Supplementary Information (SI) for Journal of Materials Chemistry A.

Supplementary Information

High-throughput computational screening of novel MA_2Z_4-type Janus structures with excellent photovoltaic and photocatalytic properties

Yongli Yang[1,2], Yadong Yu[2]*, Zhe Liu[2]*, Lijun Shang[1], Pan Xiang[2], Yu Xin[2], Tong Zhang[2], Zhonglu Guo[1]*, Mengyan Dai[2]*

[1]Hebei Key Laboratory of Boron Nitride Micro and Nano Materials, School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China

[2]Chemical Defense Institute, Academy of Military Sciences, Beijing 102205,China

*Corresponding Authors: yuyadong36@163.com (Yadong Yu), zheliu_academia@hotmail.com (Zhe Liu), zlguo@hebut.edu.cn (Zhonglu Guo), daidecai0558@163.com (Mengyan Dai)

Calculation details

The formation energy is calculated as follows

$$E_f = \frac{E_{total} - \sum_i n_i \mu_i}{\sum_i n_i} \qquad S(1)$$

where E_{total} represents the total energy of the structure in a unit cell, n_i represents the number of the ith atom, and μ_i is the cohesion energy contained in the ith atom. The formation energies obtained are shown in the following table S1.

Phonon dispersion calculations based on VASP-DFPT (Density Functional Perturbation Theory)[1, 2] are used to investigate their dynamic stability (both MA_2Z_4 are 4 × 4 × 1 supercells).The phonon dispersion curve is shown in Figure S1S2.

The thermal stability of the MA_2Z_4 structure was evaluated by performing ab initio arithmetic molecular dynamics (AIMD)1 simulations at 300 K, where sufficiently large supercells containing more than 100 atoms were used to reduce lattice translation constraints. The system was stabilized at 300 K for 5 ps with a time step of 2 fs and the Nosè algorithm was used to control the temperature.

Carrier mobility is estimated by means of the deformation potential (DP) theory defined below:

$$\mu_{2D} = \frac{2e\hbar^3 C_{2D}}{3k_B T|m*|^2 E_i^2} \qquad S(2)$$

where e, $\hbar$, k_B and T are the electron charge, the approximate Planck constant, the Boltzmann constant and the temperature (300 K), respectively. C_{2D} is the modulus of elasticity under uniaxial strain along the strain direction, calculated as follows:

$$C_{2D} = [\partial^2 E/\partial(\Delta a/a_0)^2]/S_0 \qquad S(3)$$

where S_0 is the equilibrium area. E_i is the strain–induced band–edge energy of the CBM of the electron and the VBM of the hole, calculated as follows:

$$E_i = \partial E_{edge}/\partial(\Delta a/a_0) \qquad S(4)$$

where E_{edge} is the band edge energy of CBM for electrons and VBM for holes induced by uniaxial strain. $m^*$is the effective mass of the carrier, calculated as follows:

$$m^* = \hbar^2/(\partial^2 E/\partial k^2) \qquad S(5)$$

The work function is the minimum amount of energy that must be supplied to cause an electron to immediately escape from a solid surface. The defining formula for the work function is:

$$W = -e\Phi - E_F \qquad S(6)$$

where $-e$ is the charge of an electron, Φ is the electrostatic potential in the vacuum nearby the surface, and E_F is the Fermi level (electrochemical potential of electrons) inside the material.

The investigation of optical properties begins with the calculation of the material's dielectric function $\varepsilon(\omega)$ as follows[3]:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \qquad S(7)$$

where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary parts of the dielectric function, and ω is the photon frequency. The imaginary part of the dielectric function $\varepsilon_2(\omega)$ was obtained from the following equation:

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \times \sum_{c,v,\boldsymbol{k}} 2w_{\boldsymbol{k}} \delta(E_c - E_v - \omega)|\langle c|\boldsymbol{e}\cdot\boldsymbol{q}|v\rangle|^2 \qquad S(8)$$

where $\langle c|\boldsymbol{e}\cdot\boldsymbol{q}|v\rangle$ is the integrated optical transitions from the valence states (v) to the conduction states (c), $\boldsymbol{e}$ is the polarization direction of the photon and $\boldsymbol{q}$ is the electron momentum operator. The integration over $\boldsymbol{k}$ is performed by summation over special kpoints with a corresponding weighting factor $w_{\boldsymbol{k}}$. The real part of the dielectric function $\varepsilon_1(\omega)$ can be determined from the Kramers-Kronig relation given by:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon_2(\omega')\omega'}{\omega^2 - \omega^2 + i\eta} d\omega' \qquad S(9)$$

where P denotes the principle value and η is the complex shift parameter.

Absorption coefficient $\alpha(\omega)$ can be calculated from the real $\varepsilon_1(\omega)$ and the imaginary $\varepsilon_2(\omega)$ parts:

$$\alpha(\omega) = \sqrt{2}\omega\left(\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right)^{\frac{1}{2}} \qquad S(10)$$

Additionally, in order to obtain the more accurate optical absorption of 2D materials, the optical absorption rate was calculated as follows:

$$A = \frac{\mathrm{Re}\,\tilde{\sigma}}{|1+\tilde{\sigma}/2|^2} \qquad S(11)$$

Where $R = \left|\frac{\tilde{\sigma}/2}{1+\tilde{\sigma}/2}\right|^2$ is the normalized reflectance, $\tilde{\sigma}(\omega) = \sigma_{2\mathrm{D}}(\omega)/\varepsilon_0 c$ is the normalized conductivity. σ_{2D} (ω) denotes the in-plane 2D optical conductivity, which directly related to the corresponding σ3D(ω) component through the equation of $\sigma_{2D}(\omega) = L\sigma_{3D}(\omega)$, where L is the slab thickness in the simulation cell, and 3D optical conductivity was obtained from $\sigma_{3D}(\omega) = i[1-\varepsilon(\omega)]\varepsilon_0\omega$ base on the Maxwell equation. For $\varepsilon(\omega)$, ε_0, and ω, they are the frequency-dependent complex dielectric function, permittivity of vacuum, and frequency of the incident wave, respectively.

For hydrogen evolution reaction (HER), the reaction equation at PH=0 is as follows:

$$H^+ + * + e^- \rightarrow H^* \qquad S(12)$$

$$H^* + H^+ + e^- \rightarrow H_2 \qquad S(13)$$

where * denotes the active site on the surface of the structure, H* denotes the hydrogen atoms on the surface of the adsorbed structure. The calculation of Gibbs free energy (ΔG_{H*}) under acidic conditions is as follows[4]:

$$\Delta G_{H*} = \Delta E + \Delta E_{ZPE} - T\Delta S \qquad S(14)$$

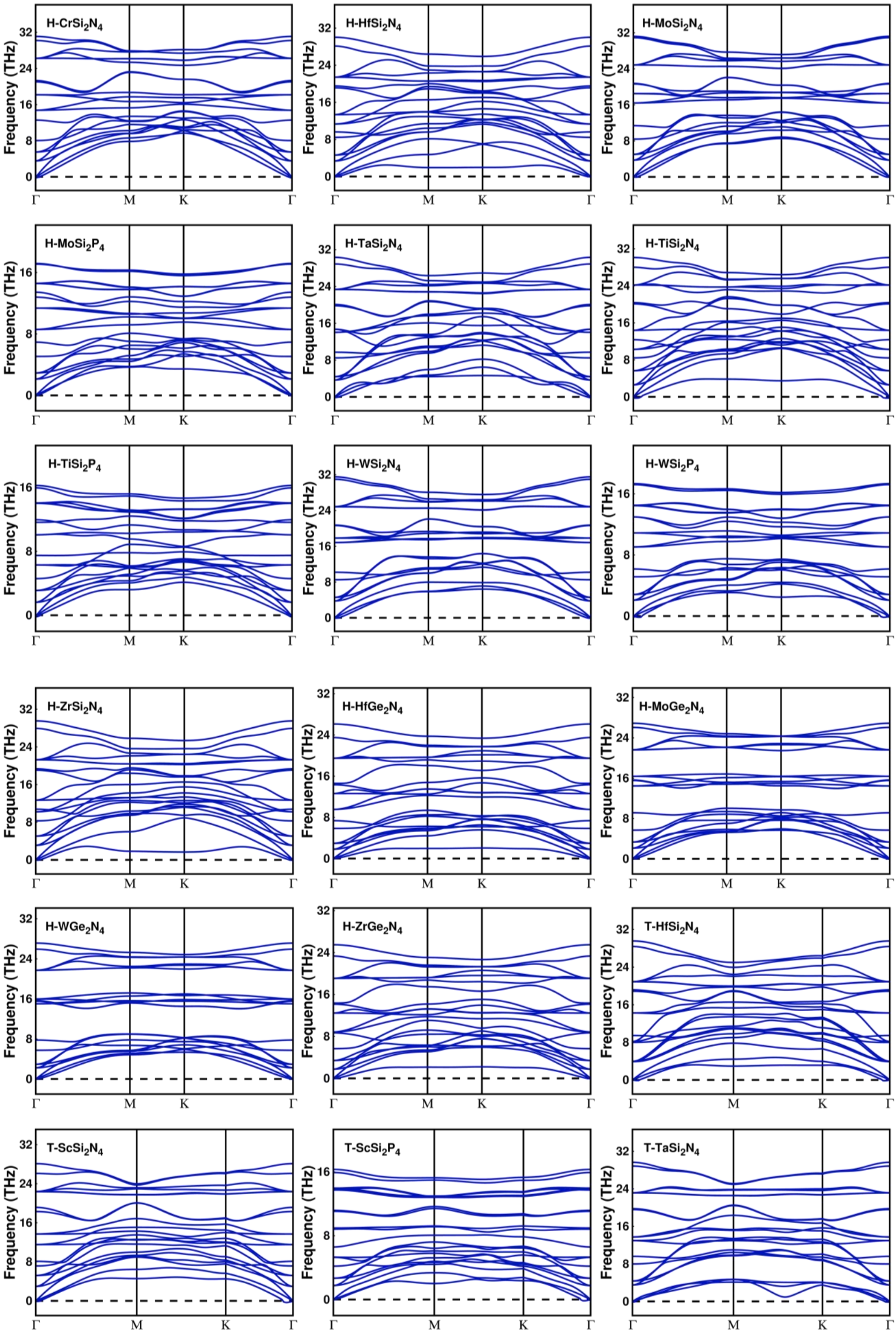
Therein ΔE denotes the energy difference between the hydrogen adsorption state and the independent state, ΔE_{ZPE}denotes the zero-point energy difference, ΔS denotes the entropy value difference, and T denotes the temperature (298.15 K).

The ΔG_{H^*} under the influence of different PH were calculated separately with the following equations:

$$\Delta G_{H^*} = G_{H^*} - 1/2G_{H_2} - G^* + 0.059 \times pH - eU \qquad S(15)$$

where 0.059 × pH is the free energy contribution under the effect of pH, eU denotes the influence of extra potential bias provided by the electrons or holes, and U is the electrode potential relative to the standard hydrogen electrode (SHE).

Supporting Figures



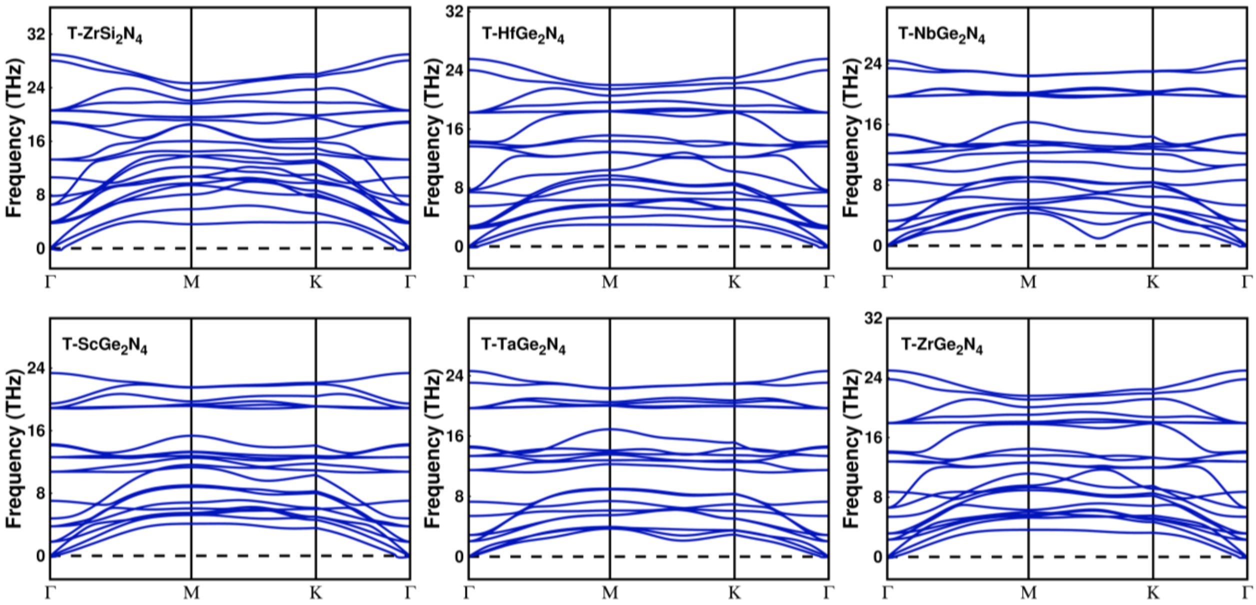
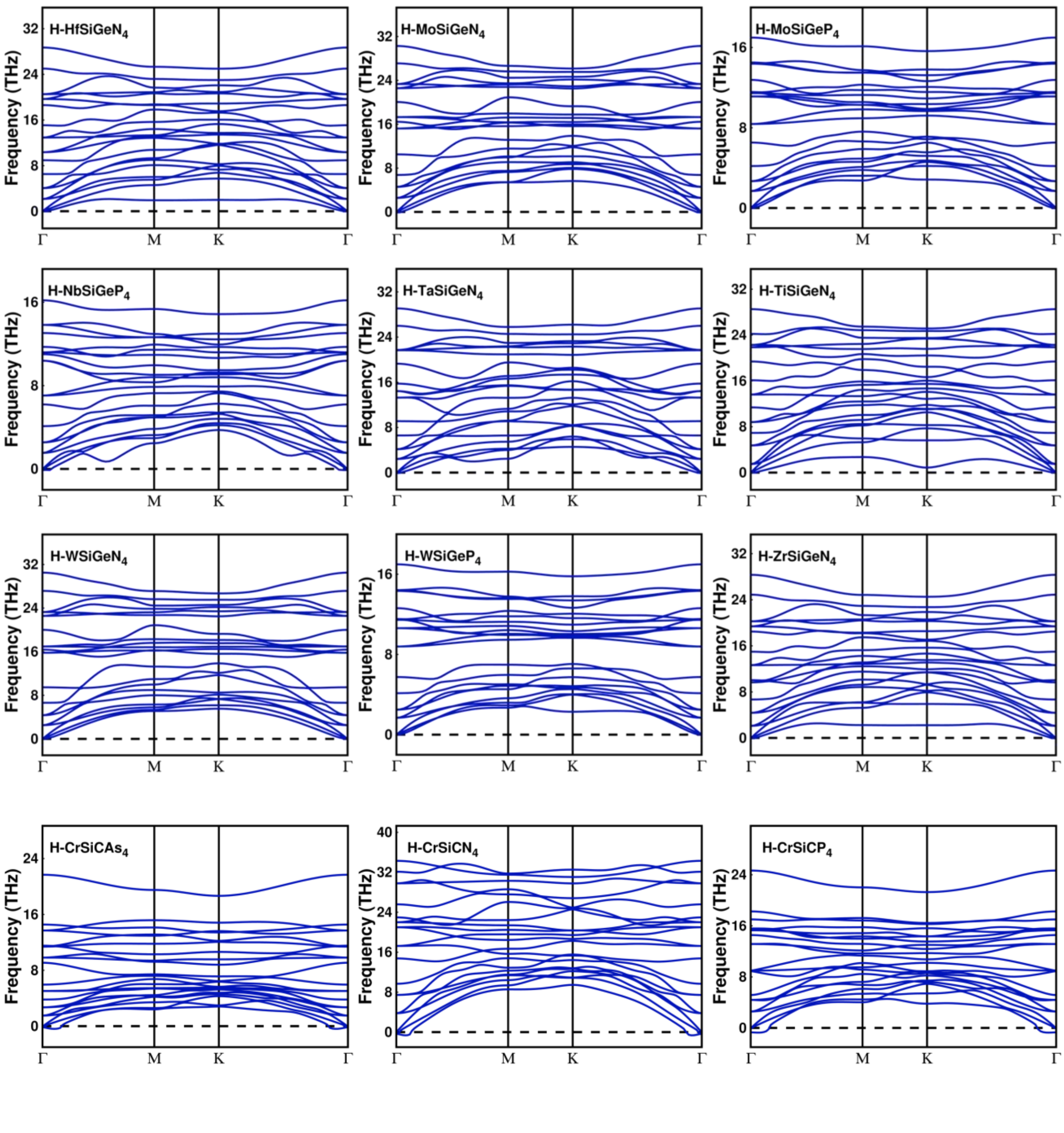
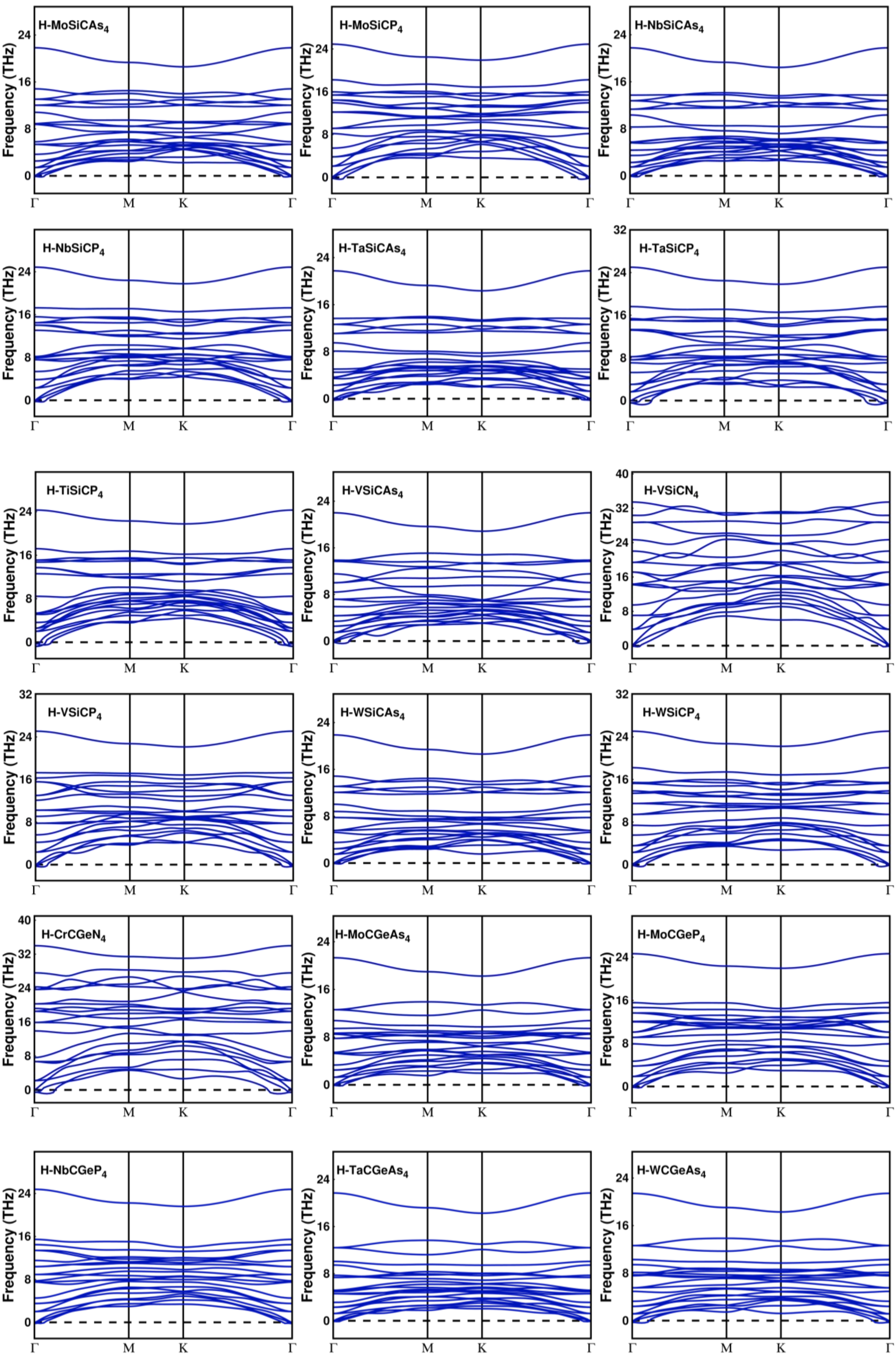


