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RESEARCH ARTICLE

Computational exploration and screening of novel Janus MA_2Z_4 (M = Sc–Zn, Y–Ag, Hf–Au; A=Si, Ge; Z=N, P) monolayers and potential application as a photocatalyst

Weibin Zhang[1,†], Woochul Yang[3], Yingkai Liu[1], Zhiyong Liu[1], Fuchun Zhang[2,‡]

[1] *College of Physics and Electronics Information, Yunnan Key Laboratory of Opto-Electronic Information Technology, Key Laboratory of Advanced Technique & Preparation for Renewable Energy Materials-Ministry of Education, Yunnan Normal University, Kunming 650500, China*
[2] *College of Physics and Electronic Information, Yan'an University, Yan'an 716000, China*
[3] *Department of Physics, Dongguk University, Seoul 04620, Republic of Korea*
Corresponding authors. E-mail: †220001@ynnu.edu.cn, ‡yadxzfc@yau.edu.cn
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Supporting Information

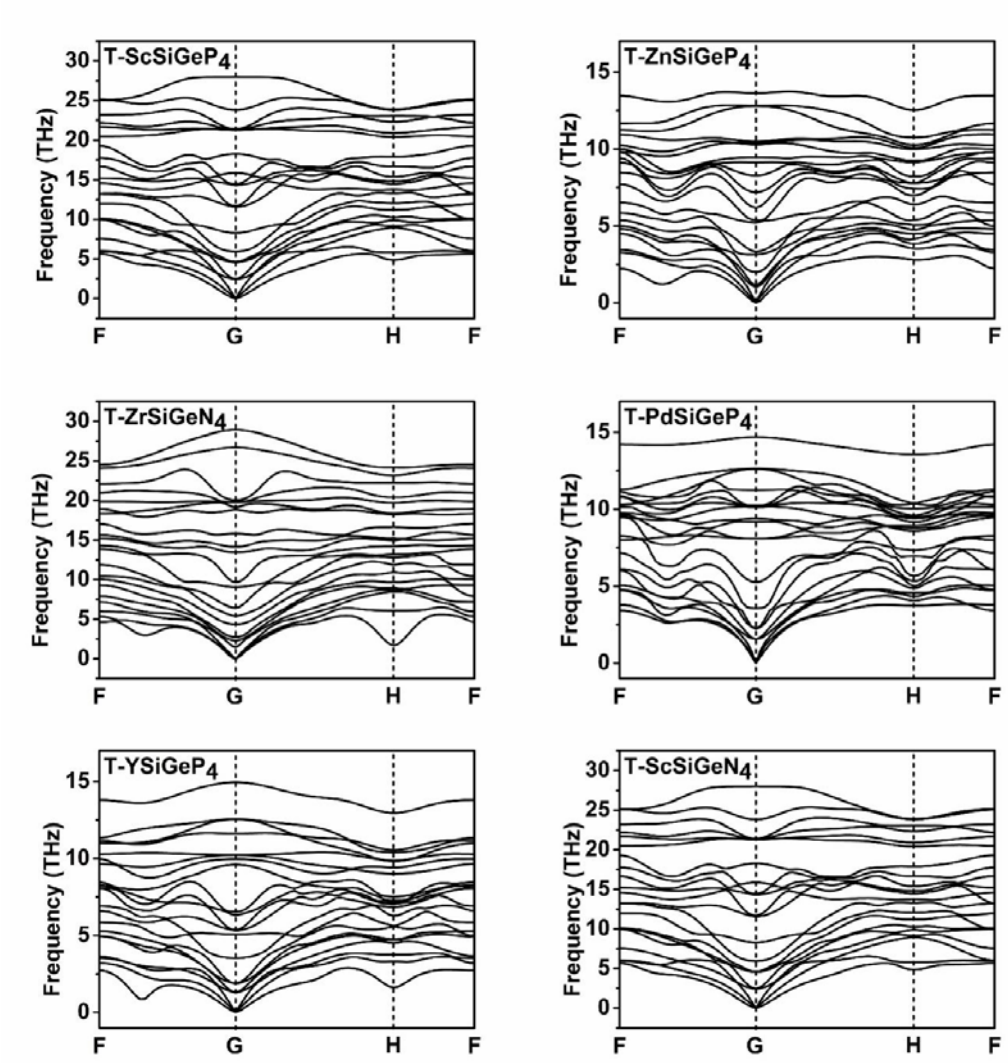

Fig. S1 Phonon bands of $T\text{-}ScSiGeP_4$, $T\text{-}ZnSiGeP_4$, $T\text{-}PdSiGeP_4$, $T\text{-}YSiGeP_4$, $T\text{-}ZrSiGeN_4$, $T\text{-}ScSiGeN_4$ monolayer.

