Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Two Janus Ga_2STe monolayers: Electronic, optical, and photocatalytic properties

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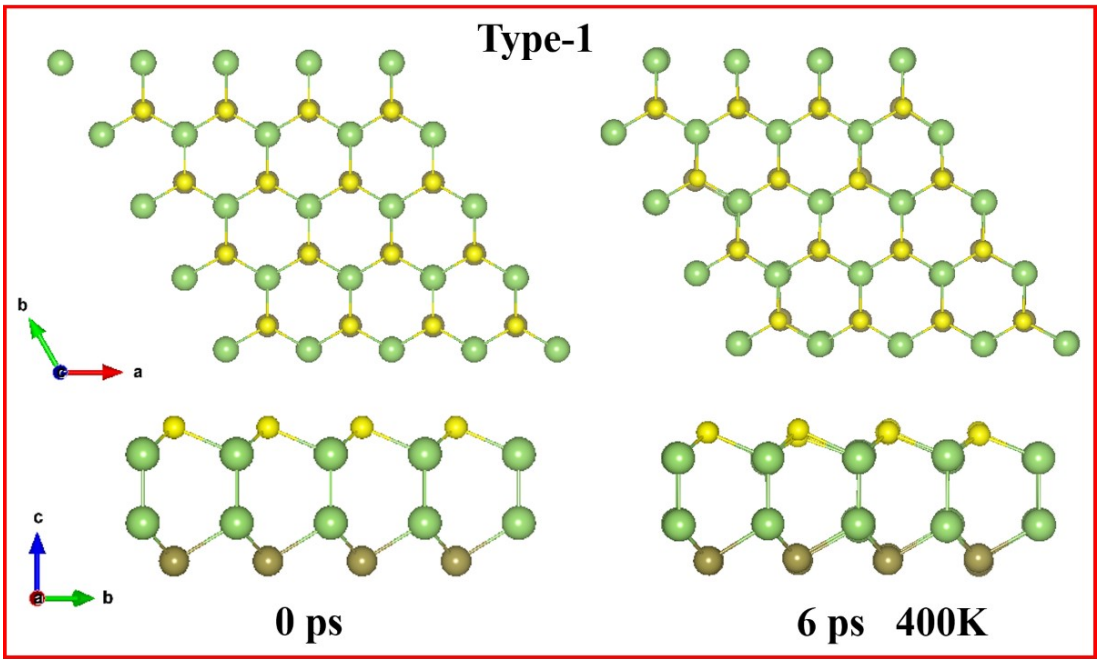

Fig. S1 Top and side views of Janus Ga_2STe monolayer with type-1 configuration at 0 ps and 6 ps at the temperature of 400 K.

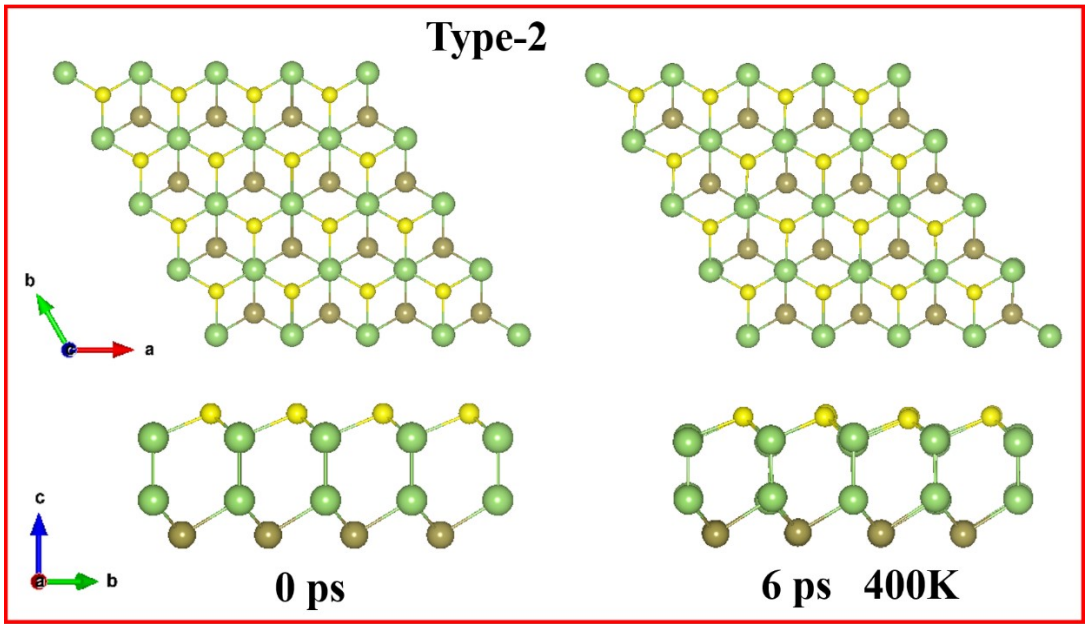

Fig. S2 Top and side views of Janus Ga_2STe monolayer with type-12 configuration at 0 ps and 6 ps at the temperature of 400 K.

