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


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# Supporting Information

## External field control and characteristic quantities of Rashba spin orbit coupling in $MA_2Z_4$ derived monolayer materials

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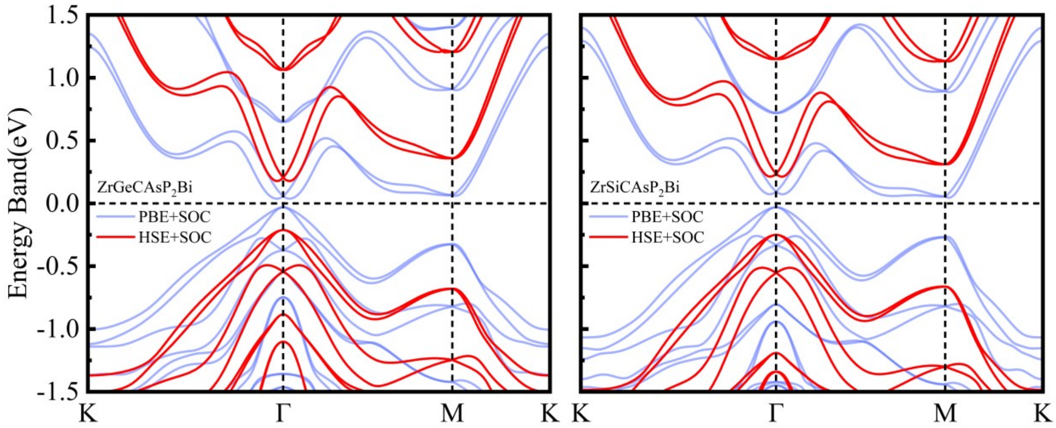



