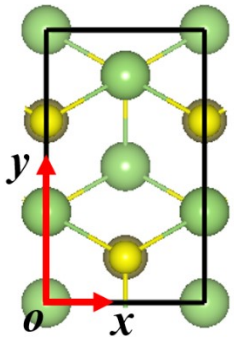

Fig. S8 An orthogonal supercell of Ga_2STe bilayer with AB_1 configuration.

References

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