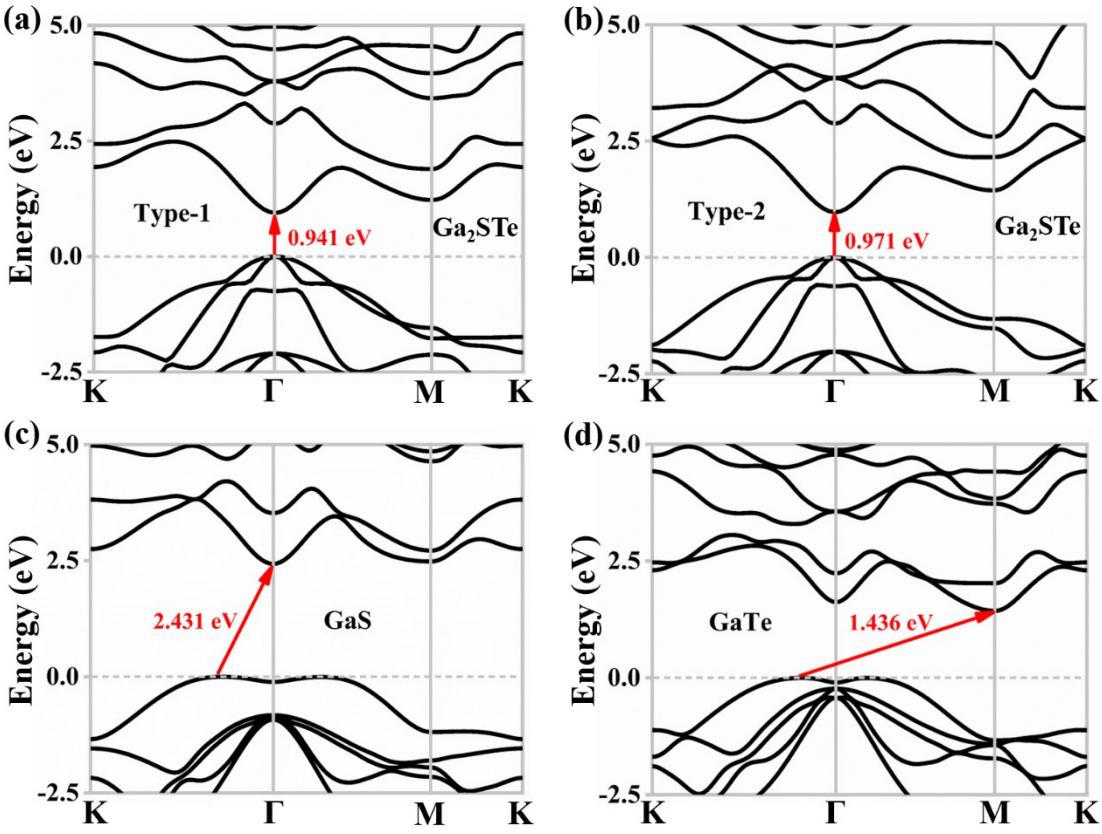

Fig. S3 Band structures of Janus Ga_2STe (a-b), GaS (c), and GaTe (d) monolayers at the PBE level.