**Figure S1.** Band structures of several materials in $MA_2Z_4$ under PBE+SOC and HSE+SOC.

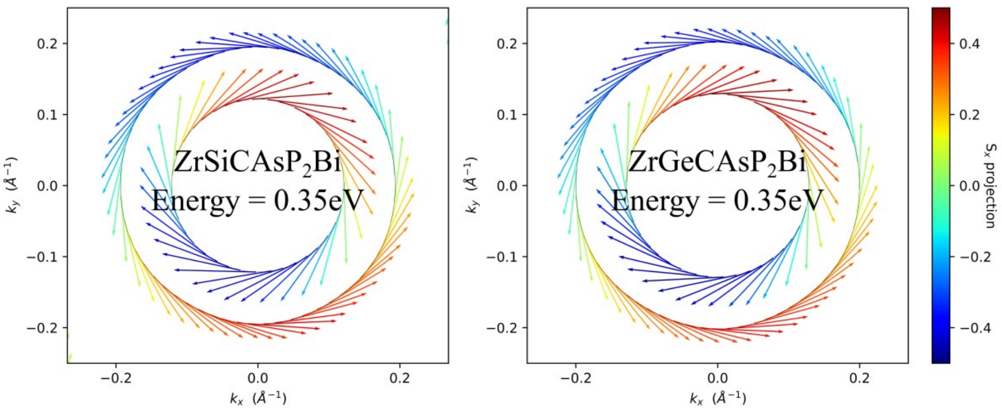
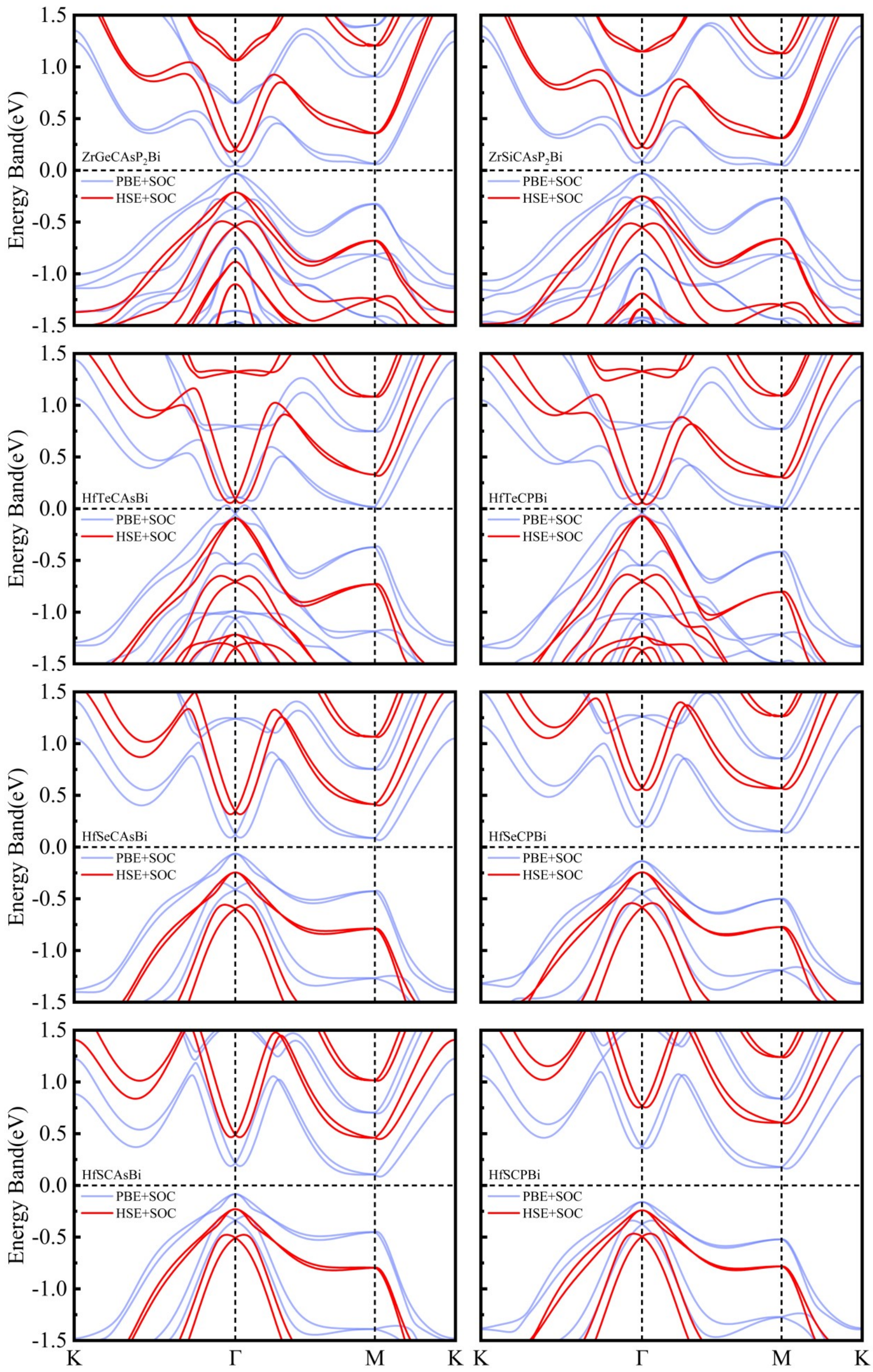
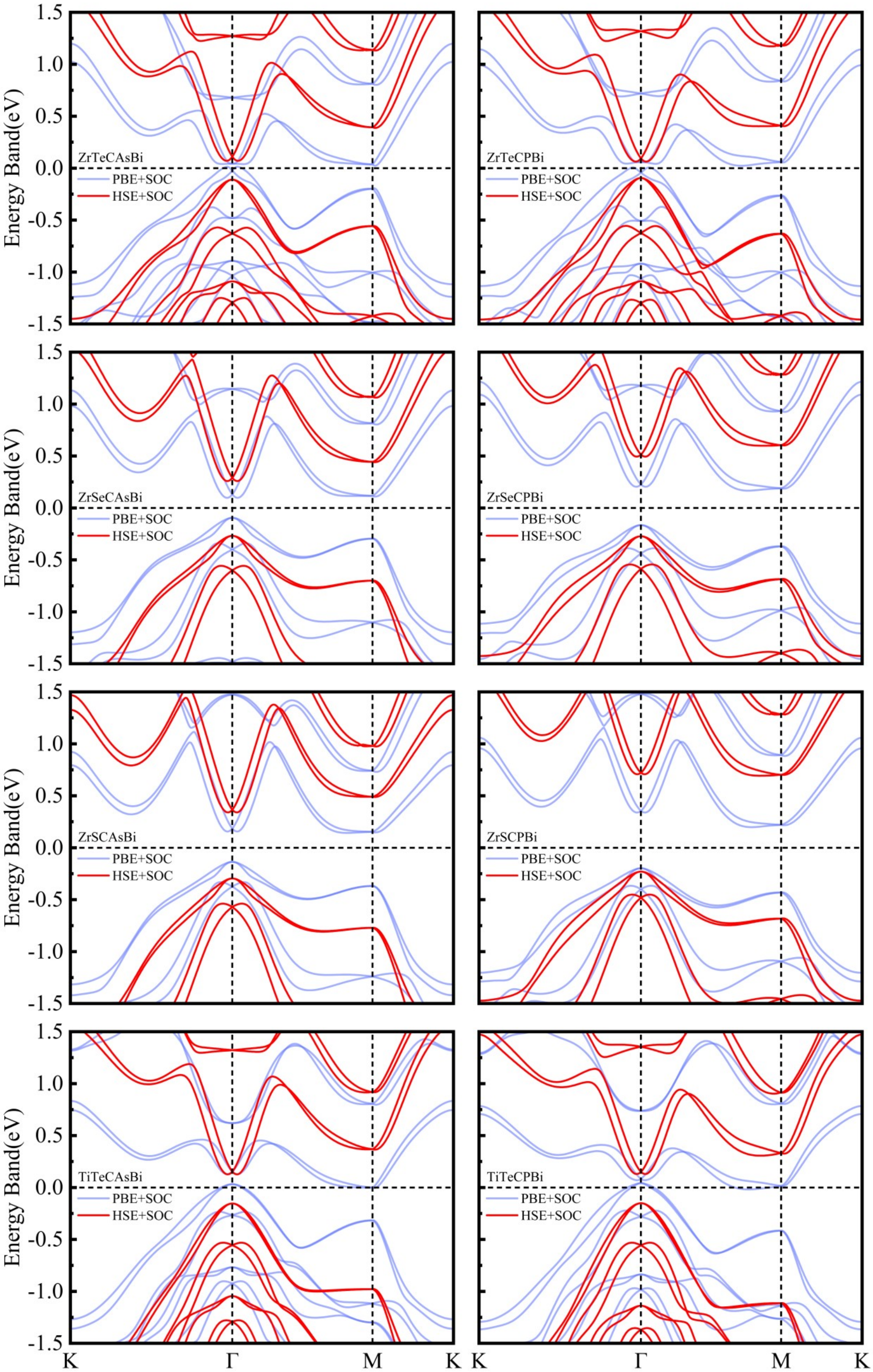



