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

Supplementary materials for "Exploring the Photocatalytic Properties and Carrier Dynamics of 2D Janus XMMX′ (X=S, Se; M = Ga, In; and X′ =Te) Materials"

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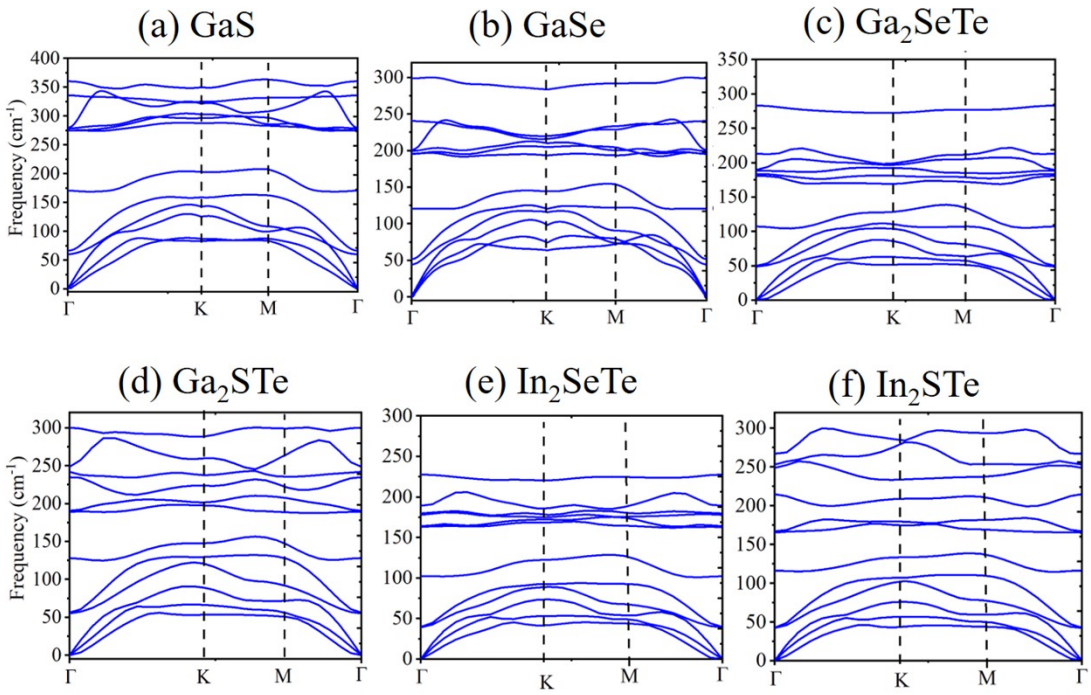

Fig. S1. (a)-(f) the phonon spectra of GaS, GaSe, Ga_2SeTe, Ga_2STe, In_2SeTe and In_2STe, respectively.