Fig. S1 Phonon dispersion curves for the symmetric structure of MA_2Z_4.




H-MoSiCAs$_4$
H-MoSiCP$_4$
H-NbSiCAs$_4$
H-NbSiCP$_4$
H-TaSiCAs$_4$
H-TaSiCP$_4$
H-TiSiCP$_4$
H-VSiCAs$_4$
H-VSiCN$_4$
H-VSiCP$_4$
H-WSiCAs$_4$
H-WSiCP$_4$
H-CrCGeN$_4$
H-MoCGeAs$_4$
H-MoCGeP$_4$
H-NbCGeP$_4$
H-TaCGeAs$_4$
H-WCGeAs$_4$
Frequency (THz)
Γ
M
K
Γ

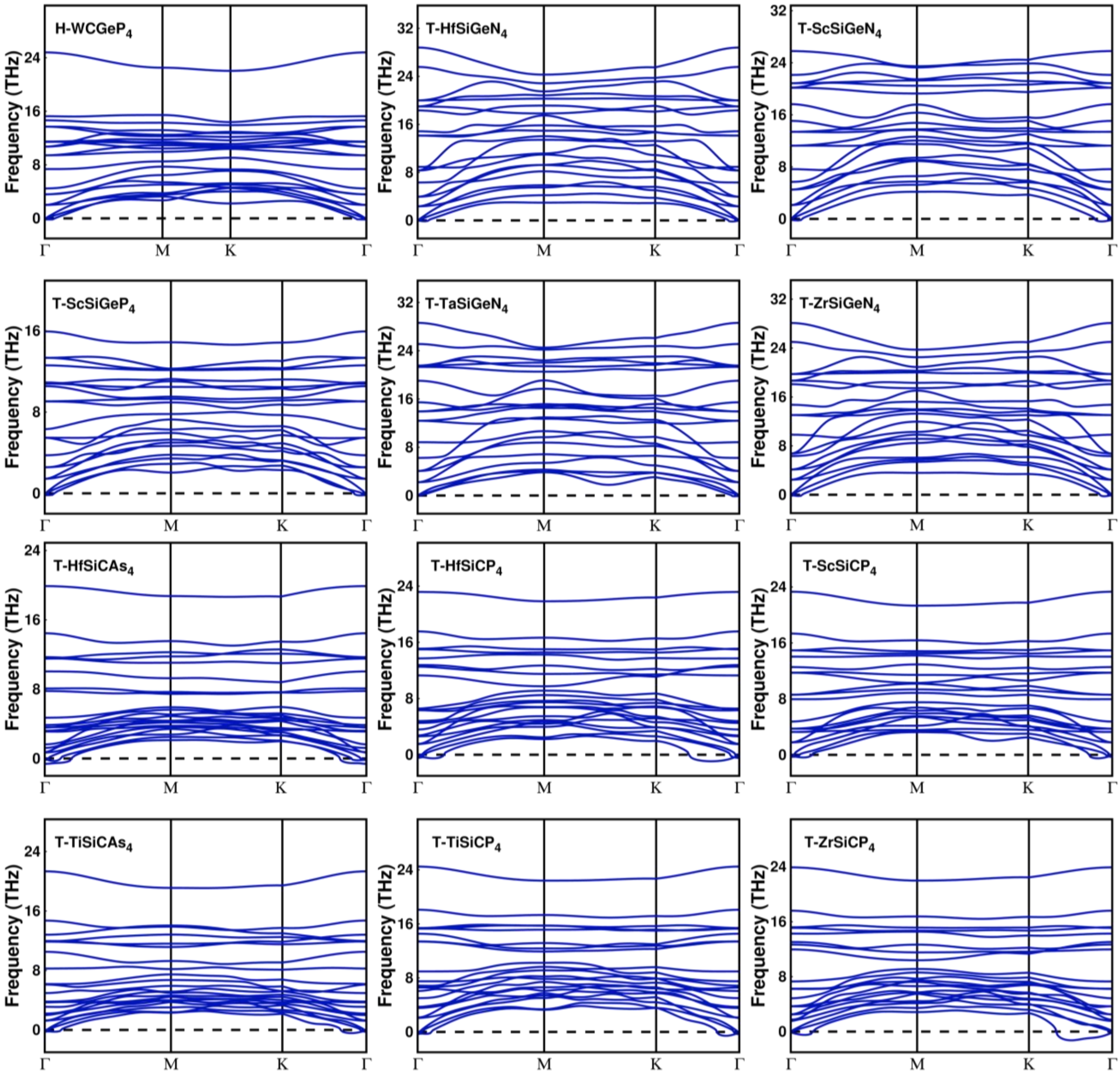
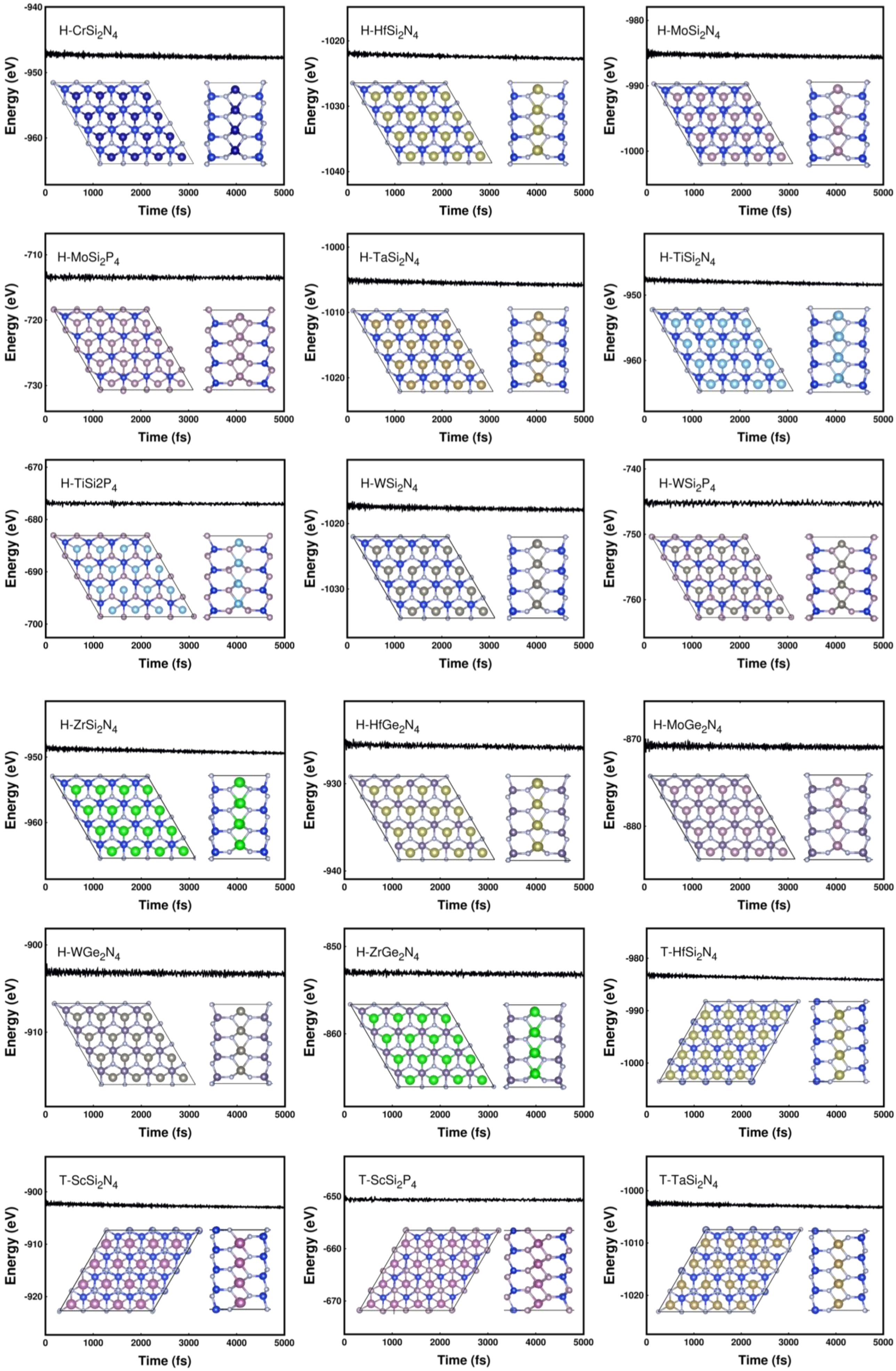


Fig. S2 Phonon dispersion curves for the asymmetric Janus structure of MA_2Z_4.



H-$CrSi_2N_4$
H-$HfSi_2N_4$
H-$MoSi_2N_4$
H-$MoSi_2P_4$
H-$TaSi_2N_4$
H-$TiSi_2N_4$
H-TiSi2P_4
H-WSi_2N_4
H-WSi_2P_4
H-$ZrSi_2N_4$
H-$HfGe_2N_4$
H-$MoGe_2N_4$
H-WGe_2N_4
H-$ZrGe_2N_4$
T-$HfSi_2N_4$
T-$ScSi_2N_4$
T-$ScSi_2P_4$
T-$TaSi_2N_4$
Energy (eV)
Time (fs)

