Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

Janus SMoZAZ'(A=Si,Ge; Z, Z'= N, P, As; Z≠Z') monolayers: potential water-splitting photocatalyst with low carrier recombination rate

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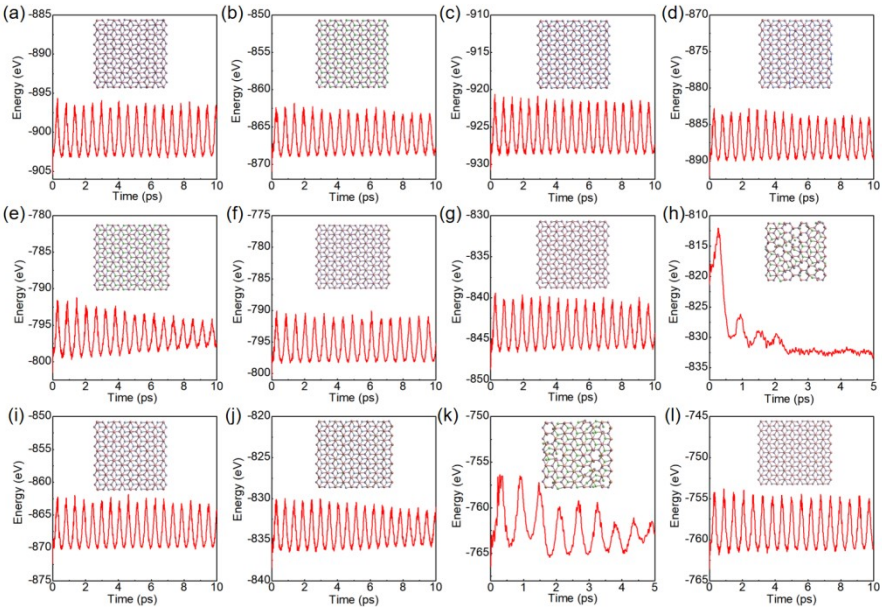

Fig S1 (a-l) Variation of the energy as a function of time for the Janus SMoNSiP, SMoNSiAs, SMoPSiN, SMoAsSiN, SMoPSiAs, SMoAsSiP, SMoNGeP, SMoNGeAs, SMoPGeN, SMoAsGeN, SMoPGeAs, and SMoAsGeP monolayer monolayers at 300K. The insets are the top view of the structure at the end of the AIMD simulation.

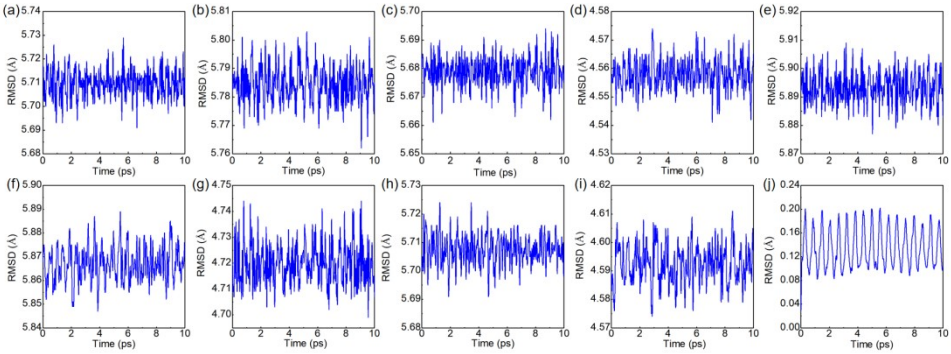

Fig S2 The RMSD variation in AIMD simulation process.