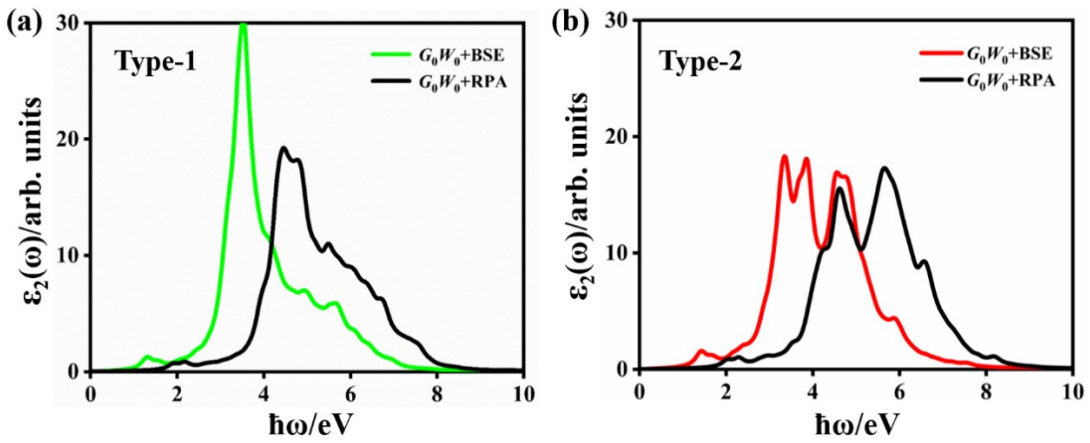

Fig. S4 (a)-(c) Imaginary parts of the dielectric functions of Janus Ga_2STe monolayers with the type-1 and type-2 configurations at the G_0W_0+RPA and G_0W_0+BSE methods. The ***a***-polarized lights are applied in these calculations.

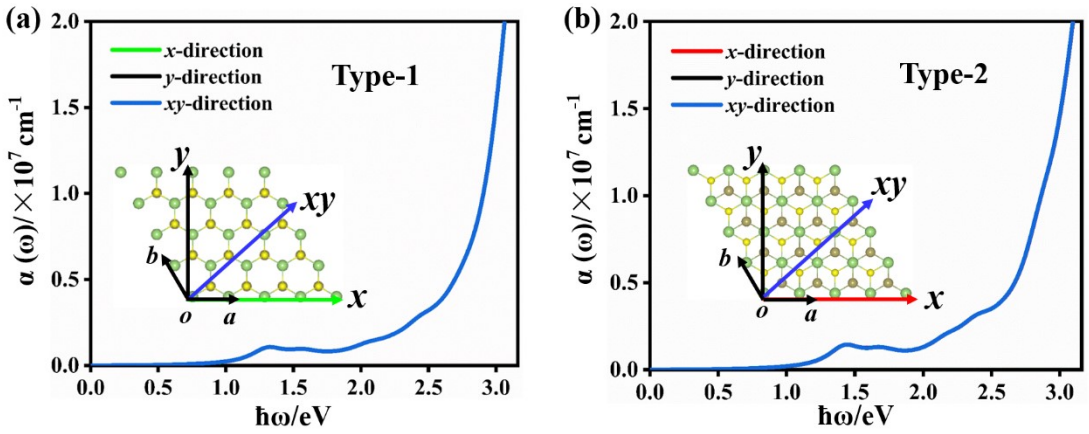

Fig. S5 Light absorption coefficient α (ω) of two Janus Ga_2STe monolayers under different photon energy ħω along three different polarized directions: (a) Type-1, (b) Type-2. The electron-hole interaction has been included in two Janus Ga_2STe monolayers by the G_0W_0+BSE method.

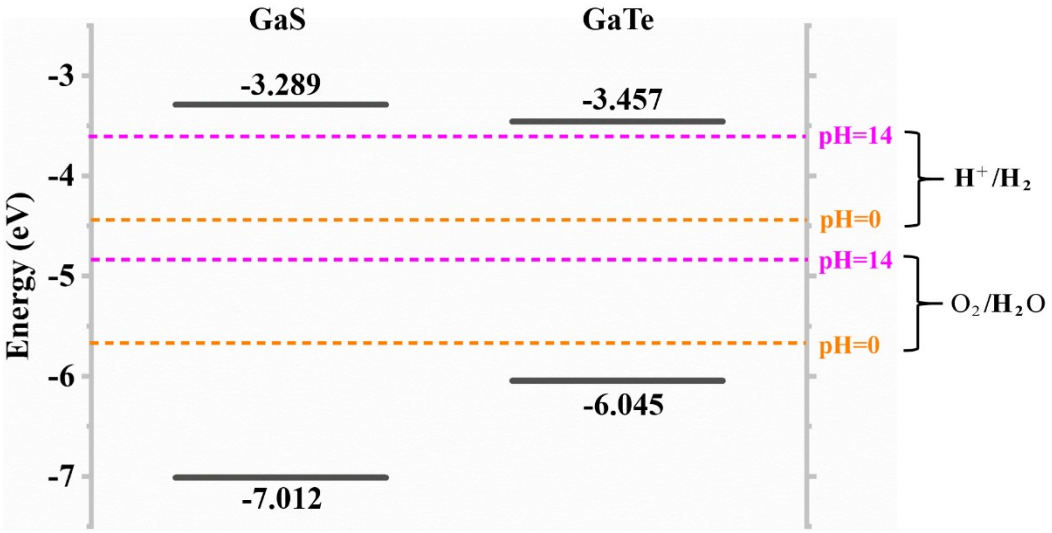

Fig. S6 Band edge alignments of the GaS and GaTe monolayers with respect to the water redox potentials at different pH values according to the G_0W_0 method.