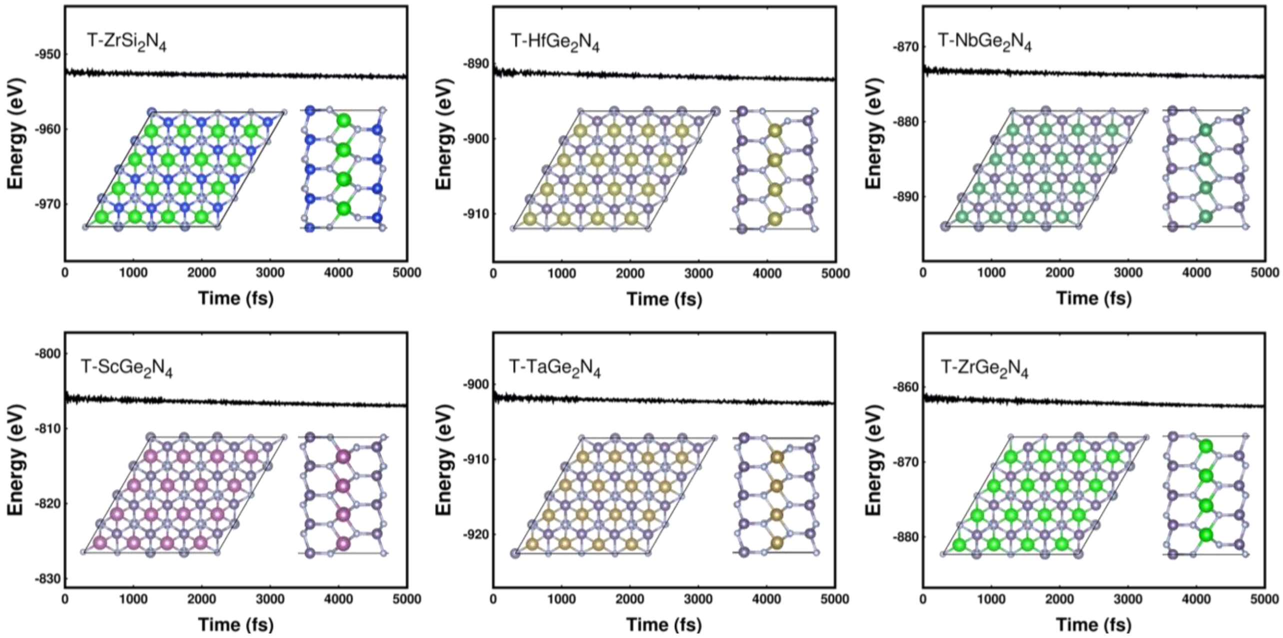
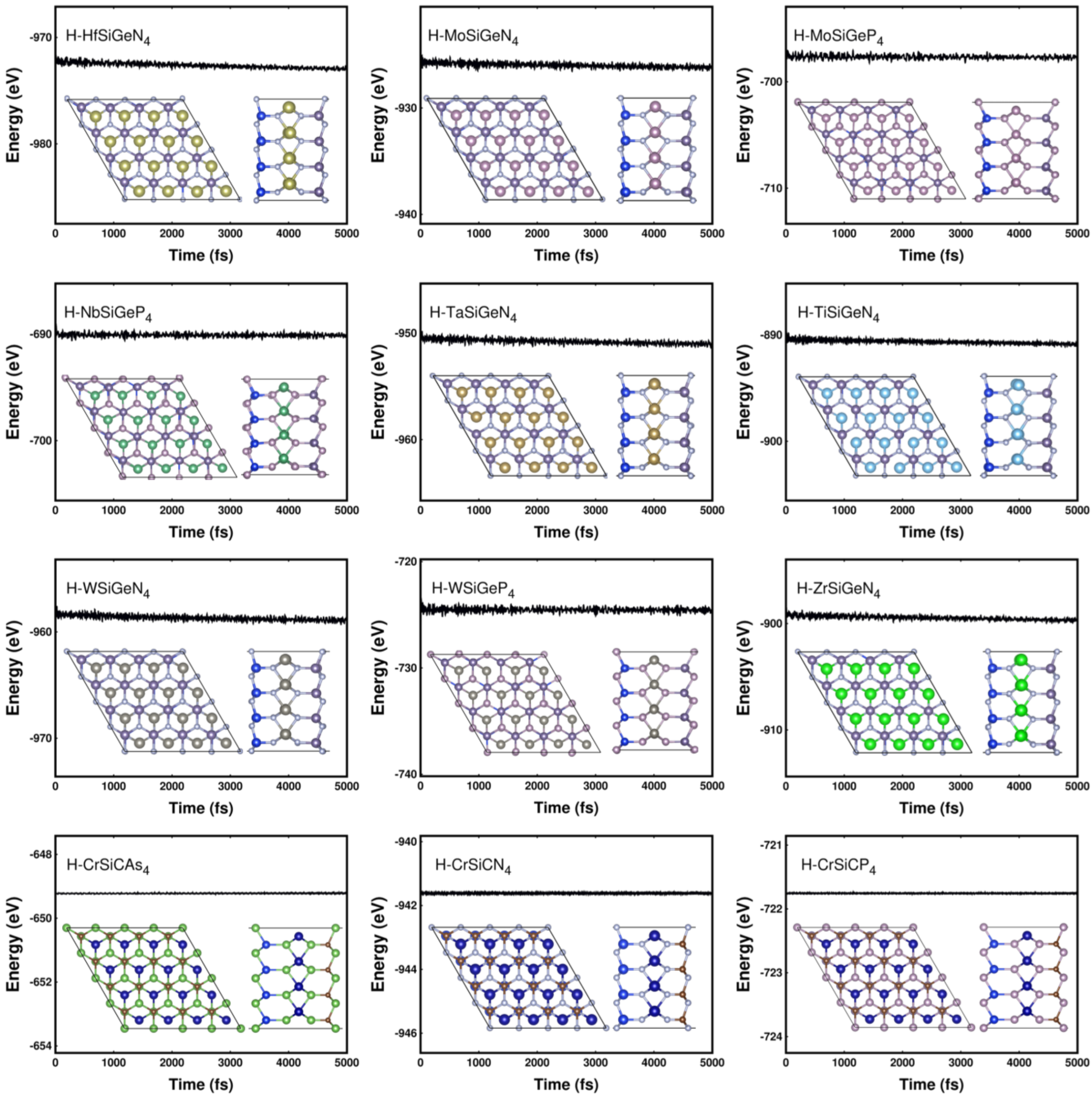
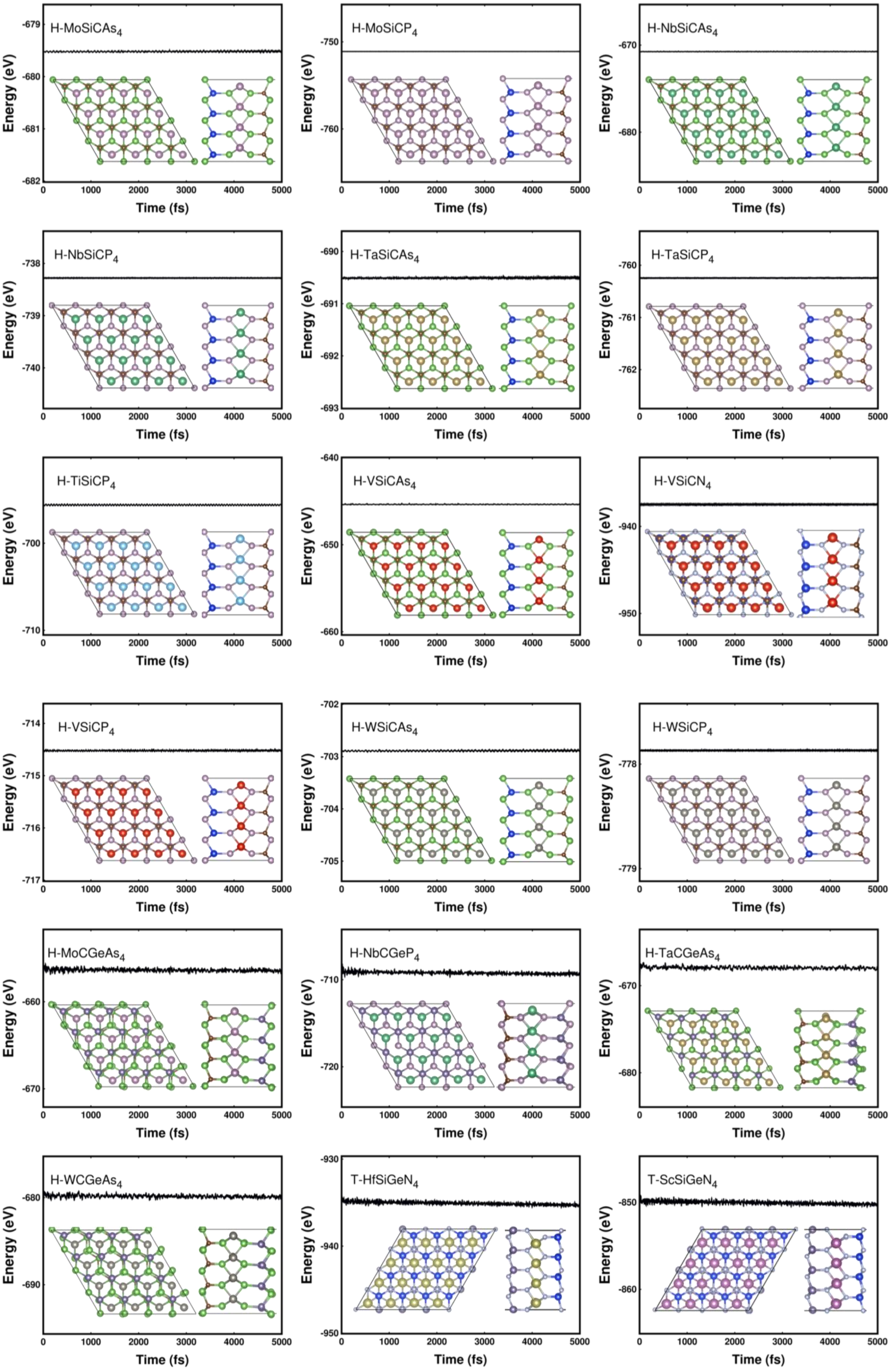


Fig. S3 Total potential energy and corresponding snapshots of symmetric MA_2Z_4 after 5 ps stabilization at 300 K obtained in AIMD simulations.




H-MoSiCAs$_4$
H-MoSiCP$_4$
H-NbSiCAs$_4$
H-NbSiCP$_4$
H-TaSiCAs$_4$
H-TaSiCP$_4$
H-TiSiCP$_4$
H-VSiCAs$_4$
H-VSiCN$_4$
H-VSiCP$_4$
H-WSiCAs$_4$
H-WSiCP$_4$
H-MoCGeAs$_4$
H-NbCGeP$_4$
H-TaCGeAs$_4$
H-WCGeAs$_4$
T-HfSiGeN$_4$
T-ScSiGeN$_4$
Energy (eV)
Time (fs)

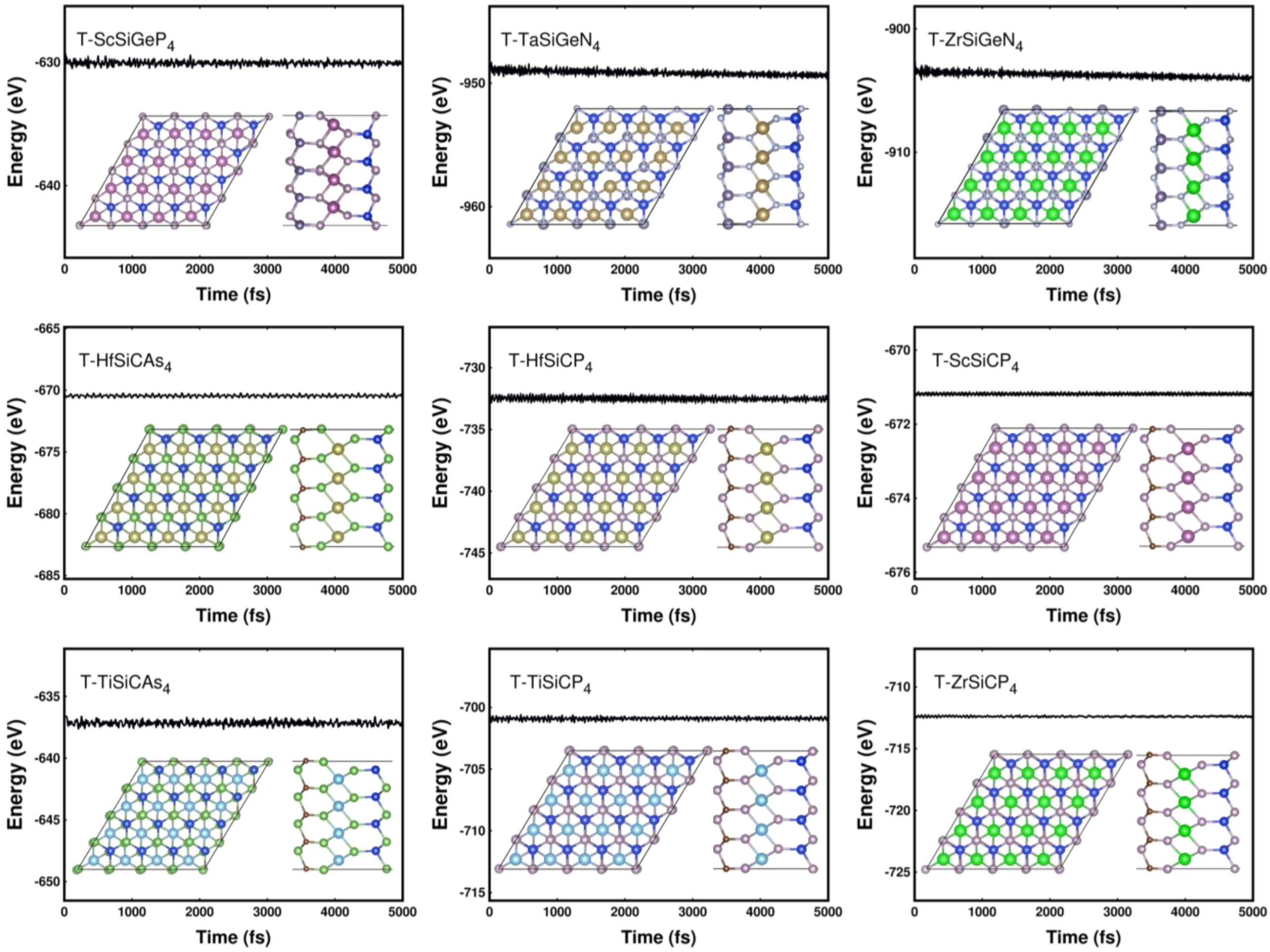
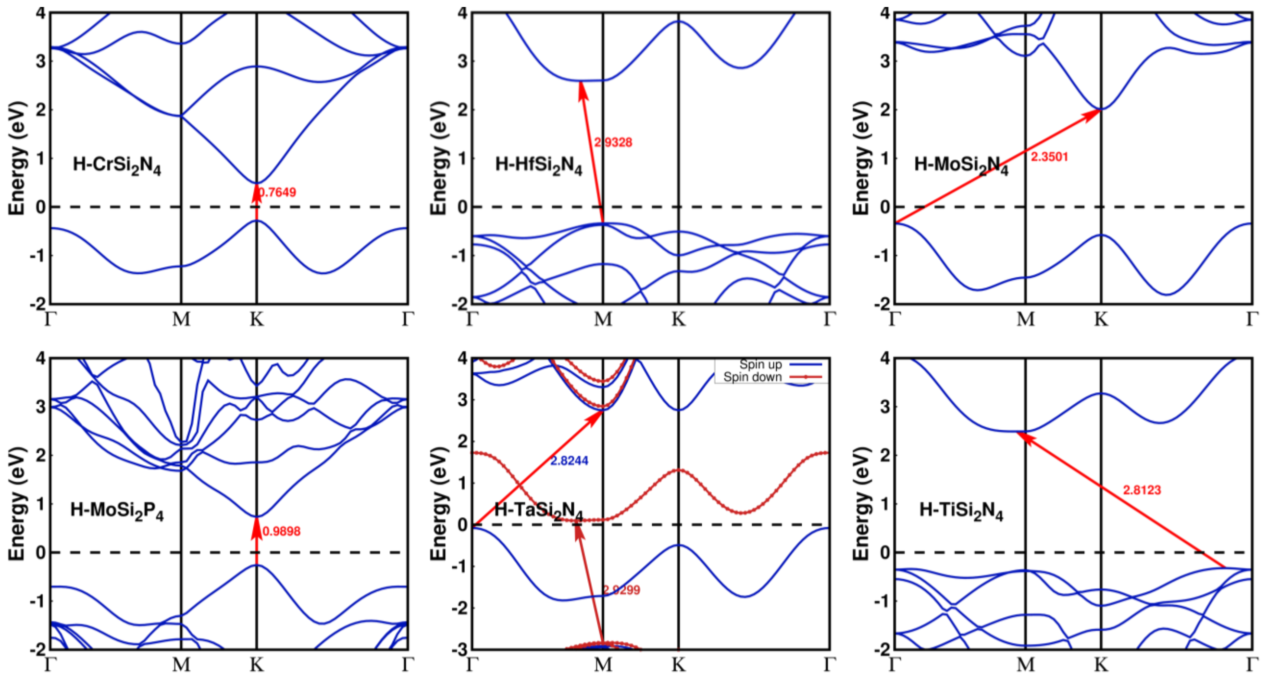


Fig. S4 The total potential energy and corresponding snapshots of the Janus MA_2Z_4 after stabilization at 300 K for 5 ps were obtained in the AIMD simulations.



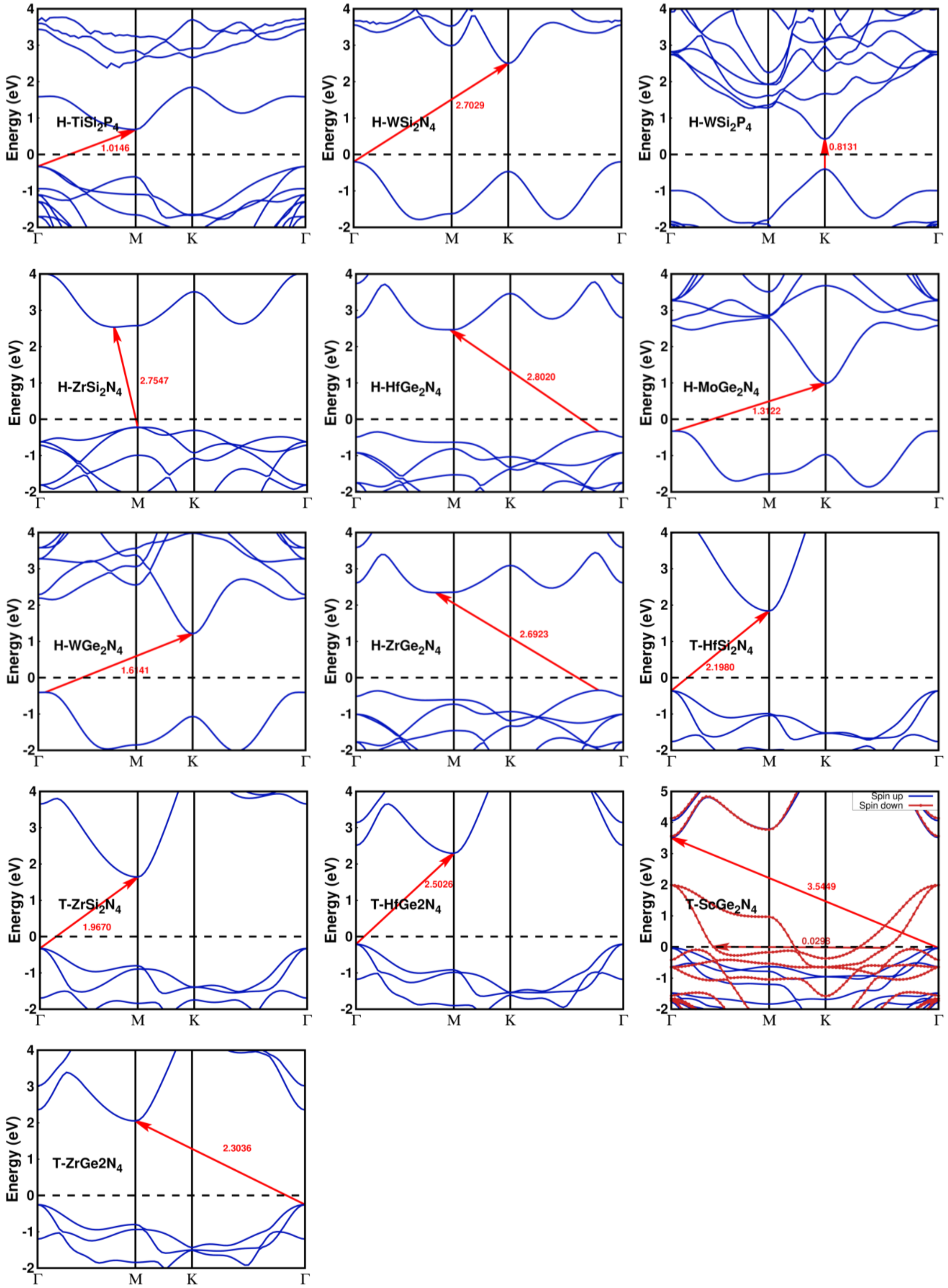
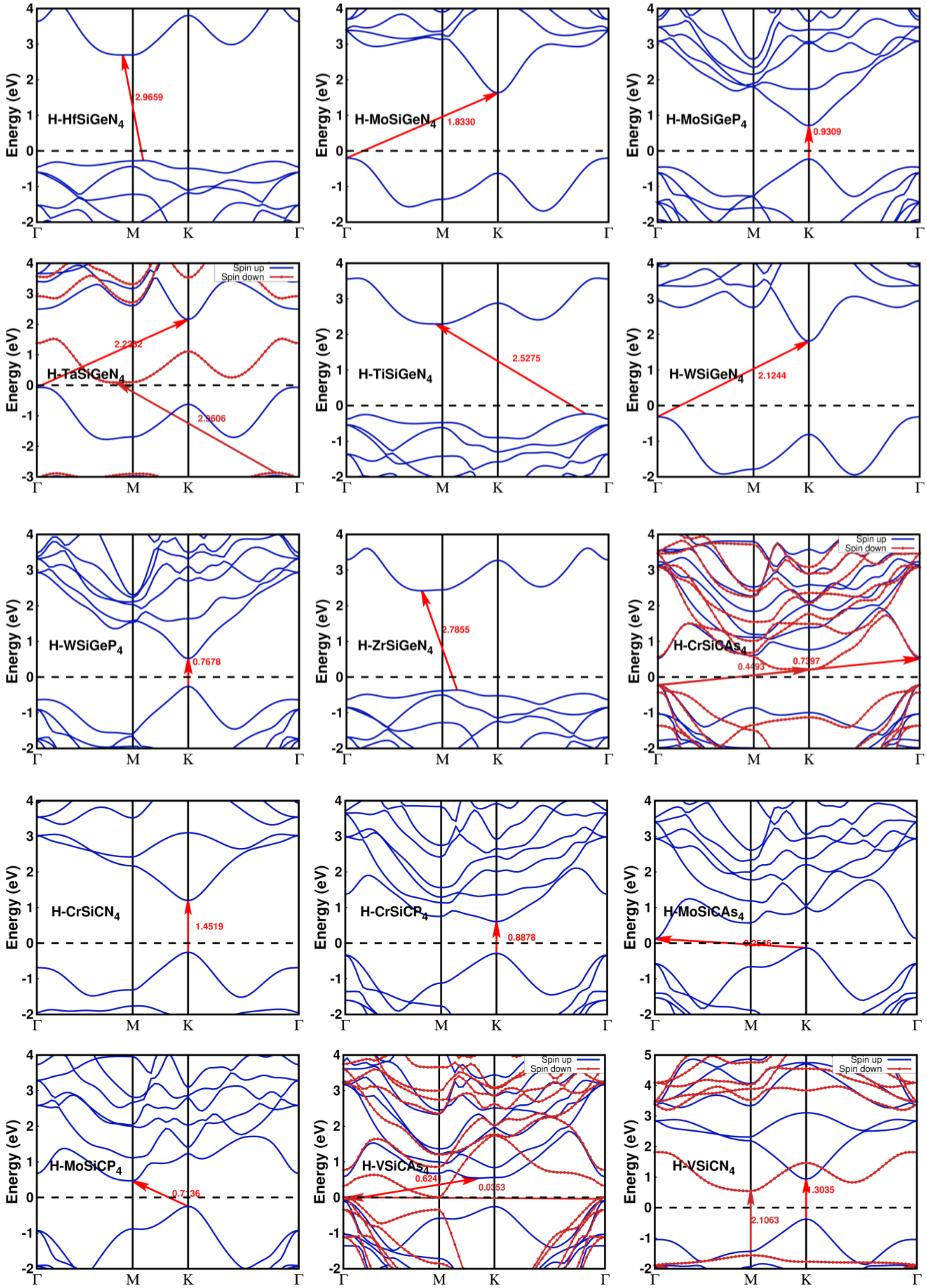