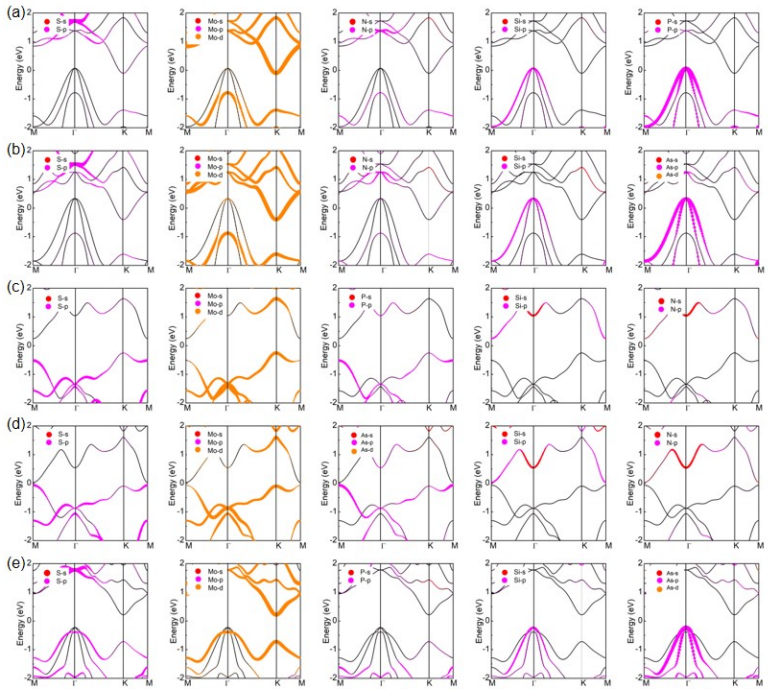

Fig S3 Projected band structure of 2D Janus (a) SMoNSiP, (b) SMoNSiAs, (c) SMoPSiN, (d) SMoAsSiN, and (e) SMoPSiAs.

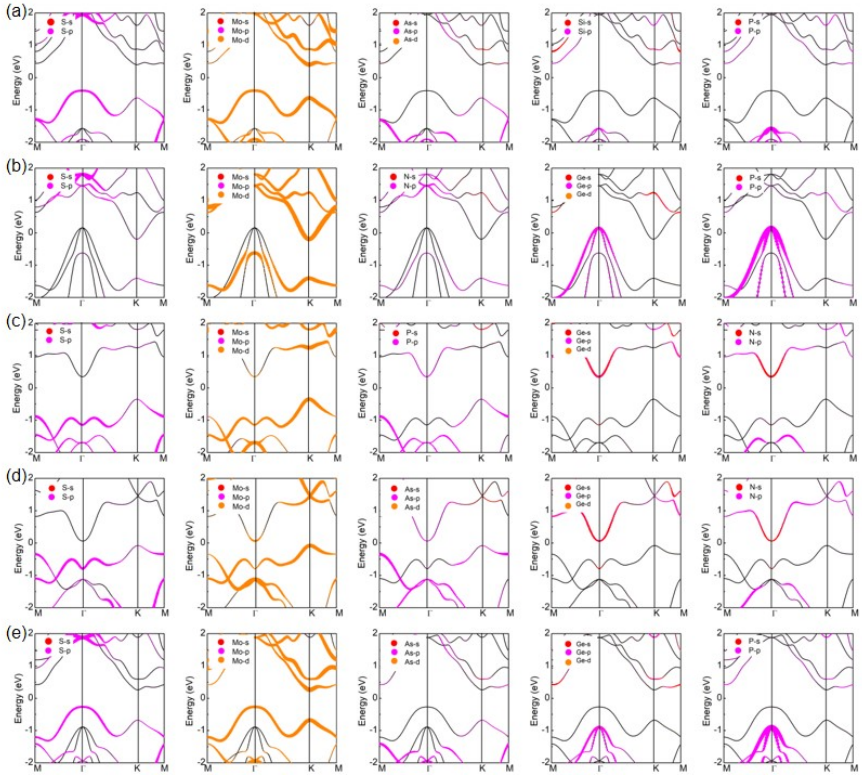

Fig S4 Projected band structure of 2D Janus (a) SMoNGeP, (b) SMoNGeAs, (c) SMoPGeN, (d) SMoAsGeN, and (e) SMoPGeAs.