**Figure S2.** Spin texture diagrams of several materials in $MA_2Z_4$ at their respective energies (referenced to the Fermi level).



Energy Band(eV)
ZrGeCAsP2Bi
ZrSiCAsP2Bi
HfTeCAsBi
HfTeCPBi
HfSeCAsBi
HfSeCPBi
HfSCAsBi
HfSCPBi
PBE+SOC
HSE+SOC
K
Γ
M
K



Energy Band(eV)
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
ZrTeCAsBi
ZrTeCPBi
ZrSeCAsBi
ZrSeCPBi
ZrSCAsBi
ZrSCPBi
TiTeCAsBi
TiTeCPBi
PBE+SOC
HSE+SOC
K
Γ
M
K

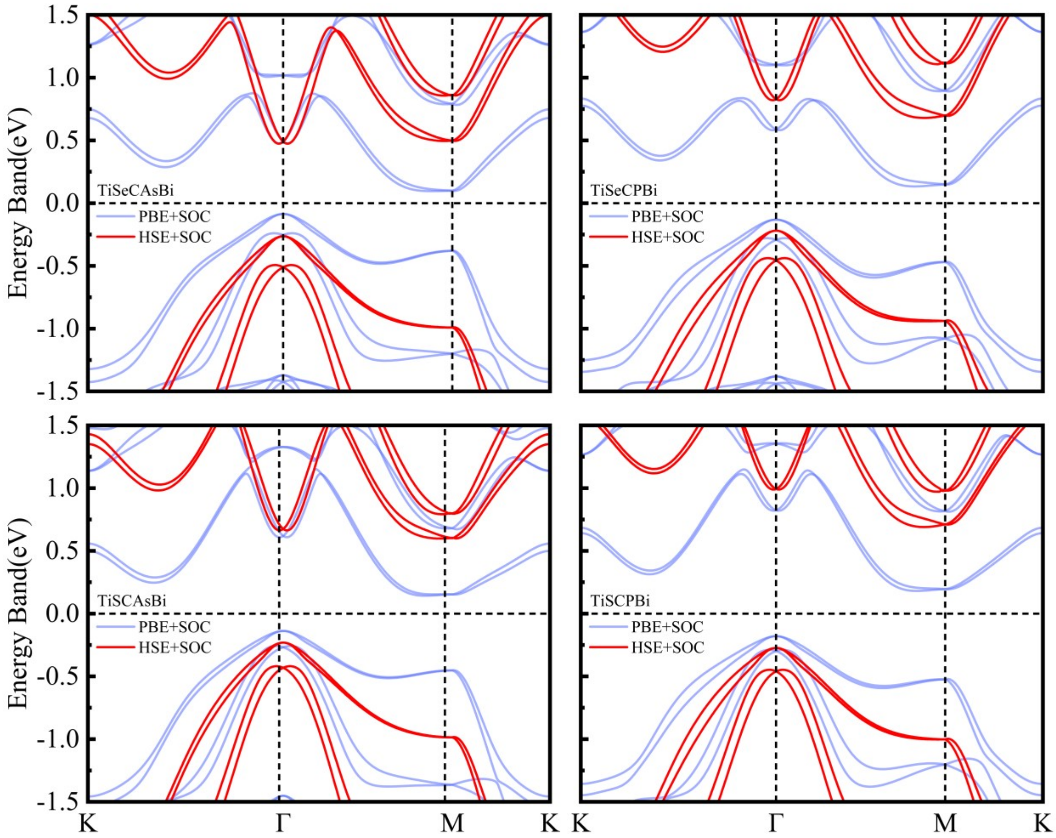
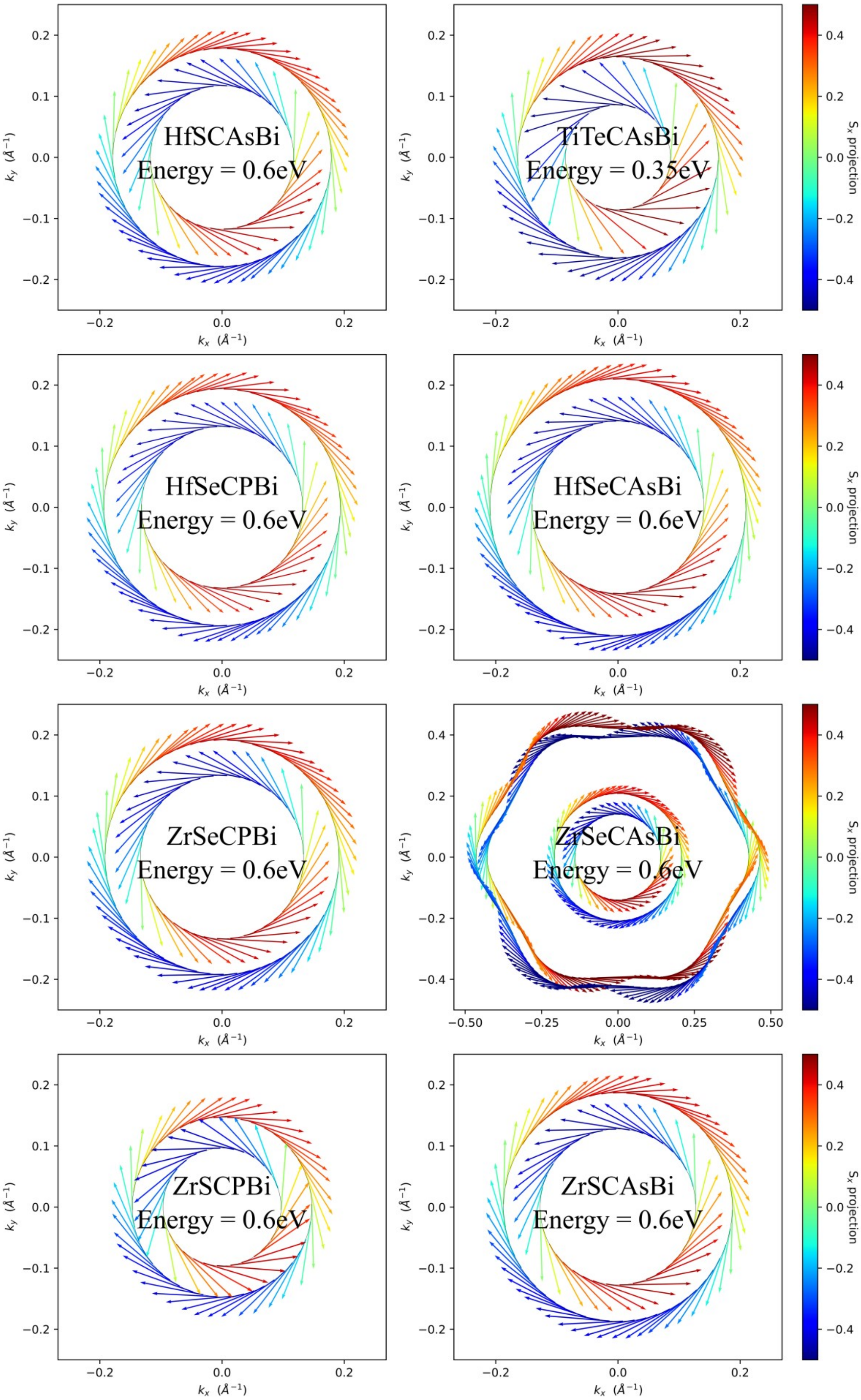