Fig. S5 Energy band structure diagrams of symmetric MA_2Z_4 structures.


Energy (eV)
Γ M K Γ
H-HfSiGeN$_4$
2.9659
H-MoSiGeN$_4$
1.8330
H-MoSiGeP$_4$
0.9309
H-TaSiGeN$_4$
Spin up
Spin down
H-TiSiGeN$_4$
2.5275
H-WSiGeN$_4$
2.1244
H-WSiGeP$_4$
0.7678
H-ZrSiGeN$_4$
2.7855
H-CrSiCAs$_4$
0.7397
H-CrSiCN$_4$
1.4519
H-CrSiCP$_4$
0.8878
H-MoSiCAs$_4$
H-MoSiCP$_4$
H-VSiCAs$_4$
H-VSiCN$_4$
2.1063

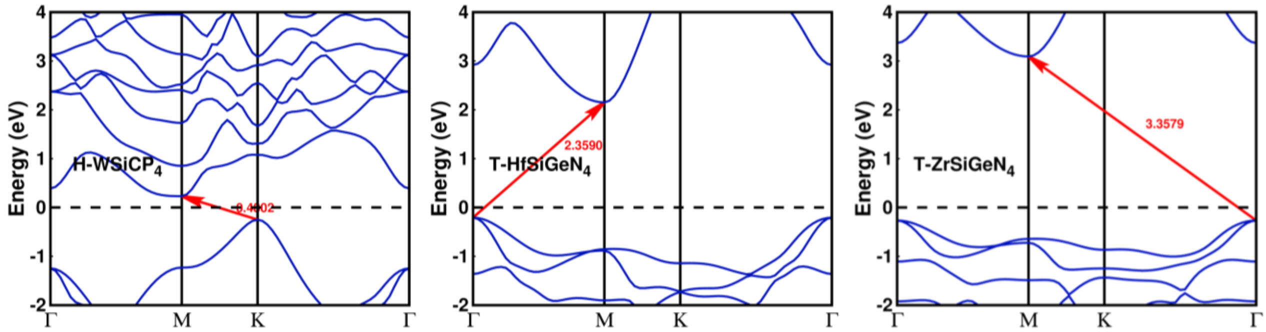
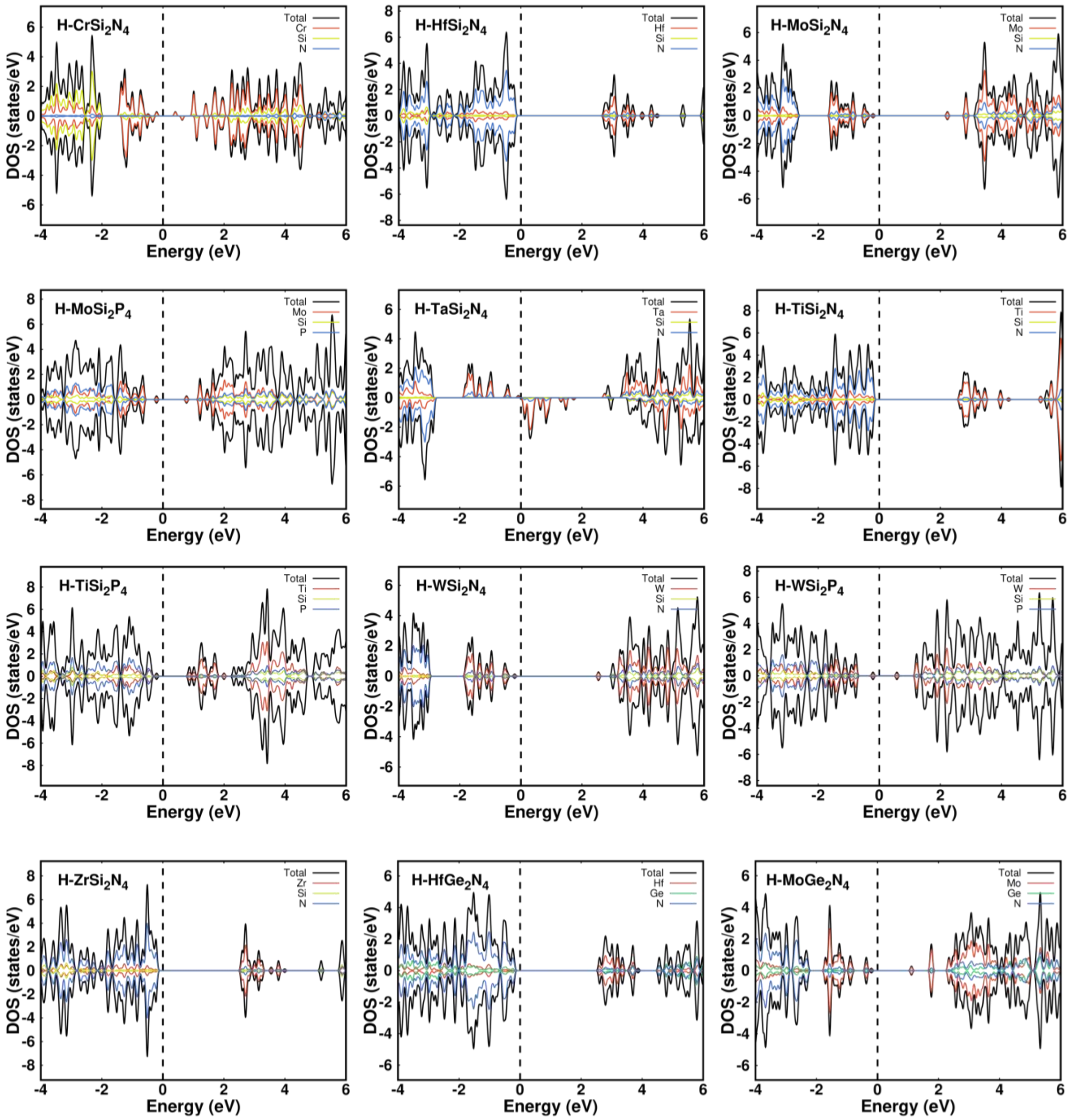


Fig. S6 Energy band structure diagrams of asymmetric Janus MA_2Z_4 structures.



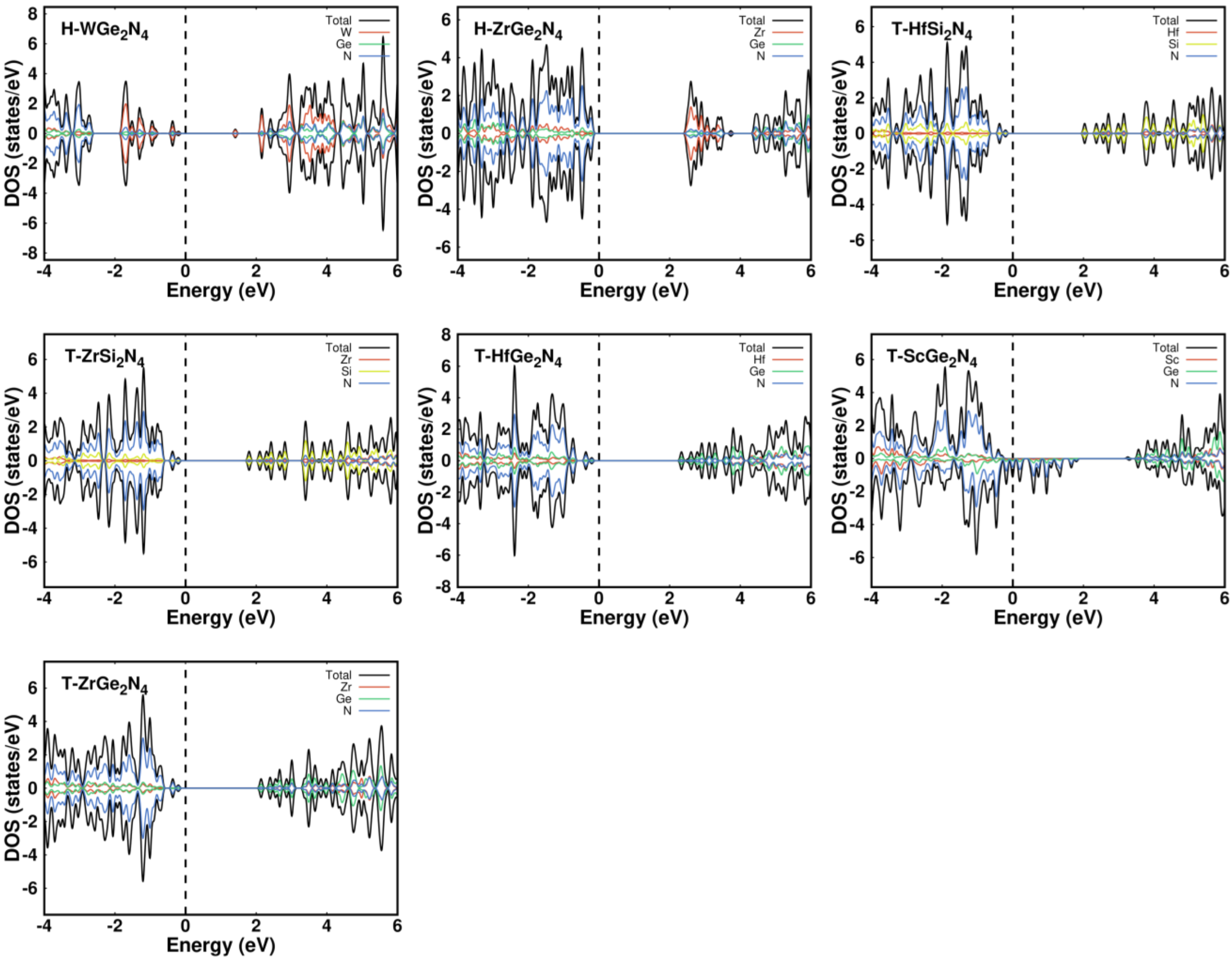
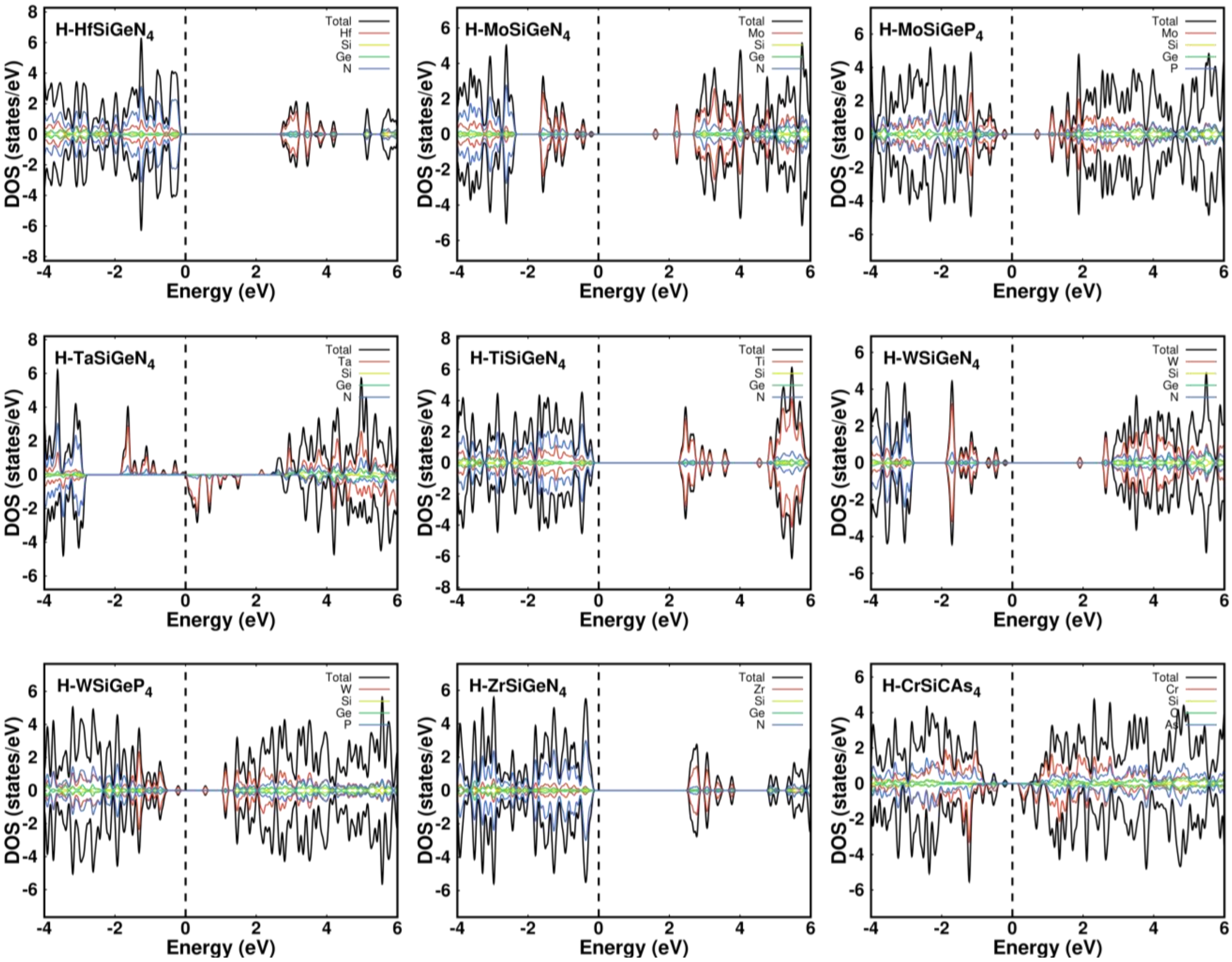


Fig. S7 TDOS and PDOS of symmetric MA_2Z_4 structure.