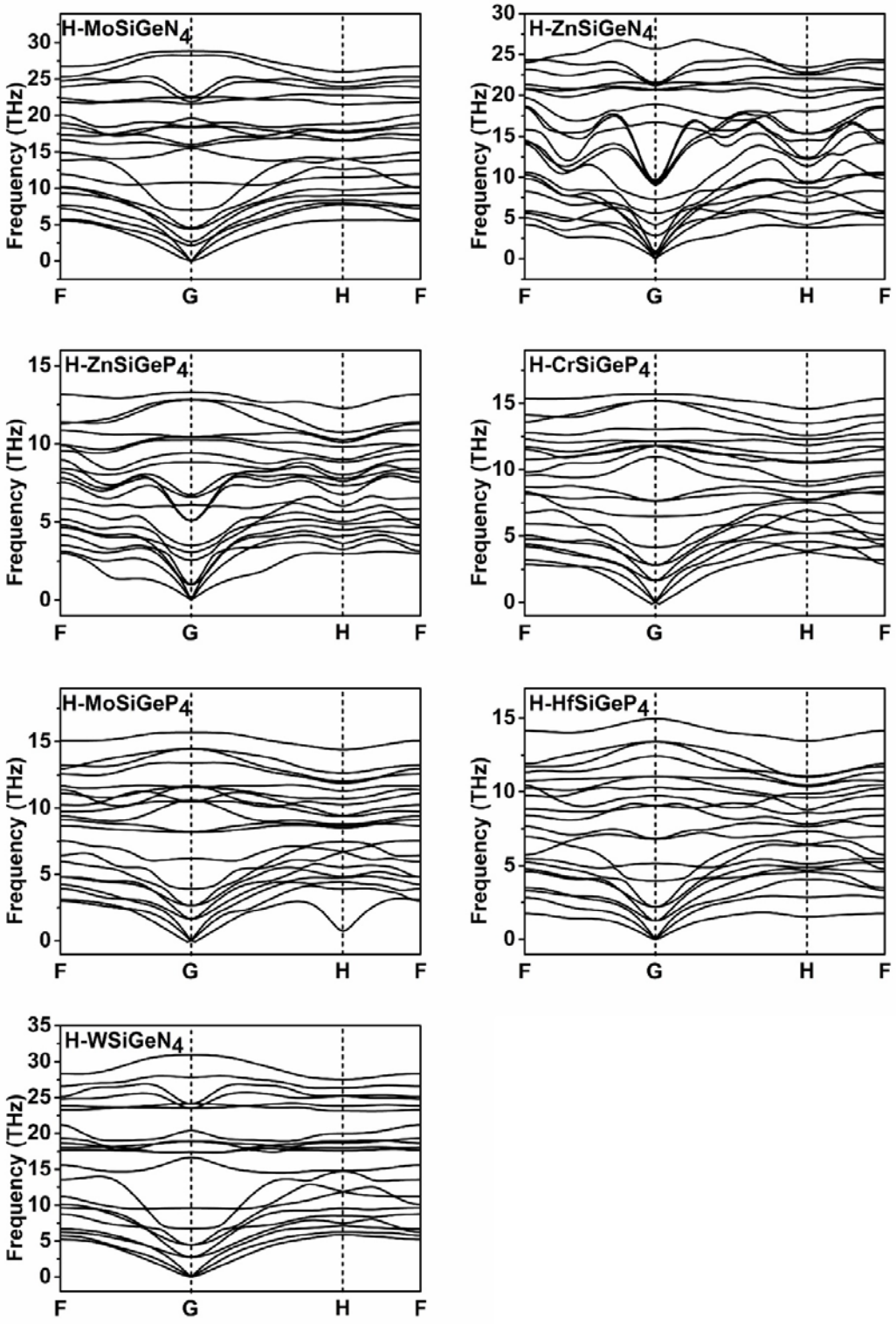

Fig. S2 Phonon bands of H-$ZnSiGeP_4$, H-$CrSiGeP_4$, H-$MoSiGeP_4$, H-$HfSiGeP_4$, H-$MoSiGeN_4$, H-$ZnSiGeN_4$, H-$WSiGeN_4$ monolayer.