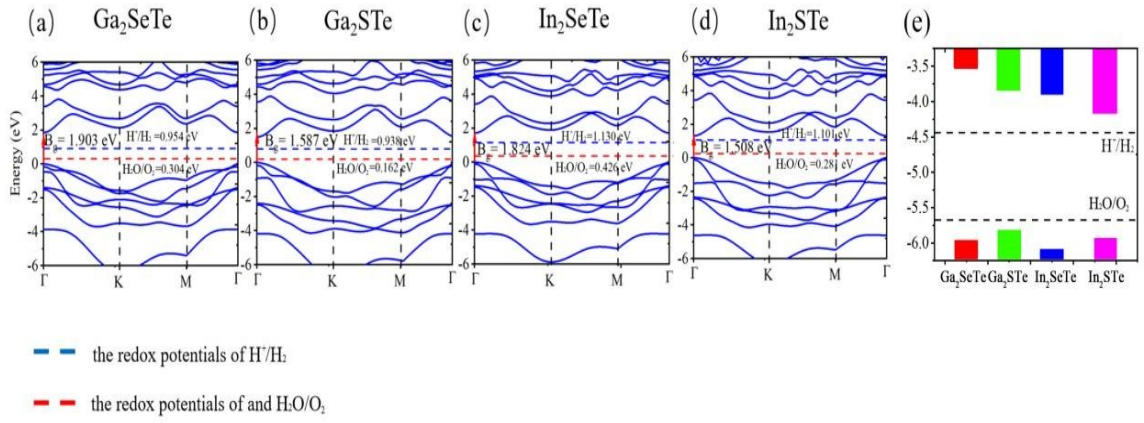

Fig. S2. (a)-(d) The band structures of Ga_2SeTe, Ga_2STe, In_2SeTe and In_2STe calculated by DFT with XC functional HSE06, compared with the standard redox potentials for water splitting shown as pink dashed lines and blue dashed lines, respectively. (e) the GW calculated band edge of Ga_2SeTe, Ga_2STe, In_2SeTe and In_2STe.