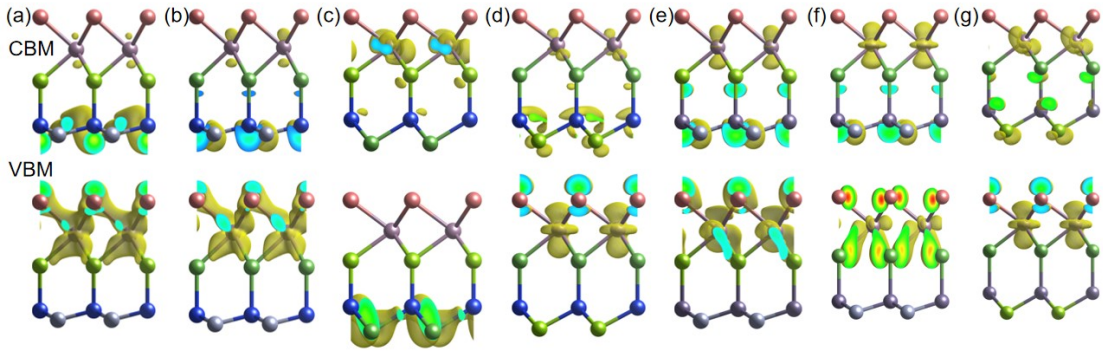

Fig S5 The charge density of the CBM and VBM of (a) SMoPSiN, (b) SMoAsSiN, (c) SMoPSiAs, (d) SMoNGeAs, (e) SMoPGeN, (f) SMoAsGeN and (g) SMoPGeAs monolayers. The isosurface values of SMoZAZ' monolayers are taken as 0.015 eÅ^{-3}.

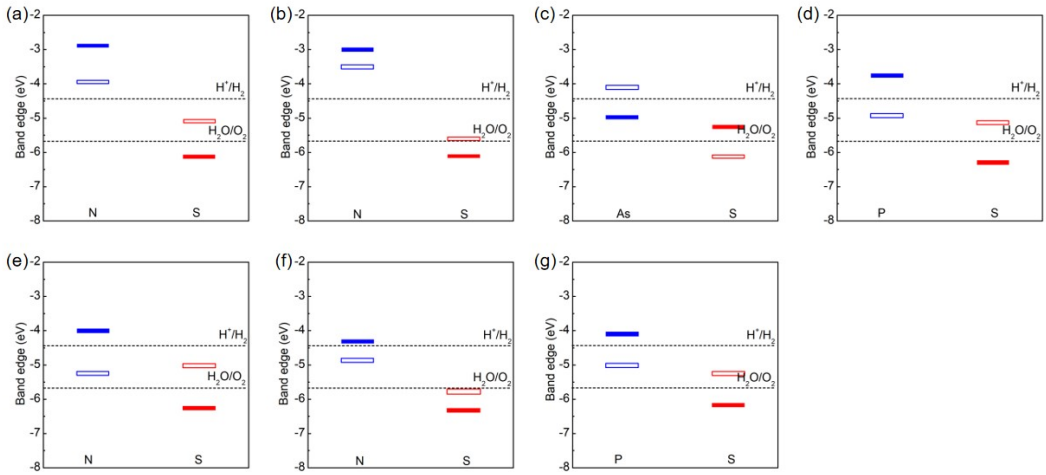

Fig S6 Theoretical band edges with respect to the redox potential of water for (a) SMoPSiN, (b) SMoAsSiN, (c) SMoPSiAs, (d) SMoAsSiP, (e) SMoPGeN, (f) SMoAsGeN and (g) SMoAsGeP monolayers. The hollow rectangle indicates the absence of CBM and VBM, and only the solid rectangles are physically meaningful.

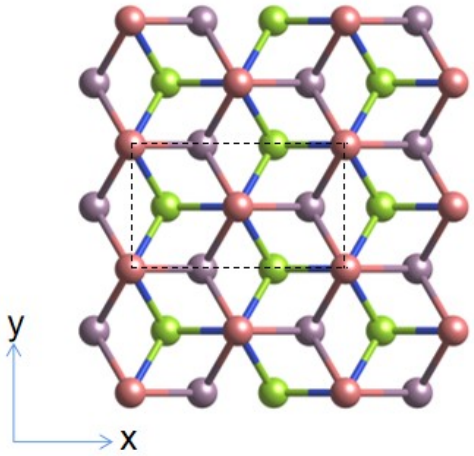

Fig S7 The calculation of carrier mobility is carried out in rectangular cell in the black dotted box, the x and y directions also been indicate.