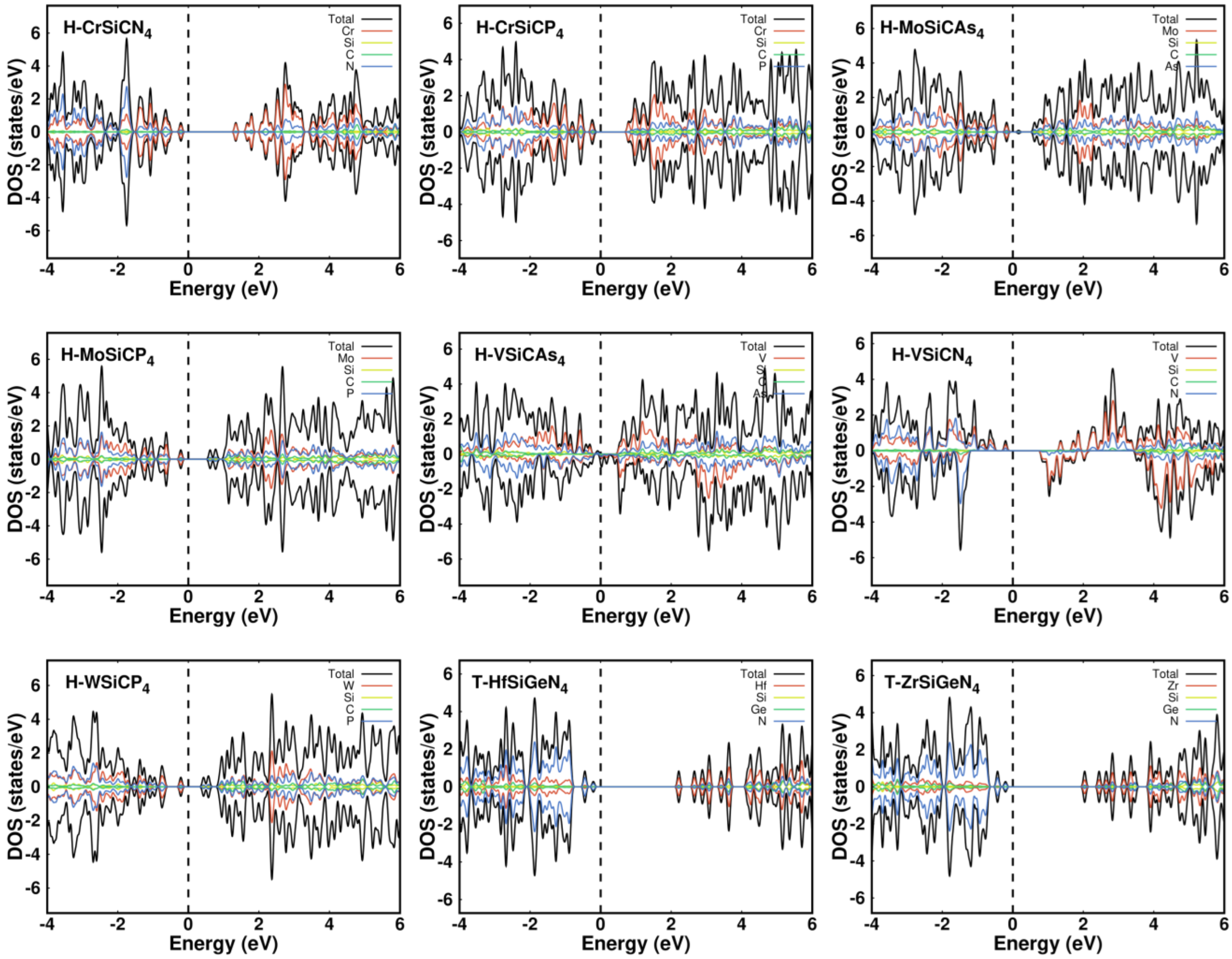
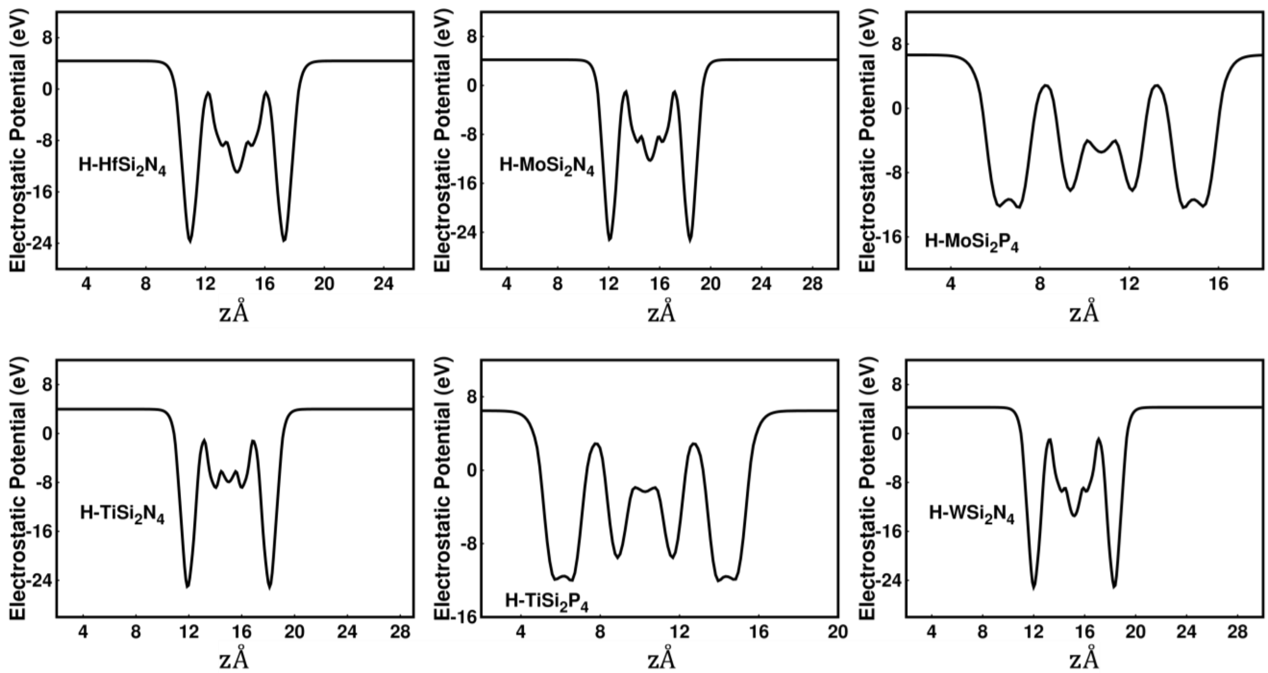


Fig. S8 TDOS and PDOS of asymmetric Janus MA_2Z_4 structures.



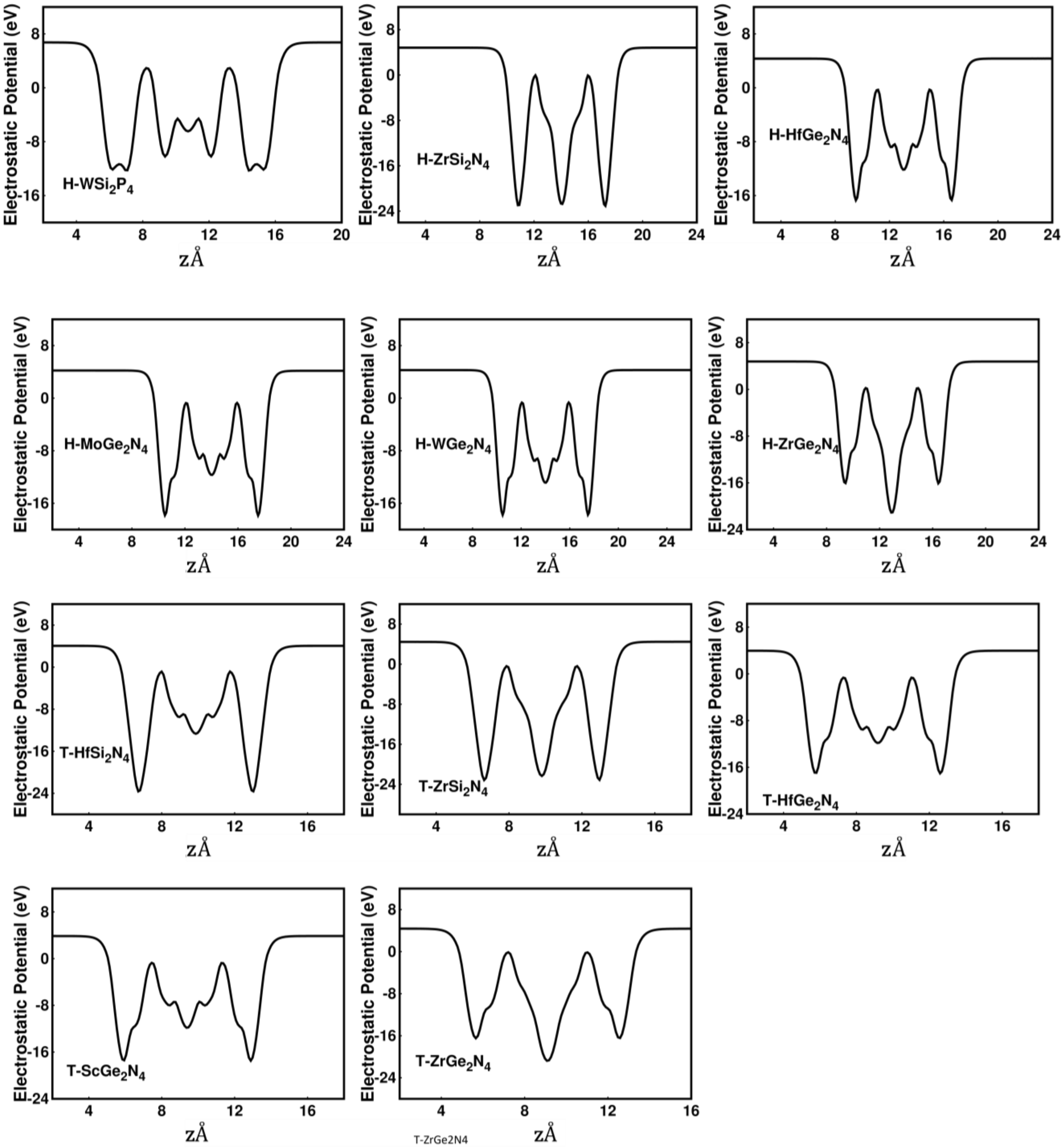
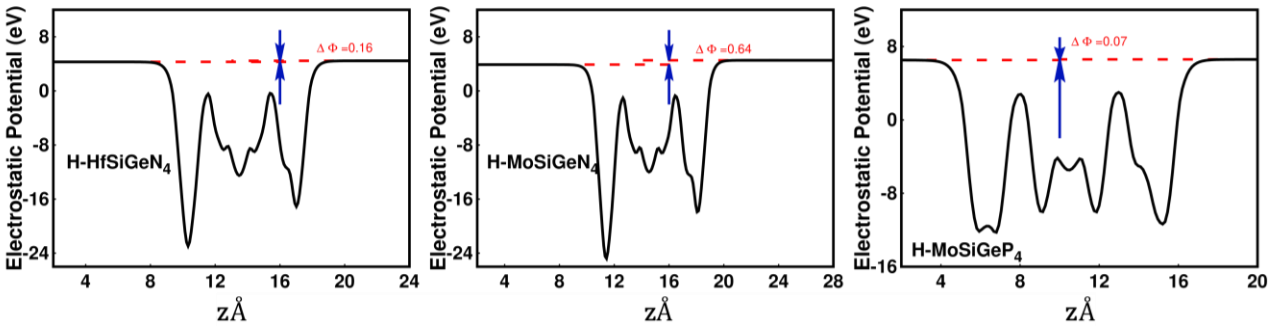


Fig. S9 Work function of symmetric structures.



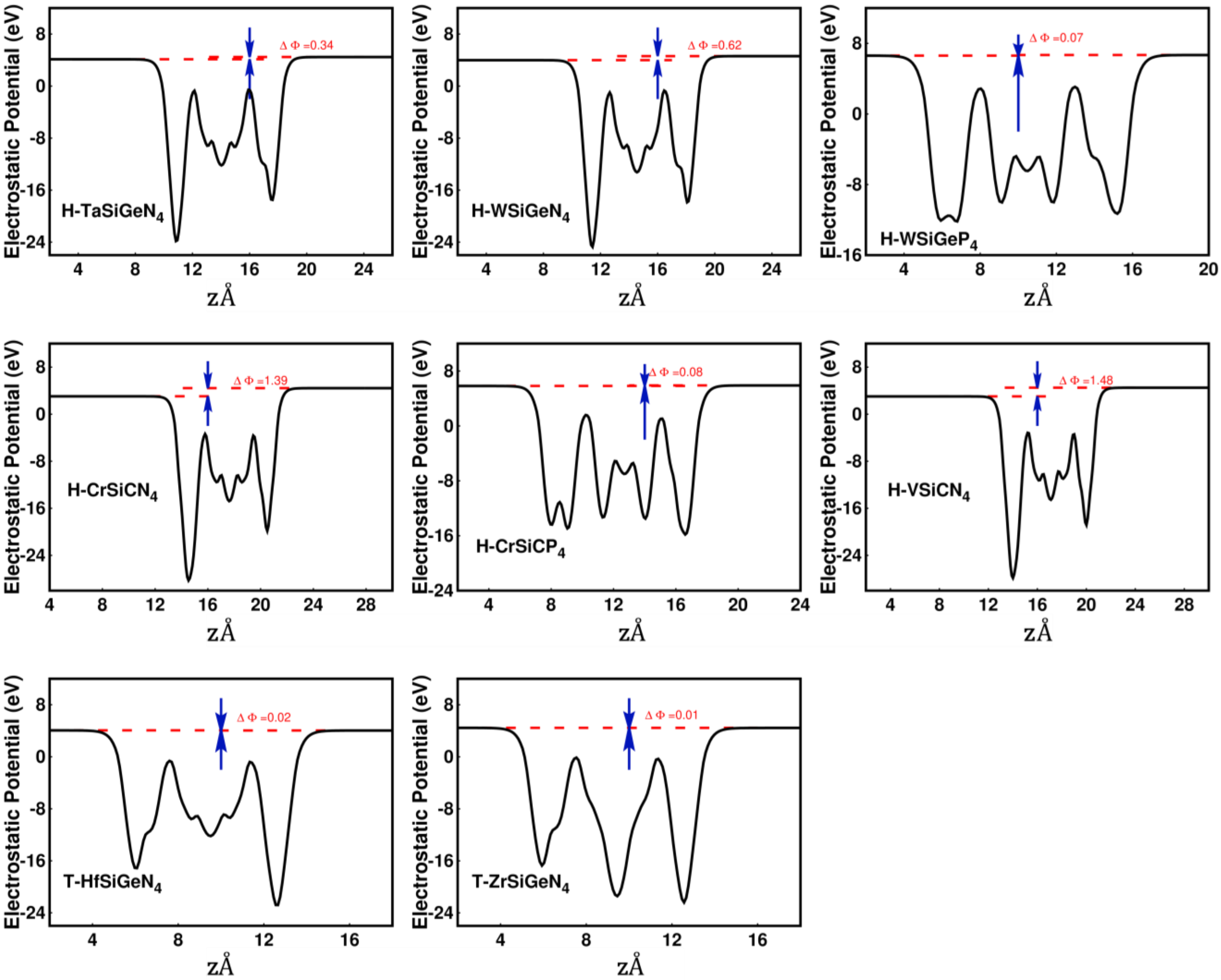


Fig. S10 work function of the Janus structures.

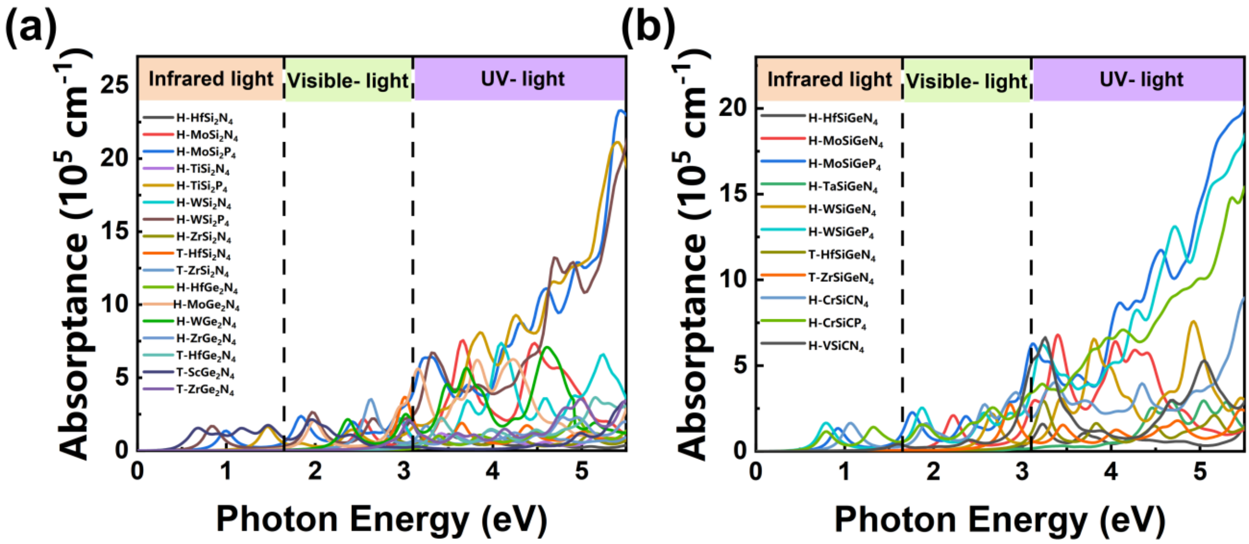


Fig. S11 Light absorption coefficients of Janus MA_2Z_4 and symmetric MA_2Z_4.