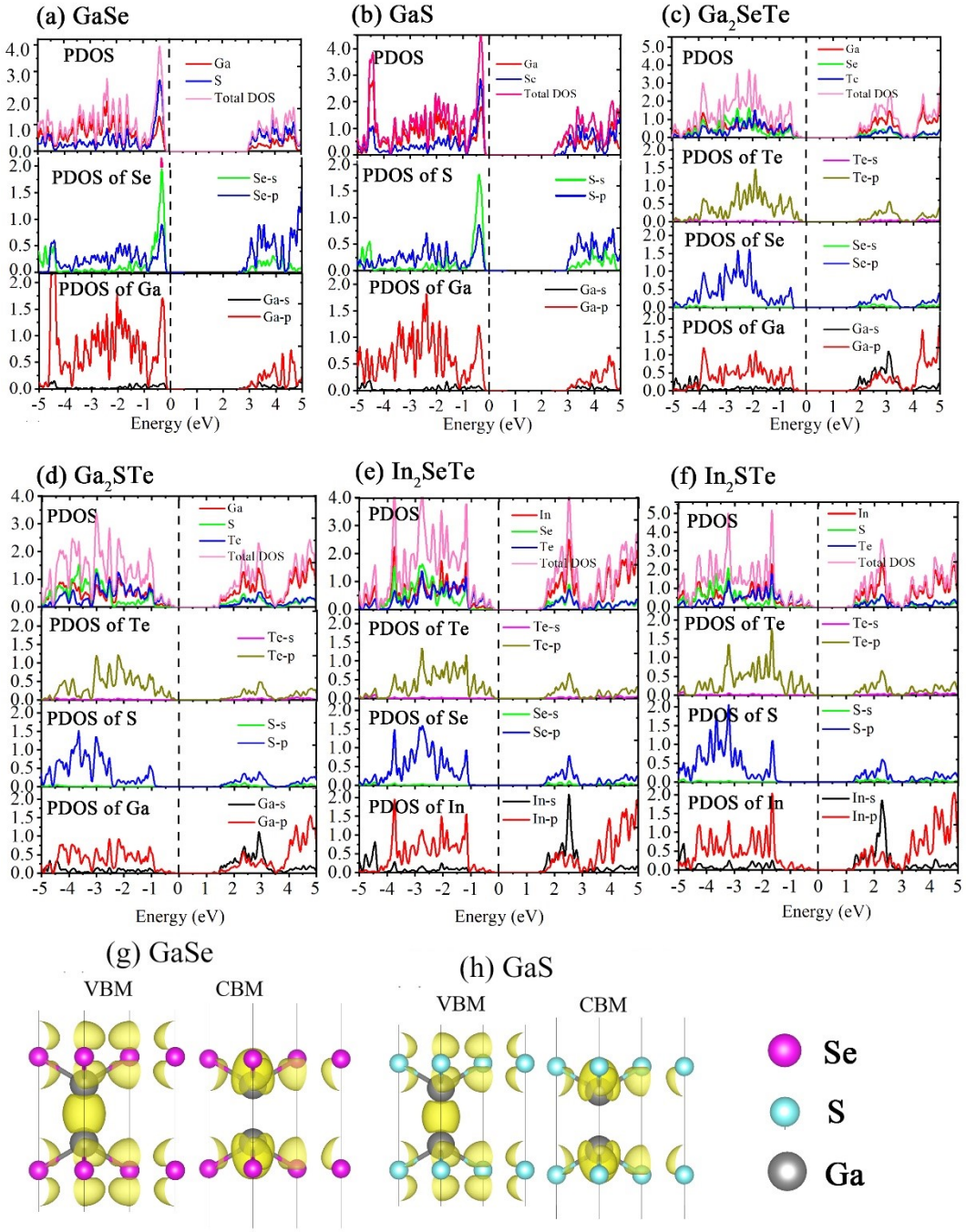

Fig. S3. (a)-(f) The PDOS of Janus XMMX′ and pristine MX monolayers. (g) and (h) charge density of CBM (right) and VBM (left) of GaSe and GaS.

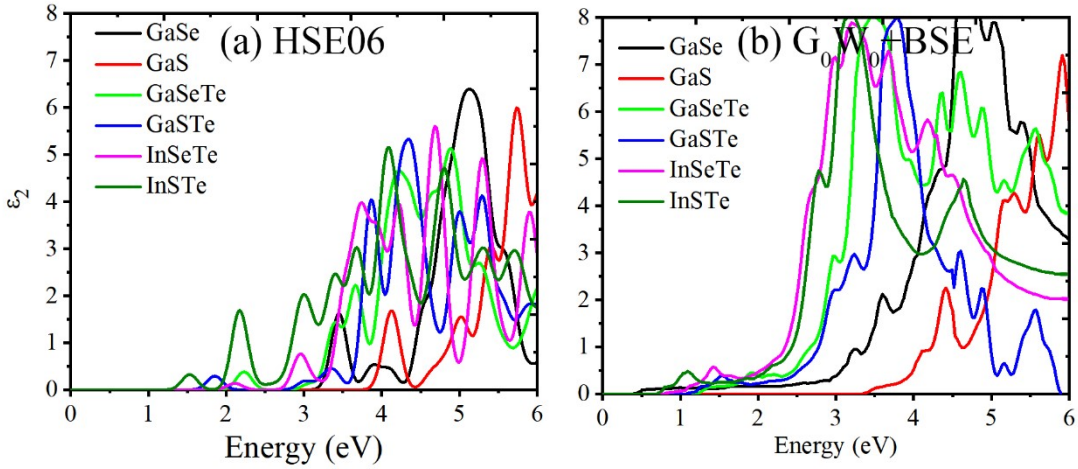

Fig. S4. (a) and (b) Imaginary parts of the dielectric functions of GaSe, GaS, Ga_2SeTe, Ga_2STe, In_2SeTe and In_2STe calculated by the independent particle model with HSE06 and the GW+BSE approach, respectively.