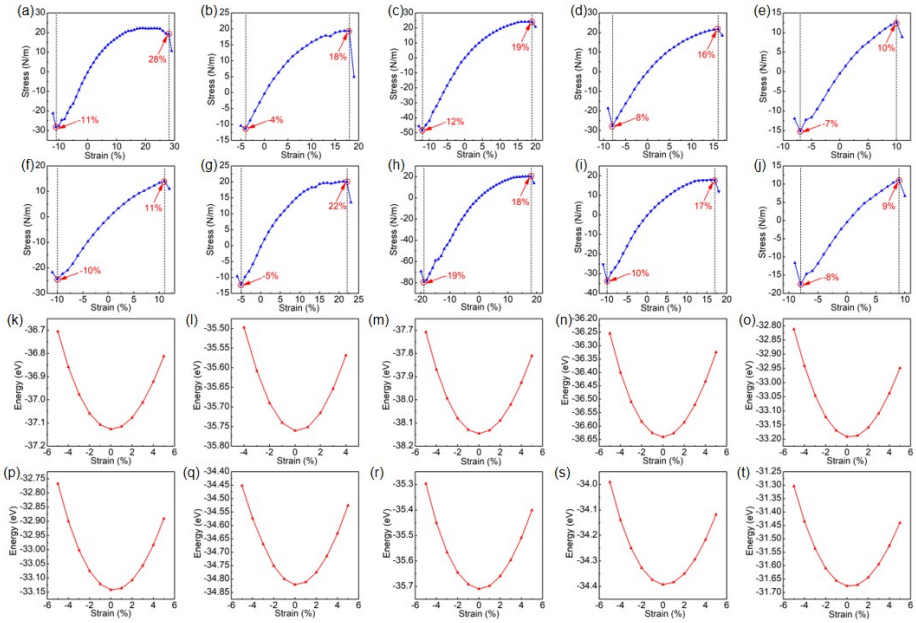

Fig S8 (a-j) Strain-stress curve and (k-t) energy-strain curve for 2D Janus SMoNSiP, SMoNSiAs, SMoPSiN, SMoAsSiN, SMoPSiAs, SMoAsSiP, SMoNGeP, SMoPGeN, SMoAsGeN and SMoAsGeP monolayers.

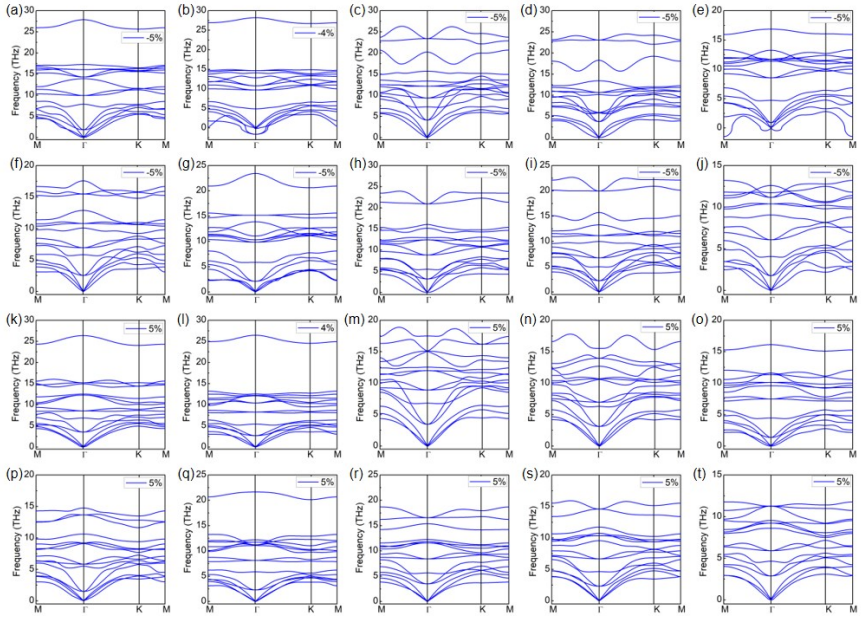

Fig S9 Phonon spectrum of SMoNSiP, SMoPSiN, SMoAsSiN, SMoPSiAs, SMoAsSiP, SMoNGeP, SMoPGeN, SMoAsGeN and SMoAsGeP monolayers under strain of (a, c-j) -5% and (k, m-t) +5%, respectively. Phonon spectrum of SMoNSiAs under strain of (b) -4% and (l) +4%,