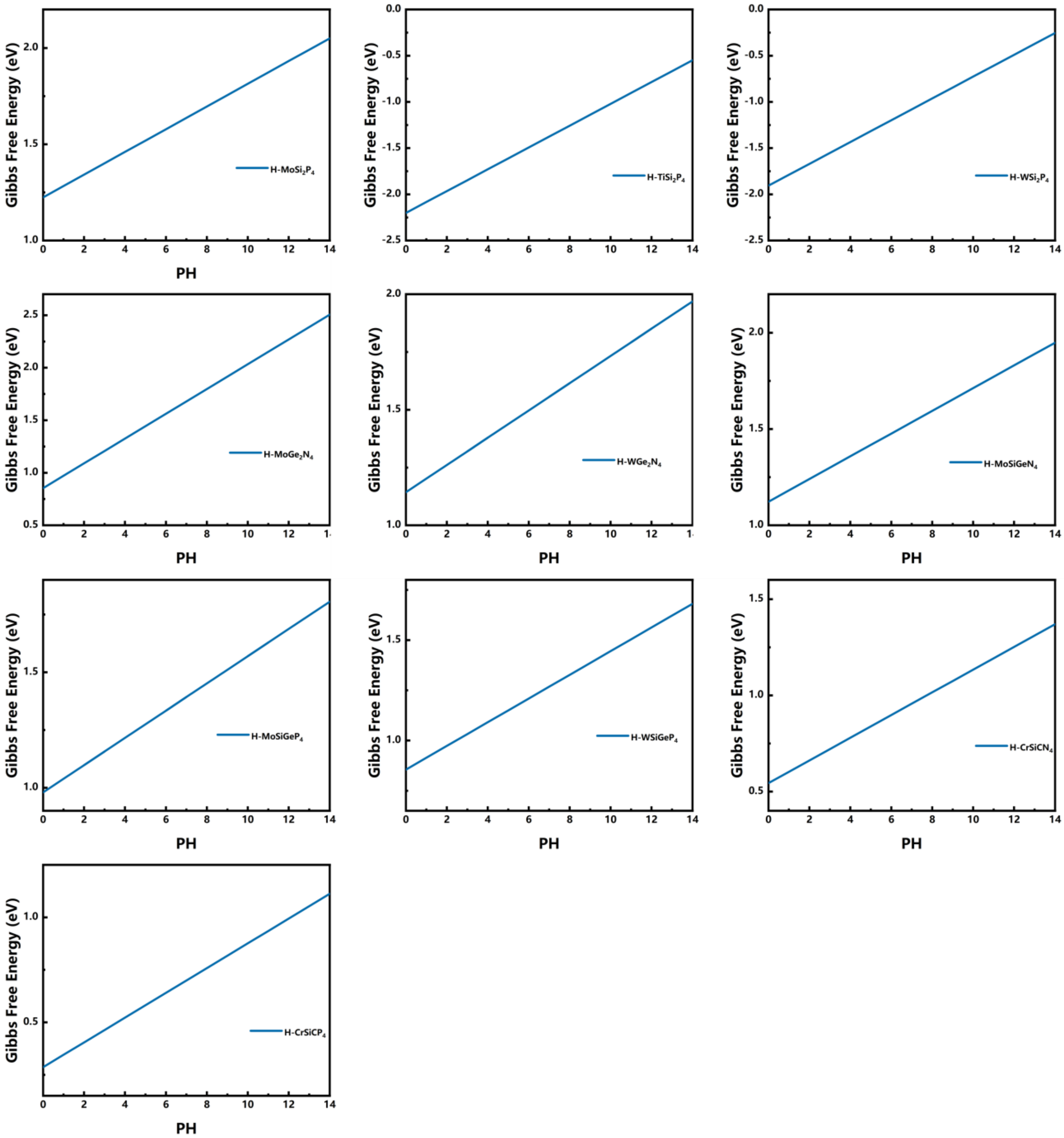


Fig. S12   HER adsorption energy at different PH.

Supporting Tables

Table S1 Formation energy of H phase symmetric MA_2Z_4 structures

Structure	$E_f(eV)$	Structure	$E_f(eV)$	Structure	$E_f(eV)$
H-$CrSi_2As_4$	-1.53621	H-$CrGe_2As_4$	-1.63928	H-CrC_2As_4	-1.56927
H-$CrSi_2N_4$	-4.55043	H-$CrGe_2N_4$	-3.73512	H-CrC_2N_4	-3.6433
H-$CrSi_2P_4$	-1.53206	H-$CrGe_2P_4$	-1.54771	H-CrC_2P_4	-1.86761
H-$CrSi_2S_4$	-2.1434	H-$CrGe_2S_4$	-2.17696	H-CrC_2S_4	-1.40492
H-$CrSi_2Se_4$	-1.42037	H-$CrGe_2Se_4$	-1.51632	H-CrC_2Se_4	-0.65914
H-$CrSi_2Te_4$	-1.07655	H-$CrGe_2Te_4$	-1.20285	H-CrC_2Te_4	-0.36513
H-$HfSi_2As_4$	-1.7447	H-$HfGe_2As_4$	-1.85079	H-HfC_2As_4	-1.69599
H-$HfSi_2N_4$	-4.89378	H-$HfGe_2N_4$	-4.63656	H-HfC_2N_4	-3.29147
H-$HfSi_2P_4$	-1.5682	H-$HfGe_2P_4$	-2.00537	H-HfC_2P_4	-1.86402
H-$HfSi_2S_4$	-2.55749	H-$HfGe_2S_4$	-3.04349	H-HfC_2S_4	-1.64121
H-$HfSi_2Se_4$	-1.85125	H-$HfGe_2Se_4$	-2.37868	H-HfC_2Se_4	-0.92946
H-$HfSi_2Te_4$	-1.46648	H-$HfGe_2Te_4$	-2.01203	H-HfC_2Te_4	-0.657
H-$MoSi_2As_4$	-1.52403	H-$MoGe_2As_4$	-1.62908	H-MoC_2As_4	-1.54983
H-$MoSi_2N_4$	-4.64147	H-$MoGe_2N_4$	-3.87599	H-MoC_2N_4	-3.4213
H-$MoSi_2P_4$	-2.13252	H-$MoGe_2P_4$	-1.46724	H-MoC_2P_4	-1.80966
H-$MoSi_2S_4$	-2.23908	H-$MoGe_2S_4$	-2.27387	H-MoC_2S_4	-1.39711
H-$MoSi_2Se_4$	-1.5073	H-$MoGe_2Se_4$	-1.59396	H-MoC_2Se_4	-0.68717
H-$MoSi_2Te_4$	-1.12603	H-$MoGe_2Te_4$	-1.24886	H-MoC_2Te_4	-0.40269
H-$ScSi_2As_4$	-1.42546	H-$ScGe_2As_4$	-1.52309	H-ScC_2As_4	-1.39678
H-$ScSi_2N_4$	-4.28884	H-$ScGe_2N_4$	-3.616	H-ScC_2N_4	-2.94745
H-$ScSi_2P_4$	-1.25203	H-$ScGe_2P_4$	-1.26996	H-ScC_2P_4	-1.54435
H-$ScSi_2S_4$	-2.23919	H-$ScGe_2S_4$	-2.27827	H-ScC_2S_4	-1.34176
H-$ScSi_2Se_4$	-1.62636	H-$ScGe_2Se_4$	-.908611	H-ScC_2Se_4	-0.66479
H-$ScSi_2Te_4$	-1.20581	H-$ScGe_2Te_4$	-1.36069	H-ScC_2Te_4	-0.34624
H-$TaSi_2As_4$	-1.73217	H-$TaGe_2As_4$	-1.82522	H-TaC_2As_4	-1.69654
H-$TaSi_2N_4$	-4.89502	H-$TaGe_2N_4$	-4.1775	H-TaC_2N_4	-3.46986
H-$TaSi_2P_4$	-1.60968	H-$TaGe_2P_4$	-1.64091	H-TaC_2P_4	-1.92664
H-$TaSi_2S_4$	-2.48561	H-$TaGe_2S_4$	-2.54342	H-TaC_2S_4	-1.52162
H-$TaSi_2Se_4$	-1.74104	H-$TaGe_2Se_4$	-1.84757	H-TaC_2Se_4	-0.8384
H-$TaSi_2Te_4$	-1.3351	H-$TaGe_2Te_4$	-1.48409	H-TaC_2Te_4	-0.57411
H-$TiSi_2As_4$	-1.61005	H-$TiGe_2As_4$	-1.71538	H-TiC_2As_4	-1.58024
H-$TiSi_2N_4$	-4.69403	H-$TiGe_2N_4$	-3.99473	H-TiC_2N_4	-3.43092
H-$TiSi_2P_4$	-2.11829	H-$TiGe_2P_4$	-1.5269	H-TiC_2P_4	-1.79553
H-$TiSi_2S_4$	-2.19883	H-$TiGe_2S_4$	-2.36603	H-TiC_2S_4	-1.46633
H-$TiSi_2Se_4$	-1.58424	H-$TiGe_2Se_4$	-1.69752	H-TiC_2Se_4	-0.74335
H-$TiSi_2Te_4$	-1.2341	H-$TiGe_2Te_4$	-1.38386	H-TiC_2Te_4	-0.48188
H-VSi_2As_4	-1.78022	H-VGe_2As_4	-1.8758	H-VC_2As_4	-1.78553
H-VSi_2N_4	-4.84383	H-VGe_2N_4	-4.07183	H-VC_2N_4	-3.77692
H-VSi_2P_4	-1.73466	H-VGe_2P_4	-1.73928	H-VC_2P_4	-2.05502
H-VSi_2S_4	-2.3912	H-VGe_2S_4	-2.44091	H-VC_2S_4	-1.52521
H-VSi_2Se_4	-1.67258	H-VGe_2Se_4	-1.77744	H-VC_2Se_4	-0.86367
H-VSi_2Te_4	-1.32609	H-VGe_2Te_4	-1.47082	H-VC_2Te_4	-0.61326

H-WSi_2As_4	-1.79064	H-WGe_2As_4	-1.89099	H-WC_2As_4	-1.7846
H-WSi_2N_4	-4.9912	H-WGe_2N_4	-4.19632	H-WC_2N_4	-3.70007
H-WSi_2P_4	-2.40938	H-WGe_2P_4	-1.74217	H-WC_2P_4	-2.06607
H-WSi_2S_4	-2.52713	H-WGe_2S_4	-2.54921	H-WC_2S_4	-1.66244
H-WSi_2Se_4	-1.776	H-WGe_2Se_4	-1.85316	H-WC_2Se_4	-0.94815
H-WSi_2Te_4	-1.35792	H-WGe_2Te_4	-1.47774	H-WC_2Te_4	-0.45626
H-$NbSi_2As_4$	-1.44653	H-$NbGe_2As_4$	-1.54459	H-NbC_2As_4	-1.4537
H-$NbSi_2N_4$	-4.56341	H-$NbGe_2N_4$	-3.85025	H-NbC_2N_4	-3.18256
H-$NbSi_2P_4$	-1.32455	H-$NbGe_2P_4$	-1.35434	H-NbC_2P_4	-1.66902
H-$NbSi_2S_4$	-2.20329	H-$NbGe_2S_4$	-2.26193	H-NbC_2S_4	-1.27631
H-$NbSi_2Se_4$	-1.47859	H-$NbGe_2Se_4$	-1.58625	H-NbC_2Se_4	-0.58924
H-$NbSi_2Te_4$	-1.10014	H-$NbGe_2Te_4$	-1.25018	H-NbC_2Te_4	-0.34493
H-$ZrSi_2As_4$	-1.59347	H-$ZrGe_2As_4$	-1.69801	H-ZrC_2As_4	-1.57142
H-$ZrSi_2N_4$	-4.66275	H-$ZrGe_2N_4$	-4.03093	H-ZrC_2N_4	-3.05984
H-$ZrSi_2P_4$	-1.40312	H-$ZrGe_2P_4$	-1.44849	H-ZrC_2P_4	-1.71953
H-$ZrSi_2S_4$	-2.38198	H-$ZrGe_2S_4$	-2.48195	H-ZrC_2S_4	-1.50525
H-$ZrSi_2Se_4$	-1.69436	H-$ZrGe_2Se_4$	-1.83438	H-ZrC_2Se_4	-0.80868
H-$ZrSi_2Te_4$	-1.14951	H-$ZrGe_2Te_4$	-1.48824	H-ZrC_2Te_4	-0.54328

Table S2 Formation energy of T phase symmetric MA_2Z_4 structures

Structure	$E_f(eV)$	Structure	$E_f(eV)$	Structure	$E_f(eV)$
T-$CrSi_2As_4$	-1.5511	T-$CrGe_2As_4$	-1.6508	T-CrC_2As_4	-1.537
T-$CrSi_2N_4$	-4.49288	T-$CrGe_2N_4$	-3.78382	T-CrC_2N_4	-3.468
T-$CrSi_2P_4$	-1.98958	T-$CrGe_2P_4$	-1.5433	T-CrC_2P_4	-1.82064
T-$CrSi_2S_4$	-2.12426	T-$CrGe_2S_4$	-2.12045	T-CrC_2S_4	-1.46269
T-$CrSi_2Se_4$	-1.34752	T-$CrGe_2Se_4$	-1.14884	T-CrC_2Se_4	-0.61724
T-$CrSi_2Te_4$	-0.70589	T-$CrGe_2Te_4$	-0.94443	T-CrC_2Te_4	-0.33027
T-$HfSi_2As_4$	-1.74432	T-$HfGe_2As_4$	-1.85592	T-HfC_2As_4	-1.70519
T-$HfSi_2N_4$	-4.93828	T-$HfGe_2N_4$	-4.35005	T-HfC_2N_4	-3.30124
T-$HfSi_2P_4$	-1.19925	T-$HfGe_2P_4$	-0.3817	T-HfC_2P_4	-1.87501
T-$HfSi_2S_4$	-2.59429	T-$HfGe_2S_4$	-2.67479	T-HfC_2S_4	-1.78399
T-$HfSi_2Se_4$	-1.87271	T-$HfGe_2Se_4$	-1.84263	T-HfC_2Se_4	-0.91709
T-$HfSi_2Te_4$	-1.24485	T-$HfGe_2Te_4$	-1.20623	T-HfC_2Te_4	-0.65717
T-$MoSi_2As_4$	-1.52782	T-$MoGe_2As_4$	-1.64113	T-MoC_2As_4	-1.5132
T-$MoSi_2N_4$	-4.50542	T-$MoGe_2N_4$	-3.79711	T-MoC_2N_4	-3.28271
T-$MoSi_2P_4$	-2.04001	T-$MoGe_2P_4$	-1.47312	T-MoC_2P_4	-1.7565
T-$MoSi_2S_4$	-2.12877	T-$MoGe_2S_4$	-2.16953	T-MoC_2S_4	-1.37282
T-$MoSi_2Se_4$	-1.36358	T-$MoGe_2Se_4$	-1.49855	T-MoC_2Se_4	-0.60782
T-$MoSi_2Te_4$	-0.87196	T-$MoGe_2Te_4$	-0.95342	T-MoC_2Te_4	-0.36418
T-$ScSi_2As_4$	-1.43117	T-$ScGe_2As_4$	-1.54375	T-ScC_2As_4	-1.40608
T-$ScSi_2N_4$	-4.36035	T-$ScGe_2N_4$	-3.75179	T-ScC_2N_4	-2.95526
T-$ScSi_2P_4$	-1.97251	T-$ScGe_2P_4$	-1.27643	T-ScC_2P_4	-1.55778
T-$ScSi_2S_4$	-2.30833	T-$ScGe_2S_4$	-2.27294	T-ScC_2S_4	-1.40089
T-$ScSi_2Se_4$	-1.54098	T-$ScGe_2Se_4$	-1.53522	T-ScC_2Se_4	-0.72684
T-$ScSi_2Te_4$	-0.94383	T-$ScGe_2Te_4$	-0.90861	T-ScC_2Te_4	-0.34375