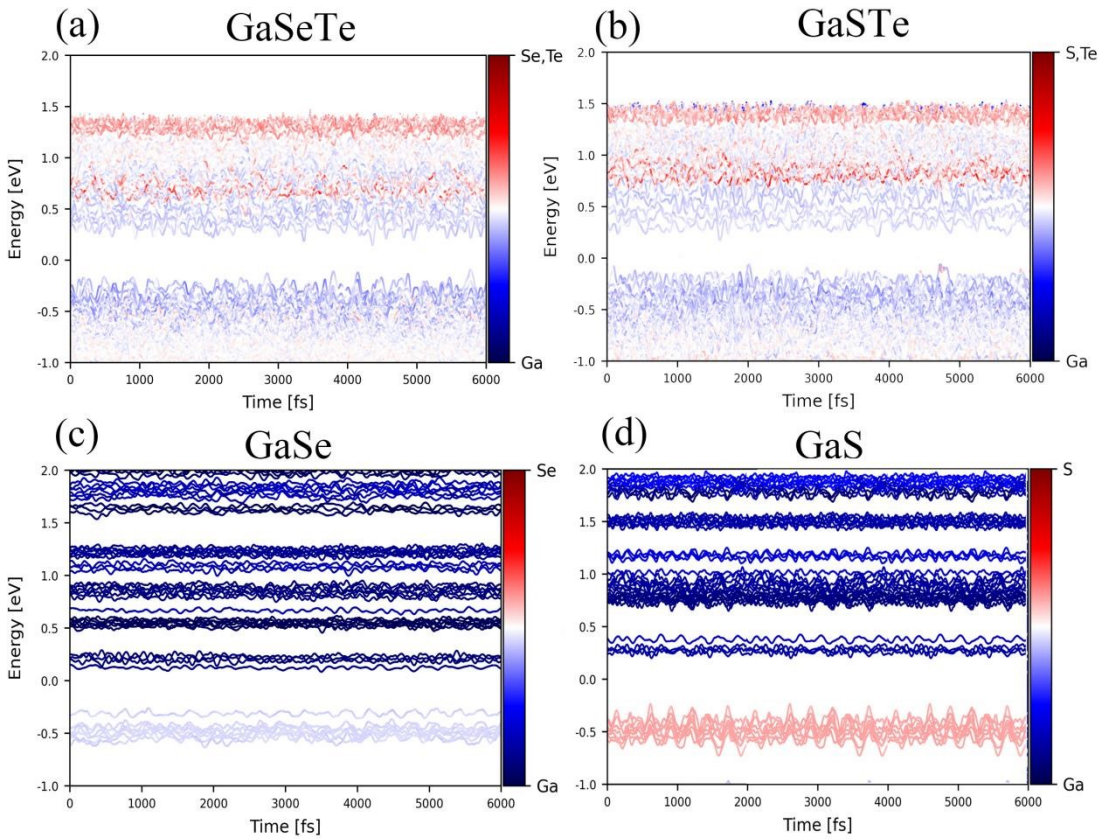

Fig. S5 (a)-(d) Time evolutions of the energy states for the Ga_2SeTe, Ga_2STe, GaSe and GaS, respectively, and the color map indicates the orbital localization. The red lines and blue lines stand for the contribution from X and X′ atoms and M atoms, respectively.

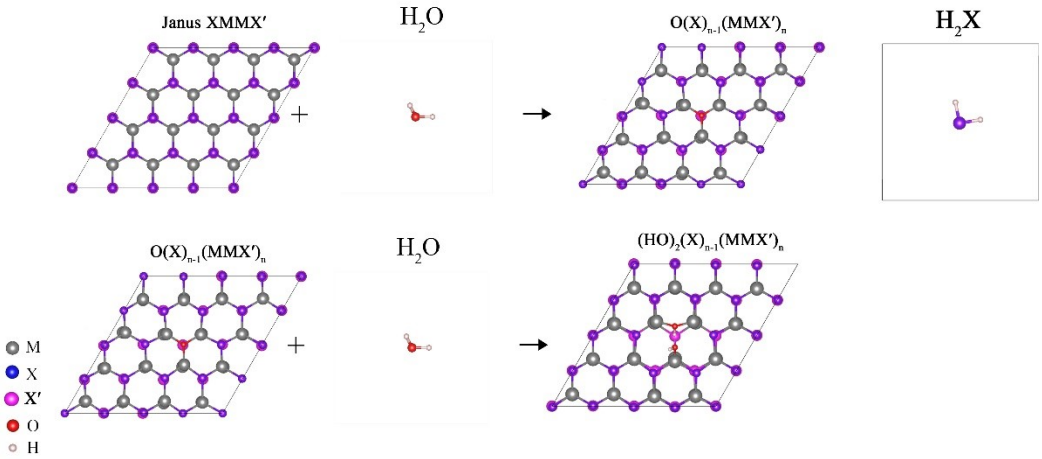

Fig. S6 Diagram of hydration reaction of Janus XMMX′.