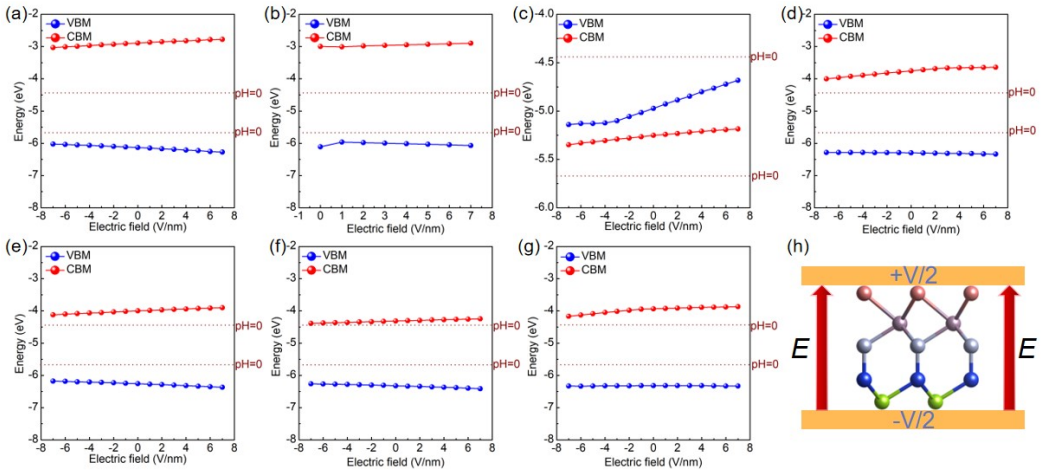

Fig S10 Band alignments of Janus (a) SMoPSiN, (b) SMoAsSiN, (c) SMoPSiAs, (d) SMoAsSiP, (e) SMoPGeN, (f) SMoAsGeN and (g) SMoAsGeP under external electric field. (f) The top view of Janus SMoZAZ' (A=Si, Ge; Z, Z'=N, P, As, Z≠Z') under external electric field.

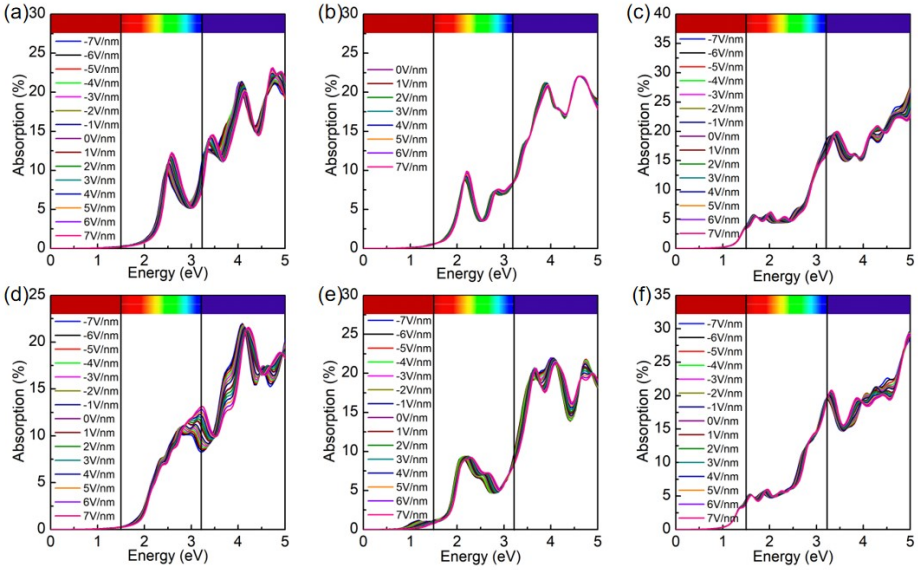

Fig S11 The light absorption of Janus(a) SMoPSiN, (b) SMoAsSiN, (c) SMoAsSiP, (d) SMoPGeN, (e) SMoAsGeN and (f) SMoAsGeP with biaxial strain.