T-$TaSi_2As_4$	-1.72198	T-$TaGe_2As_4$	-1.89299	T-TaC_2As_4	-1.69568
T-$TaSi_2N_4$	-4.85765	T-$TaGe_2N_4$	-4.20077	T-TaC_2N_4	-3.42461
T-$TaSi_2P_4$	-2.28187	T-$TaGe_2P_4$	-2.13653	T-TaC_2P_4	-1.91821
T-$TaSi_2S_4$	-2.46455	T-$TaGe_2S_4$	-0.5596	T-TaC_2S_4	-1.64813
T-$TaSi_2Se_4$	-1.6546	T-$TaGe_2Se_4$	-1.79115	T-TaC_2Se_4	-0.83719
T-$TaSi_2Te_4$	-1.19429	T-$TaGe_2Te_4$	-1.0918	T-TaC_2Te_4	-0.57685
T-$TiSi_2As_4$	-1.81111	T-$TiGe_2As_4$	-1.72396	T-TiC_2As_4	-1.61246
T-$TiSi_2N_4$	-4.79721	T-$TiGe_2N_4$	-4.12206	T-TiC_2N_4	-3.42972
T-$TiSi_2P_4$	-1.69661	T-$TiGe_2P_4$	-1.53292	T-TiC_2P_4	-1.83015
T-$TiSi_2S_4$	-2.36102	T-$TiGe_2S_4$	-2.48353	T-TiC_2S_4	-1.62283
T-$TiSi_2Se_4$	-1.57864	T-$TiGe_2Se_4$	-1.75388	T-TiC_2Se_4	-0.75634
T-$TiSi_2Te_4$	-1.07956	T-$TiGe_2Te_4$	-1.06497	T-TiC_2Te_4	-0.43615
T-VSi_2As_4	-1.79358	T-VGe_2As_4	-1.89761	T-VC_2As_4	-1.78014
T-VSi_2N_4	-4.85948	T-VGe_2N_4	-4.13912	T-VC_2N_4	-3.70041
T-VSi_2P_4	-1.77239	T-VGe_2P_4	-1.76557	T-VC_2P_4	-2.04167
T-VSi_2S_4	-2.4109	T-VGe_2S_4	-2.38913	T-VC_2S_4	-1.68442
T-VSi_2Se_4	-1.65409	T-VGe_2Se_4	-1.78961	T-VC_2Se_4	-0.86798
T-VSi_2Te_4	-1.22613	T-VGe_2Te_4	-1.26821	T-VC_2Te_4	-0.64419
T-WSi_2As_4	-1.85038	T-WGe_2As_4	-1.90214	T-WC_2As_4	-1.74249
T-WSi_2N_4	-4.80486	T-WGe_2N_4	-4.09966	T-WC_2N_4	-3.55408
T-WSi_2P_4	-2.30652	T-WGe_2P_4	-2.15299	T-WC_2P_4	-2.00976
T-WSi_2S_4	-2.39804	T-WGe_2S_4	-2.43973	T-WC_2S_4	-1.56022
T-WSi_2Se_4	-1.6157	T-WGe_2Se_4	-1.67523	T-WC_2Se_4	-0.86096
T-WSi_2Te_4	-1.18264	T-WGe_2Te_4	-1.16778	T-WC_2Te_4	-0.51633
T-$NbSi_2As_4$	-1.45194	T-$NbGe_2As_4$	-1.56846	T-NbC_2As_4	-1.4479
T-$NbSi_2N_4$	-4.53975	T-$NbGe_2N_4$	-3.87861	T-NbC_2N_4	-3.14413
T-$NbSi_2P_4$	-1.32485	T-$NbGe_2P_4$	-1.69598	T-NbC_2P_4	-1.65539
T-$NbSi_2S_4$	-2.18617	T-$NbGe_2S_4$	-1.78242	T-NbC_2S_4	-1.42672
T-$NbSi_2Se_4$	-1.50848	T-$NbGe_2Se_4$	-1.39576	T-NbC_2Se_4	-0.58621
T-$NbSi_2Te_4$	-1.51507	T-$NbGe_2Te_4$	-0.79837	T-NbC_2Te_4	-0.38353
T-$ZrSi_2As_4$	-1.60182	T-$ZrGe_2As_4$	-1.7262	T-ZrC_2As_4	-1.58788
T-$ZrSi_2N_4$	-4.69926	T-$ZrGe_2N_4$	-4.12463	T-ZrC_2N_4	-3.08332
T-$ZrSi_2P_4$	-1.4071	T-$ZrGe_2P_4$	-1.44973	T-ZrC_2P_4	-1.73552
T-$ZrSi_2S_4$	-2.48172	T-$ZrGe_2S_4$	-2.49479	T-ZrC_2S_4	-1.67933
T-$ZrSi_2Se_4$	-1.61098	T-$ZrGe_2Se_4$	-1.68485	T-ZrC_2Se_4	-0.79306
T-$ZrSi_2Te_4$	-1.18479	T-$ZrGe_2Te_4$	-1.07389	T-ZrC_2Te_4	-0.50584

Table S3 Formation energy of asymmetric H-MA_2Z_4 Janus structures

Structure	$E_f(eV)$	Structure	$E_f(eV)$		$E_f(eV)$
H-$CrSiGeAs_4$	-1.36623	H-$CrCGeAs_4$	-1.59844	H-$CrSiCAs_4$	-1.66695
H-$CrSiGeN_4$	-4.10545	H-$CrCGeN_4$	-3.42759	H-$CrSiCN_4$	-3.95802
H-$CrSiGeP_4$	-1.52787	H-$CrCGeP_4$	-1.66665	H-$CrSiCP_4$	-1.85087
H-$CrSiGeS_4$	-2.14441	H-$CrCGeS_4$	-1.69714	H-$CrSiCS_4$	-1.67321
H-$CrSiGeSe_4$	-1.45521	H-$CrCGeSe_4$	-1.02063	H-$CrSiCSe_4$	-1.00171
H-$CrSiGeTe_4$	-1.06429	H-$CrCGeTe_4$	-0.8259	H-$CrSiCTe_4$	-0.69743

H-$HfSiGeAs_4$	-1.80188	H-$HfCGeAs_4$	-1.78439	H-$HfSiCAs_4$	-1.85057
H-$HfSiGeN_4$	-4.55369	H-$HfCGeN_4$	-3.66795	H-$HfSiCN_4$	-4.04652
H-$HfSiGeP_4$	-1.58375	H-$HfCGeP_4$	-1.83137	H-$HfSiCP_4$	-1.94328
H-$HfSiGeS_4$	-2.60136	H-$HfCGeS_4$	-2.15277	H-$HfSiCS_4$	-2.10656
H-$HfSiGeSe_4$	-1.91645	H-$HfCGeSe_4$	-1.46882	H-$HfSiCSe_4$	-1.39863
H-$HfSiGeTe_4$	-1.54028	H-$HfCGeTe_4$	-1.14284	H-$HfSiCTe_4$	-1.06871
H-$MoSiGeAs_4$	-1.58236	H-$MoCGeAs_4$	-1.63811	H-$MoSiCAs_4$	-1.70428
H-$MoSiGeN_4$	-4.23105	H-$MoCGeN_4$	-3.44157	H-$MoSiCN_4$	-3.92125
H-$MoSiGeP_4$	-2.04205	H-$MoCGeP_4$	-1.75658	H-$MoSiCP_4$	-1.87895
H-$MoSiGeS_4$	-2.2499	H-$MoCGeS_4$	-1.76548	H-$MoSiCS_4$	-1.77623
H-$MoSiGeSe_4$	-1.54721	H-$MoCGeSe_4$	-1.09144	H-$MoSiCSe_4$	-1.06706
H-$MoSiGeTe_4$	-1.18682	H-$MoCGeTe_4$	-0.77586	H-$MoSiCTe_4$	-0.73034
H-$NbSiGeAs_4$	-1.50375	H-$ScCGeAs_4$	-1.46302	H-$ScSiCAs_4$	-1.53061
H-$NbSiGeN_4$	-4.1886	H-$ScCGeN_4$	-3.21557	H-$ScSiCN_4$	-3.58331
H-$NbSiGeP_4$	-1.3337	H-$ScCGeP_4$	-1.405	H-$ScSiCP_4$	-1.57326
H-$NbSiGeS_4$	-2.22911	H-$ScCGeS_4$	-1.85511	H-$ScSiCS_4$	-1.75155
H-$NbSiGeSe_4$	-1.5304	H-$ScCGeSe_4$	-1.20225	H-$ScSiCSe_4$	-1.13049
H-$NbSiGeTe_4$	-1.17419	H-$ScCGeTe_4$	-0.89171	H-$ScSiCTe_4$	-0.8138
H-$ScSiGeAs_4$	-1.48104	H-$TaCGeAs_4$	-1.79874	H-$TaSiCAs_4$	-1.85904
H-$ScSiGeN_4$	-3.93607	H-$TaCGeN_4$	-3.66914	H-$TaSiCN_4$	-4.10121
H-$ScSiGeP_4$	-1.25656	H-$TaCGeP_4$	-1.79773	H-$TaSiCP_4$	-2.01707
H-$ScSiGeS_4$	-2.30731	H-$TaCGeS_4$	-2.06128	H-$TaSiCS_4$	-2.03189
H-$ScSiGeSe_4$	-1.62742	H-$TaCGeSe_4$	-1.31135	H-$TaSiCSe_4$	-1.27265
H-$ScSiGeTe_4$	-1.28841	H-$TaCGeTe_4$	-1.01779	H-$TaSiCTe_4$	-0.94233
H-$TaSiGeAs_4$	-1.78539	H-$TiCGeAs_4$	-1.63682	H-$TiSiCAs_4$	-1.69721
H-$TaSiGeN_4$	-4.51876	H-$TiCGeN_4$	-3.5046	H-$TiSiCN_4$	-3.95433
H-$TaSiGeP_4$	-1.62439	H-$TiCGeP_4$	-1.6395	H-$TiSiCP_4$	-1.7968
H-$TaSiGeS_4$	-2.51037	H-$TiCGeS_4$	-1.92019	H-$TiSiCS_4$	-1.88852
H-$TaSiGeSe_4$	-1.79234	H-$TiCGeSe_4$	-1.23887	H-$TiSiCSe_4$	-1.17979
H-$TaSiGeTe_4$	-1.40845	H-$TiCGeTe_4$	-0.92773	H-$TiSiCTe_4$	-0.85283
H-$TiSiGeAs_4$	-1.65926	H-$VCGeAs_4$	-1.81125	H-$VSiCAs_4$	-1.88248
H-$TiSiGeN_4$	-4.30737	H-$VCGeN_4$	-3.68159	H-$VSiCN_4$	-4.17761
H-$TiSiGeP_4$	-1.50932	H-$VCGeP_4$	-1.85986	H-$VSiCP_4$	-2.03935
H-$TiSiGeS_4$	-2.27897	H-$VCGeS_4$	-2.01622	H-$VSiCS_4$	-1.99869
H-$TiSiGeSe_4$	-1.6376	H-$VCGeSe_4$	-1.31813	H-$VSiCSe_4$	-1.26749
H-$TiSiGeTe_4$	-1.21804	H-$VCGeTe_4$	-1.02639	H-$VSiCTe_4$	-0.95792
H-$VSiGeAs_4$	-1.82414	H-$WCGeAs_4$	-1.88417	H-$WSiCAs_4$	-1.94967
H-$VSiGeN_4$	-4.42516	H-$WCGeN_4$	-3.78308	H-$WSiCN_4$	-4.26092
H-$VSiGeP_4$	-1.73073	H-$WCGeP_4$	-2.03259	H-$WSiCP_4$	-2.15376
H-$VSiGeS_4$	-2.40363	H-$WCGeS_4$	-2.05362	H-$WSiCS_4$	-2.063
H-$VSiGeSe_4$	-1.71578	H-$WCGeSe_4$	-1.36187	H-$WSiCSe_4$	-1.33768
H-$VSiGeTe_4$	-3.171	H-$WCGeTe_4$	-1.01684	H-$WSiCTe_4$	-0.96323
H-$WSiGeAs_4$	-1.84705	H-$NbCGeAs_4$	-1.50099	H-$NbSiCAs_4$	-1.60596
H-$WSiGeN_4$	-4.58006	H-$NbCGeN_4$	-3.34495	H-$NbSiCN_4$	-3.77865
H-$WSiGeP_4$	-2.31957	H-$NbCGeP_4$	-1.6288	H-$NbSiCP_4$	-1.74694
H-$WSiGeS_4$	-2.3799	H-$NbCGeS_4$	-1.80353	H-$NbSiCS_4$	-1.77366

H-WSiGeSe_4	-1.81506	H-NbCGeSe_4	-1.10172	H-NbSiCSe_4	-1.04456
H-WSiGeTe_4	-1.41998	H-NbCGeTe_4	-0.78532	H-NbSiCTe_4	-0.71373
H-ZrSiGeAs_4	-1.65061	H-ZrCGeAs_4	-1.64529	H-ZrSiCAs_4	-1.72663
H-ZrSiGeN_4	-4.32969	H-ZrCGeN_4	-3.44086	H-ZrSiCN_4	-3.80896
H-ZrSiGeP_4	-2.10452	H-ZrCGeP_4	-1.59924	H-ZrSiCP_4	-1.80263
H-ZrSiGeS_4	-2.41149	H-ZrCGeS_4	-1.99426	H-ZrSiCS_4	-1.94607
H-ZrSiGeSe_4	-1.76241	H-ZrCGeSe_4	-1.32332	H-ZrSiCSe_4	-1.25506
H-ZrSiGeTe_4	-1.40952	H-ZrCGeTe_4	-1.03285	H-ZrSiCTe_4	-0.95487

Table S4 Formation energy of asymmetric T-MA_2Z_4 Janus structures

Structure	$E_f(eV)$	Structure	$E_f(eV)$	Structure	$E_f(eV)$
T-CrSiGeAs_4	-1.59324	T-CrCGeAs_4	-1.56369	T-CrSiCAs_4	-1.62663
T-CrSiGeN_4	-4.07856	T-CrCGeN_4	-3.41207	T-CrSiCN_4	-3.83853
T-CrSiGeP_4	-1.88767	T-CrCGeP_4	-1.65354	T-CrSiCP_4	-1.79108
T-CrSiGeS_4	-2.08851	T-CrCGeS_4	-1.89621	T-CrSiCS_4	-1.83343
T-CrSiGeSe_4	-1.45314	T-CrCGeSe_4	-1.14886	T-CrSiCSe_4	-0.97089
T-CrSiGeTe_4	-0.89211	T-CrCGeTe_4	-0.76139	T-CrSiCTe_4	-0.74577
T-HfSiGeAs_4	-1.812	T-HfCGeAs_4	-1.83824	T-HfSiCAs_4	-1.89724
T-HfSiGeN_4	-4.61513	T-HfCGeN_4	-3.6932	T-HfSiCN_4	-4.06455
T-HfSiGeP_4	-1.58474	T-HfCGeP_4	-1.87852	T-HfSiCP_4	-1.98977
T-HfSiGeS_4	-2.63783	T-HfCGeS_4	-2.26249	T-HfSiCS_4	-2.20809
T-HfSiGeSe_4	-1.91767	T-HfCGeSe_4	-1.4733	T-HfSiCSe_4	-1.43856
T-HfSiGeTe_4	-1.25119	T-HfCGeTe_4	-0.98712	T-HfSiCTe_4	-0.9848
T-MoSiGeAs_4	-1.83865	T-MoCGeAs_4	-1.58361	T-MoSiCAs_4	-1.64624
T-MoSiGeN_4	-4.08388	T-MoCGeN_4	-3.30393	T-MoSiCN_4	-3.77869
T-MoSiGeP_4	-1.94876	T-MoCGeP_4	-1.62043	T-MoSiCP_4	-1.80545
T-MoSiGeS_4	-2.13487	T-MoCGeS_4	-1.76009	T-MoSiCS_4	-1.76098
T-MoSiGeSe_4	-1.46604	T-MoCGeSe_4	-0.98835	T-MoSiCSe_4	-0.96936
T-MoSiGeTe_4	-0.89296	T-MoCGeTe_4	-0.69851	T-MoSiCTe_4	-0.69578
T-NbSiGeAs_4	-1.57146	T-ScCGeAs_4	-1.47432	T-ScSiCAs_4	-1.57574
T-NbSiGeN_4	-4.16629	T-ScCGeN_4	-3.35448	T-ScSiCN_4	-3.72055
T-NbSiGeP_4	-1.91651	T-ScCGeP_4	-1.41799	T-ScSiCP_4	-1.61195
T-NbSiGeS_4	-2.20838	T-ScCGeS_4	-2.00956	T-ScSiCS_4	-1.93393
T-NbSiGeSe_4	-1.50284	T-ScCGeSe_4	-1.22012	T-ScSiCSe_4	-1.10121
T-NbSiGeTe_4	-0.93978	T-ScCGeTe_4	-0.72507	T-ScSiCTe_4	-0.66915
T-ScSiGeAs_4	-1.48293	T-TaCGeAs_4	-1.78487	T-TaSiCAs_4	-1.84647
T-ScSiGeN_4	-4.01767	T-TaCGeN_4	-3.6311	T-TaSiCN_4	-4.06422
T-ScSiGeP_4	-1.89887	T-TaCGeP_4	-1.88281	T-TaSiCP_4	-1.99984
T-ScSiGeS_4	-2.27891	T-TaCGeS_4	-2.094	T-TaSiCS_4	-2.07424
T-ScSiGeSe_4	-1.63514	T-TaCGeSe_4	-1.30283	T-TaSiCSe_4	-1.2607
T-ScSiGeTe_4	-0.95849	T-TaCGeTe_4	-0.87775	T-TaSiCTe_4	-0.82831
T-TaSiGeAs_4	-1.8369	T-TiCGeAs_4	-1.66481	T-TiSiCAs_4	-1.73691
T-TaSiGeN_4	-4.49585	T-TiCGeN_4	-3.53526	T-TiSiCN_4	-3.97939
T-TaSiGeP_4	-1.69691	T-TiCGeP_4	-1.67474	T-TiSiCP_4	-1.84688
T-TaSiGeS_4	-2.49377	T-TiCGeS_4	-2.02092	T-TiSiCS_4	-1.982
T-TaSiGeSe_4	-1.76544	T-TiCGeSe_4	-1.2406	T-TiSiCSe_4	-1.22313