Table SI Calculated formation enthalpy, ΔH (in eV), for the hydration reaction of Janus XMMX′. Here $H_A = H_{O(X)_{n-1}(MMX')_n} + H_{H_2S} - H_{XMMX'} - H_{H_2O}$. $H_B = H_{(HO)_2(X)_{n-1}(MMX')_n} - H_{O(X)_{n-1}(MMX')_n} - H_{H_2O}$ and $\Delta H = H_A + H_B$.

	H_A	H_B	ΔH
Ga_2SeTe	49.027	8.7772	57.8042
Ga_2STe	50.431	8.3285	58.7595
In_2SeTe	9.157	6.9261	16.0831
In_2STe	10.932	6.5423	17.4743

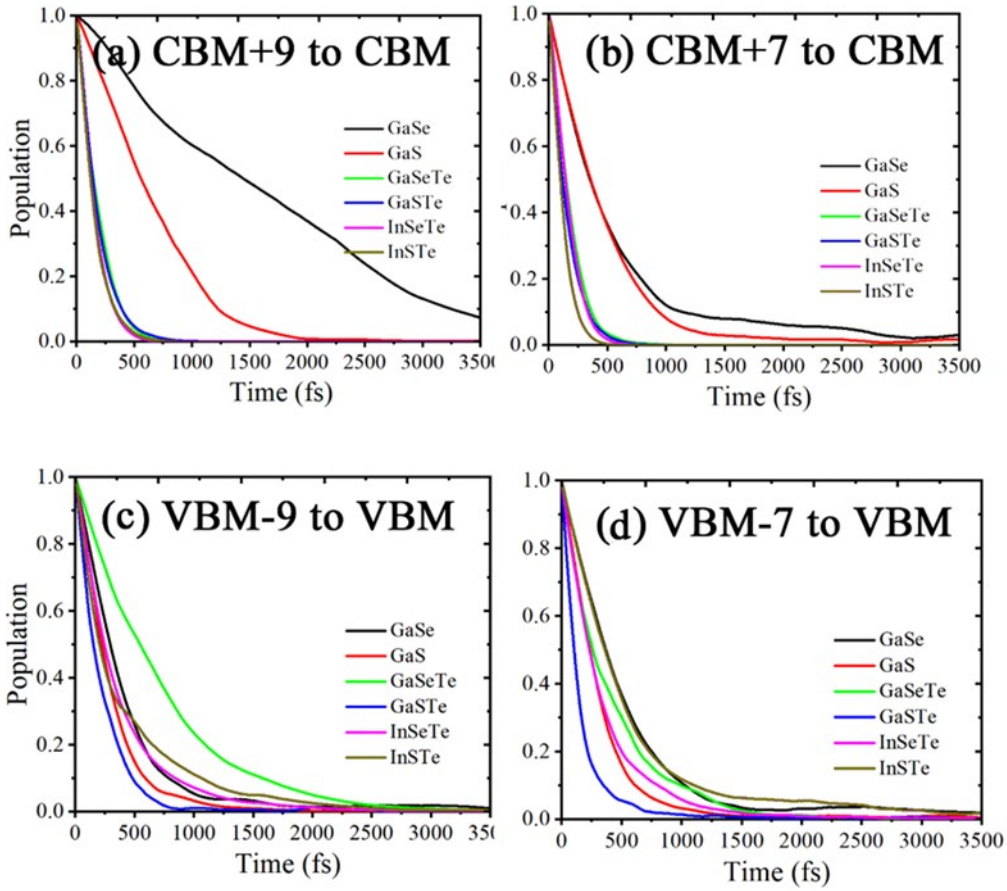

Fig. S7 (a)(b) Electron relaxation dynamics from CBM+9 and CBM+7 to CBM in Janus XMMX′ and pristine MX. (c)(d) Hole relaxation dynamics from VBM-9 and VBM-7 to VBM in Janus XMMX′ and pristine MX.