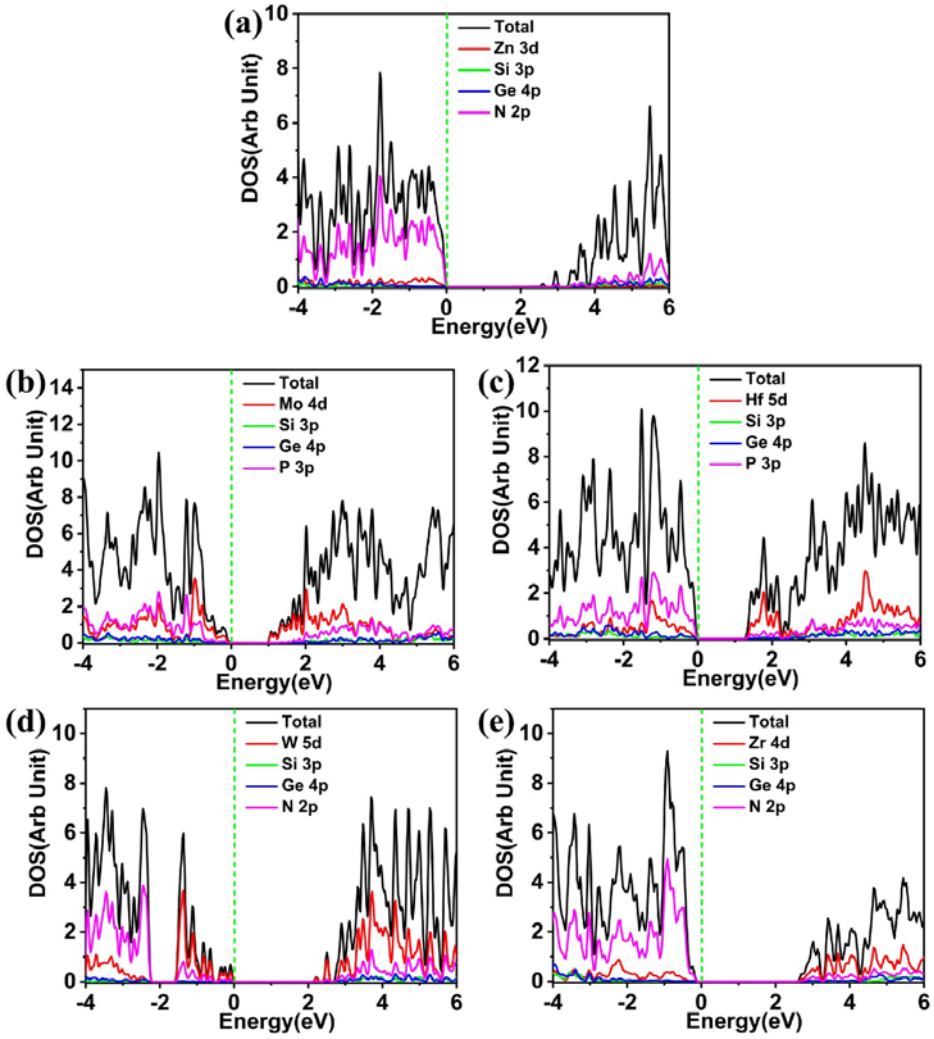

Fig. S3 Density of state of **(a)** H-$ZnSiGeN_4$, **(b)** H-$MoSiGeP_4$, **(c)** H- $HfSiGeP_4$, **(d)** H-$WSiGeN_4$, **(e)** T-$ZrSiGeN_4$. The fermi level was set to be 0.

Table S1 The calculated electron effective mass (m_e^*) at the conduction band minimum, the hole effective masses (m_h^*) at the valence band maximum, and the relative ratio of effective masses (D) of Janus MA_2Z_4 materials.

	m_e^*	m_h^*	D
H-$ZnSiGeN_4$	0.11	1.55	14.73
H-$MoSiGeN_4$	0.19	4.83	26.06
H-$MoSiGeP_4$	0.15	1.26	8.54
H-$HfSiGeP_4$	0.19	0.73	3.87
H-$WSiGeN_4$	0.13	1.80	14.41
T-$ScSiGeN_4$	0.12	0.39	3.23
T-$ZrSiGeN_4$	0.26	0.55	2.12
$Bi_4O_5Br_2$[39]	0.38	1.59	4.18
$BiVO_4$ [40]	0.896	3.04	3.39
g-C_3N_4[41]	3.9	29	7.4
TiO_2 [42]	0.62	1.70	2.74