T-$TaSiGeTe_4$	-0.93815	T-$TiCGeTe_4$	-0.81788	T-$TiSiCTe_4$	-0.80941
T-$TiSiGeAs_4$	-1.75798	T-$VCGeAs_4$	-1.82913	T-$VSiCAs_4$	-1.87554
T-$TiSiGeN_4$	-4.37416	T-$VCGeN_4$	-3.64982	T-$VSiCN_4$	-4.14359
T-$TiSiGeP_4$	-1.51387	T-$VCGeP_4$	-1.89329	T-$VSiCP_4$	-2.02708
T-$TiSiGeS_4$	-1.93326	T-$VCGeS_4$	-2.0634	T-$VSiCS_4$	-2.05173
T-$TiSiGeSe_4$	-1.71227	T-$VCGeSe_4$	-1.26178	T-$VSiCSe_4$	-1.23422
T-$TiSiGeTe_4$	-1.10734	T-$VCGeTe_4$	-0.93025	T-$VSiCTe_4$	-0.8792
T-$VSiGeAs_4$	-1.8489	T-$WCGeAs_4$	-1.8274	T-$WSiCAs_4$	-1.88769
T-$VSiGeN_4$	-4.42421	T-$WCGeN_4$	-3.62841	T-$WSiCN_4$	-4.10095
T-$VSiGeP_4$	-1.74859	T-$WCGeP_4$	-1.95672	T-$WSiCP_4$	-2.07714
T-$VSiGeS_4$	-2.40557	T-$WCGeS_4$	-2.01637	T-$WSiCS_4$	-0.16581
T-$VSiGeSe_4$	-1.74368	T-$WCGeSe_4$	-1.2414	T-$WSiCSe_4$	-1.22912
T-$VSiGeTe_4$	-1.21655	T-$WCGeTe_4$	-0.96134	T-$WSiCTe_4$	-0.80058
T-$WSiGeAs_4$	-1.86184	T-$NbCGeAs_4$	-1.53052	T-$NbSiCAs_4$	-1.59116
T-$WSiGeN_4$	-4.4146	T-$NbCGeN_4$	-3.31368	T-$NbSiCN_4$	-3.74878
T-$WSiGeP_4$	-2.22493	T-$NbCGeP_4$	-1.60749	T-$NbSiCP_4$	-1.72652
T-$WSiGeS_4$	-2.4189	T-$NbCGeS_4$	-1.84878	T-$NbSiCS_4$	-1.80371
T-$WSiGeSe_4$	-1.64655	T-$NbCGeSe_4$	-1.0368	T-$NbSiCSe_4$	-1.00669
T-$WSiGeTe_4$	-0.95374	T-$NbCGeTe_4$	-0.64273	T-$NbSiCTe_4$	-0.59199
T-$ZrSiGeAs_4$	-1.83279	T-$ZrCGeAs_4$	-1.70415	T-$ZrSiCAs_4$	-1.76797
T-$ZrSiGeN_4$	-4.37667	T-$ZrCGeN_4$	-3.45851	T-$ZrSiCN_4$	-3.82305
T-$ZrSiGeP_4$	-2.11956	T-$ZrCGeP_4$	-1.73073	T-$ZrSiCP_4$	-1.84415
T-$ZrSiGeS_4$	-2.45802	T-$ZrCGeS_4$	-2.07956	T-$ZrSiCS_4$	-2.04684
T-$ZrSiGeSe_4$	-2.09302	T-$ZrCGeSe_4$	-1.32428	T-$ZrSiCSe_4$	-1.27479
T-$ZrSiGeTe_4$	-1.09395	T-$ZrCGeTe_4$	-0.84266	T-$ZrSiCTe_4$	-0.79327

Table S5 The elastic constants of MA_2Z_4 structures (in Nm^{-1})

Structure	C_{11}	C_{12}	C_{22}	C_{44}	$C_{11}C_{22}-C_{12}^2$
H-$CrSi_2N_4$	517.55	156.89	156.89	180.33	56583.01
H-$HfSi_2N_4$	466.43	153.54	153.54	156.44	48041.15
H-$MoSi_2N_4$	548.07	158.42	158.42	194.82	61728.60
H-$MoSi_2P_4$	219.20	56.79	56.79	81.21	9222.97
H-$TaSi_2N_4$	523.57	163.91	163.91	179.83	58952.28
H-$TiSi_2N_4$	495.98	156.72	156.72	169.63	53169.81
H-$TiSi_2P_4$	189.62	46.40	46.40	71.61	6645.02
H-WSi_2N_4	568.24	158.30	158.30	204.97	64893.70
H-WSi_2P_4	223.95	54.53	54.53	84.71	9238.59
H-$ZrSi_2N_4$	442.01	144.25	144.25	148.88	42952.16
H-$HfGe_2N_4$	405.60	142.67	142.67	131.46	37511.60
H-$MoGe_2N_4$	443.25	145.43	145.43	148.91	43311.54
H-WGe_2N_4	460.18	144.96	144.96	157.61	45693.98
H-$ZrGe_2N_4$	382.10	133.53	133.53	124.28	33192.34
T-$HfSi_2N_4$	464.62	123.57	123.57	171.05	42143.94
T-$ScSi_2N_4$	395.96	131.62	131.62	126.15	34793.40
T-$ScSi_2P_4$	168.06	47.77	47.77	36.17	5746.08
T-$TaSi_2N_4$	481.74	143.83	143.83	158.79	48601.61
T-$ZrSi_2N_4$	442.34	117.44	117.44	163.29	38155.03
T-$HfGe_2N_4$	413.47	124.29	124.29	145.82	35941.36

T-$NbGe_2N_4$	397.98	126.40	126.40	133.07	34328.11
T-$ScGe_2N_4$	334.35	123.01	123.01	102.81	25996.62
T-$TaGe_2N_4$	404.93	127.26	127.26	134.66	35336.89
T-$ZrGe_2N_4$	394.02	118.84	118.84	138.61	32702.38
H-$HfSiGeN_4$	429.53	146.72	146.72	141.41	41494.03
H-$MoSiGeN_4$	489.65	148.53	148.53	170.56	50665.94
H-$MoSiGeP_4$	209.34	57.97	57.97	75.68	8775.22
H-$NbSiGeP_4$	35.84	230.92	230.92	-97.54	-45048.92
H-$TaSiGeN_4$	480.88	154.51	154.51	163.18	50427.10
H-$TiSiGeN_4$	444.87	145.44	145.44	149.71	43549.51
H-$WSiGeN_4$	512.16	150.39	150.39	180.88	54407.10
H-$WSiGeP_4$	214.60	56.18	56.18	79.21	8900.31
H-$ZrSiGeN_4$	407.09	138.69	138.69	134.20	37224.92
H-$CrSiCAs_4$	192.83	61.73	61.73	65.55	8092.93
H-$CrSiCN_4$	473.42	155.51	155.51	158.96	49438.51
H-$CrSiCP_4$	235.59	59.62	59.62	87.99	10490.86
H-$MoSiCAs_4$	196.71	50.58	50.58	73.06	7391.02
H-$MoSiCP_4$	234.37	49.75	49.75	92.31	9185.21
H-$NbSiCAs_4$	149.93	72.07	72.07	38.93	5611.62
H-$NbSiCP_4$	206.44	72.98	72.98	66.73	9740.14
H-$TaSiCAs_4$	123.55	80.20	80.20	21.68	3477.04
H-$TaSiCP_4$	189.35	85.54	85.54	51.91	8880.02
H-$TiSiCP_4$	89.07	-1.24	-1.24	45.15	-111.54
H-$VSiCAs_4$	140.90	63.73	63.73	38.58	4917.91
H-$VSiCN_4$	432.40	166.79	166.79	132.80	44300.91
H-$VSiCP_4$	184.79	66.83	66.83	58.98	7883.03
H-$WSiCAs_4$	199.42	45.30	45.30	77.06	6981.25
H-$WSiCP_4$	235.01	46.33	46.33	94.34	8742.20
H-$MoCGeAs_4$	170.58	55.07	55.07	57.76	6361.23
H-$NbCGeP_4$	203.62	55.33	55.33	74.14	8205.10
H-$TaCGeAs_4$	156.05	49.48	49.48	53.29	5273.52
H-$WCGeAs_4$	171.23	52.11	52.11	59.56	6207.23
T-$HfSiGeN_4$	428.46	117.91	117.91	154.74	36616.82
T-$ScSiGeN_4$	352.19	117.86	117.86	116.57	27618.56
T-$ScSiGeP_4$	149.64	54.51	54.51	25.18	5185.22
T-$TaSiGeN_4$	437.27	126.54	126.54	154.67	39319.86
T-$ZrSiGeN_4$	408.71	112.71	112.71	147.55	33361.87
T-$HfSiCAs_4$	109.41	31.28	31.28	38.50	2443.92
T-$HfSiCP_4$	104.38	34.99	34.99	-185.26	2427.81
T-$ScSiCP_4$	132.56	36.63	36.63	54.54	3514.13
T-$TiSiCAs_4$	71.27	88.40	88.40	-14.97	-1513.51
T-$TiSiCP_4$	138.81	50.56	50.56	-30.98	4461.68
T-$ZrSiCP_4$	111.52	67.29	67.29	-580.09	2975.96

Table S6 Effective mass ($m^{\star}$), elastic modulus (C_{2D}), variable situation constant Ei and carrier mobility (μ_{2D}) in the xy direction for electrons and holes

Structure name		$m^{*}{}_{x}/m_0$	$m^{*}{}_{y}/m_0$	E_{ix}(eV)	E_{iy}(eV)	C_{2Dx}(eV)	C_{2Dy}(eV)	μ_x($cm^2/(Vs)$)	μ_y($cm^2/(Vs)$)
H-$HfSi_2N_4$	electron	0.80	0.86	452.55	452.41	2.94	2.93	1.17E+03	1.01E+03
	hole	2.35	2.48	452.55	452.41	2.47	2.67	1.90E+02	1.47E+02
H-$MoSi_2N_4$	electron	0.43	0.44	540.10	539.35	2.86	2.51	5.17E+03	6.42E+03
	hole	1.63	1.63	540.10	539.35	5.41	5.40	9.86E+01	9.92E+01

H-$MoSi_2P_4$	electron	0.32	0.33	221.09	220.41	4.51	4.31	1.48E+03	1.53E+03
	hole	0.34	0.38	221.09	220.41	2.16	2.43	5.90E+03	3.75E+03
H-$TaSi_2N_4$	electron	0.83	0.83	492.28	495.83	8.59	8.76	1.38E+02	1.33E+02
	hole	1.06	5.15	492.28	495.83	6.73	5.93	1.38E+02	7.56E+00
H-$TiSi_2N_4$	electron	1.44	3.26	471.90	471.89	3	4.08	3.61E+02	3.80E+01
	hole	3.84	1.13	471.90	471.89	3.47	3.05	3.78E+01	5.66E+02
H-$TiSi_2P_4$	electron	0.62	0.24	193.76	191.52	0.89	0.80	9.08E+03	7.27E+04
	hole	1.09	0.94	193.76	191.52	4.63	4.54	1.08E+02	1.51E+02
H-WSi_2N_4	electron	0.34	0.34	565.23	564.82	3.72	3.91	4.98E+03	4.66E+03
	hole	1.53	1.52	565.23	564.82	5.64	5.05	1.08E+02	1.37E+02
H-WSi_2P_4	electron	0.18	0.19	228.38	227.89	3.72	4.14	7.10E+03	5.42E+03
	hole	0.24	0.24	228.38	227.89	2.43	2.40	9.53E+03	9.61E+03
H-$ZrSi_2N_4$	electron	2.30	1.37	431.38	430.36	2.26	2.59	2.27E+02	4.88E+02
	hole	3.61	2.26	431.38	430.36	3.95	3.97	3.02E+01	7.60E+01
T-$HfSi_2N_4$	electron	0.52	0.24	492.89	491.44	5.1	5.79	1.00E+03	3.50E+03
	hole	-1.09	1.08	492.89	491.44	3.52	3.04	4.74E+02	6.43E+02
T-$ZrSi_2N_4$	electron	0.54	0.25	471.67	470.46	3.95	4.77	1.46E+03	4.74E+03
	hole	-1.10	-1.4	471.67	470.46	3.51	3.23	4.48E+02	3.30E+02
H-$HfGe_2N_4$	electron	0.72	2.2	383.63	381.39	2.17	2.00	2.26E+03	2.78E+02
	hole	1.86	1.8	383.63	381.39	3.09	3.13	1.66E+02	1.71E+02
H-$MoGe_2N_4$	electron	0.38	0.39	434.55	433.35	2.02	2.81	1.03E+04	5.11E+03
	hole	1.10	1.1	434.55	433.35	3.5	3.43	4.21E+02	4.38E+02
H-WGe_2N_4	electron	0.30	0.31	457.89	457.19	2.86	2.50	8.61E+03	1.09E+04
	hole	0.80	0.8	457.89	457.19	3.4	3.32	8.77E+02	9.22E+02
H-$ZrGe_2N_4$	electron	1.50	1.7	364.79	362.43	3.35	3.50	2.04E+02	1.45E+02
	hole	1.77	1.52	364.79	362.43	2.78	2.81	2.15E+02	2.81E+02
T-$HfGe_2N_4$	electron	0.21	0.21	416.89	415.66	8.47	8.62	1.86E+03	1.79E+03
	hole	1.29	0.97	416.89	415.66	2.28	2.05	6.84E+02	1.50E+03
T-$ScGe_2N_4$	electron	0.45	-0.99	413.62	413.16	3.98	3.56	1.80E+03	4.79E+02
	hole	0.65	0.66	413.62	413.16	4.64	4.29	6.46E+02	7.42E+02
T-$ZrGe_2N_4$	electron	0.31	0.65	401.27	400.01	3.84	3.72	4.08E+03	9.67E+02
	hole	-0.97	-1.03	401.27	400.01	4.54	4.54	2.94E+02	2.58E+02
H-$HfSiGeN_4$	electron	0.78	0.86	414.51	414.32	3.08	2.98	1.04E+03	8.93E+02
	hole	2.91	2.97	414.51	414.32	3.23	3.49	6.66E+01	5.50E+01
H-$MoSiGeN_4$	electron	0.40	0.41	484.97	484.22	1.94	1.63	1.16E+04	1.56E+04
	hole	-6.20	-6.2	484.97	484.22	4.79	4.74	7.83E+00	7.96E+00
H-$MoSiGeP_4$	electron	0.33	0.33	209.52	209.20	4.04	4.06	1.73E+03	1.62E+03
	hole	0.34	0.37	209.52	209.20	2.31	2.56	4.99E+03	3.25E+03
H-$TaSiGeN_4$	electron	1.57	1.8	468.55	476.69	3.27	2.51	2.52E+02	3.30E+02
	hole	1.52	1.27	468.55	476.69	4.27	3.79	1.58E+02	2.93E+02
H-$TiSiGeN_4$	electron	2.11	3	427.59	426.66	4.11	3.34	8.08E+01	6.04E+01
	hole	2.44	1.33	427.59	426.66	4.32	4.75	5.50E+01	1.51E+02
H-$WSiGeN_4$	electron	0.32	0.32	511.54	509.90	2.89	2.55	8.44E+03	1.09E+04
	hole	16.50	16.84	511.54	509.90	4.81	4.70	1.15E+00	1.16E+00
H-$WSiGeP_4$	electron	0.21	0.2	216.98	215.76	3.98	3.64	4.34E+03	5.79E+03
	hole	0.24	0.24	216.98	215.76	2.37	2.78	9.30E+03	6.69E+03
H-$ZrSiGeN_4$	electron	1.64	1.92	394.27	393.35	3.77	3.97	1.47E+02	9.60E+01
	hole	2.19	2.33	394.27	393.35	3.17	3.37	1.16E+02	9.10E+01
T-$HfSiGeN_4$	electron	0.56	0.27	449.62	449.21	2.32	5.72	3.75E+03	2.70E+03
	hole	1.08	1.11	449.62	449.21	8.61	8.75	7.41E+01	6.82E+01
T-$ZrSiGeN_4$	electron	0.22	0.61	431.75	431.04	3.48	2.68	1.01E+04	2.31E+03
	hole	1.01	1.28	431.75	431.04	5.34	5.48	2.11E+02	1.25E+02
H-$CrSiCN_4$	electron	0.95	1.03	490.90	478.38	6.93	6.62	1.62E+02	1.48E+02
	hole	0.95	1.05	490.90	478.38	3.45	3.68	6.56E+02	4.55E+02
H-$CrSiCP_4$	electron	0.25	0.76	224.25	228.76	1.25	2.12	3.33E+04	1.27E+03
	hole	0.51	0.6	224.25	228.76	2.05	2.53	2.98E+03	1.40E+03
H-$VSiCN_4$	electron	0.72	0.82	372.21	371.14	3	3.13	1.13E+03	8.01E+02
	hole	5.55	0.99	372.21	371.14	2.9	2.47	2.04E+01	8.83E+02

References

1 Atsushi, Togo, Fumiyasu, Oba, Isao and Tanaka, *Phys. Rev. B*, 2008, **78** 134106.

2 X. Gonze and C. Lee, *Phys. Rev. B*, 1997, **55**, 10355--10368.

3 V. Wang, N. Xu, J.-C. Liu, G. Tang and W.-T. Geng, *Comput. Phys. Commun.*, 2021, **267**, 108033.

4 J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. R. Kitchin, T. Bligaard and H. Jónsson, *J. Phys. Chem. B*, 2004, **108**, 17886-17892.