**Figure S3.** Band structures of several materials in $MXAZ_2$ under PBE+SOC and HSE+SOC.


HfSCAsBi
Energy = 0.6eV
TiTeCAsBi
Energy = 0.35eV
HfSeCPBi
Energy = 0.6eV
HfSeCAsBi
Energy = 0.6eV
ZrSeCPBi
Energy = 0.6eV
ZrSeCAsBi
Energy = 0.6eV
ZrSCPBi
Energy = 0.6eV
ZrSCAsBi
Energy = 0.6eV
$k_x$ ($Å^{-1}$)
$k_y$ ($Å^{-1}$)
$S_x$ projection

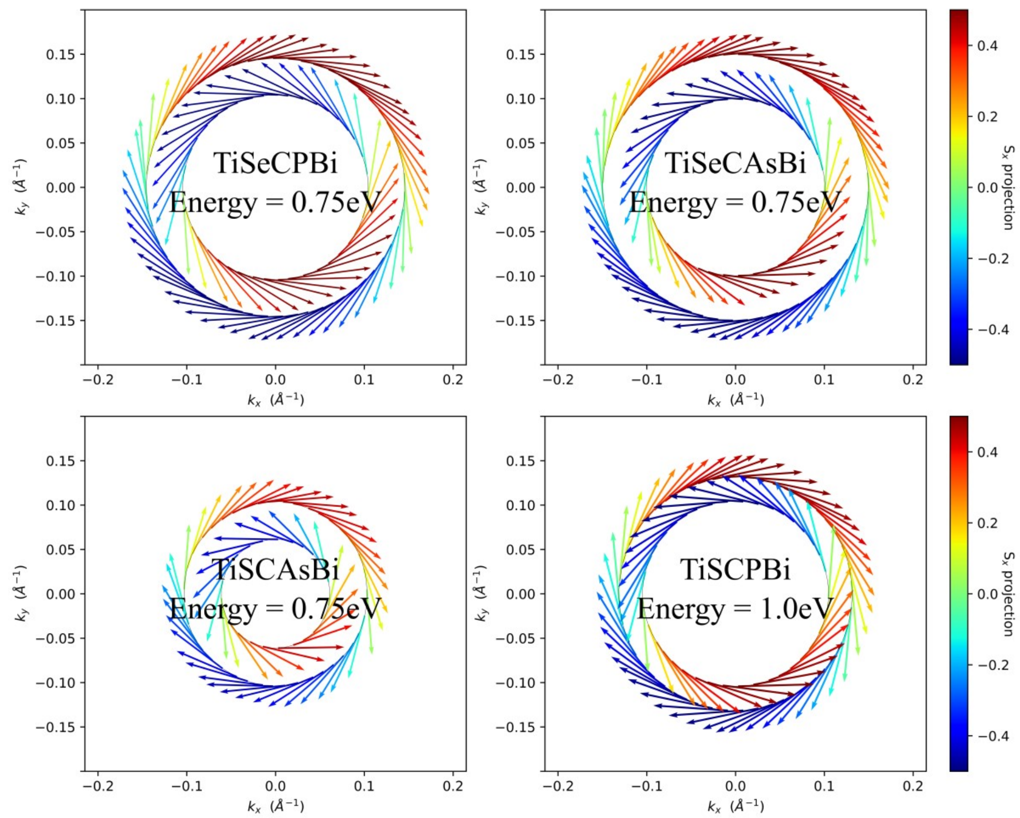
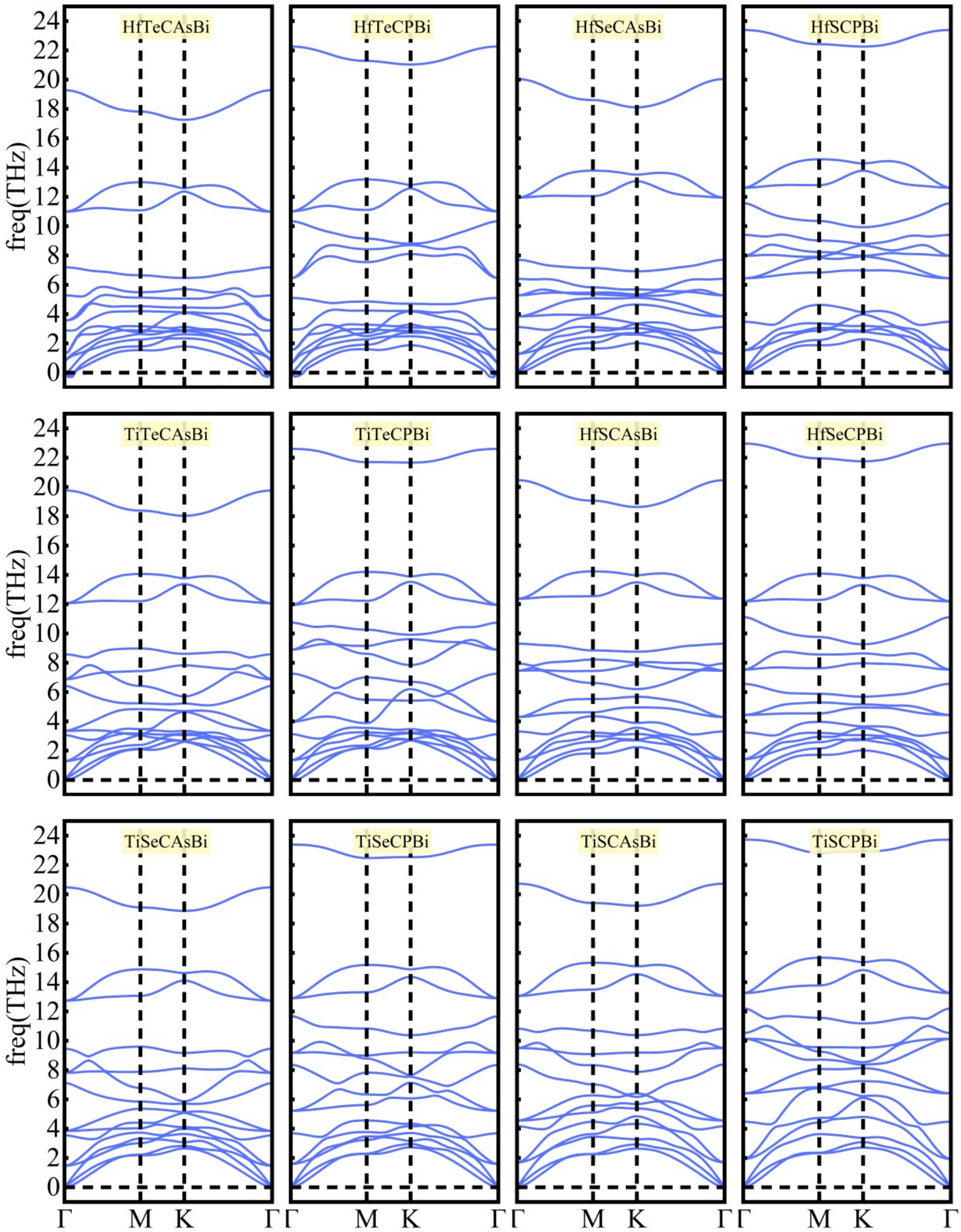



**Figure S4.** Spin texture diagrams of several materials in $MXAZ_2$ at their respective energies (referenced to the Fermi level).



HfTeCAsBi
HfTeCPBi
HfSeCAsBi
HfSCPBi
TiTeCAsBi
TiTeCPBi
HfSCAsBi
HfSeCPBi
TiSeCAsBi
TiSeCPBi
TiSCAsBi
TiSCPBi
freq(THz)
Γ M K Γ

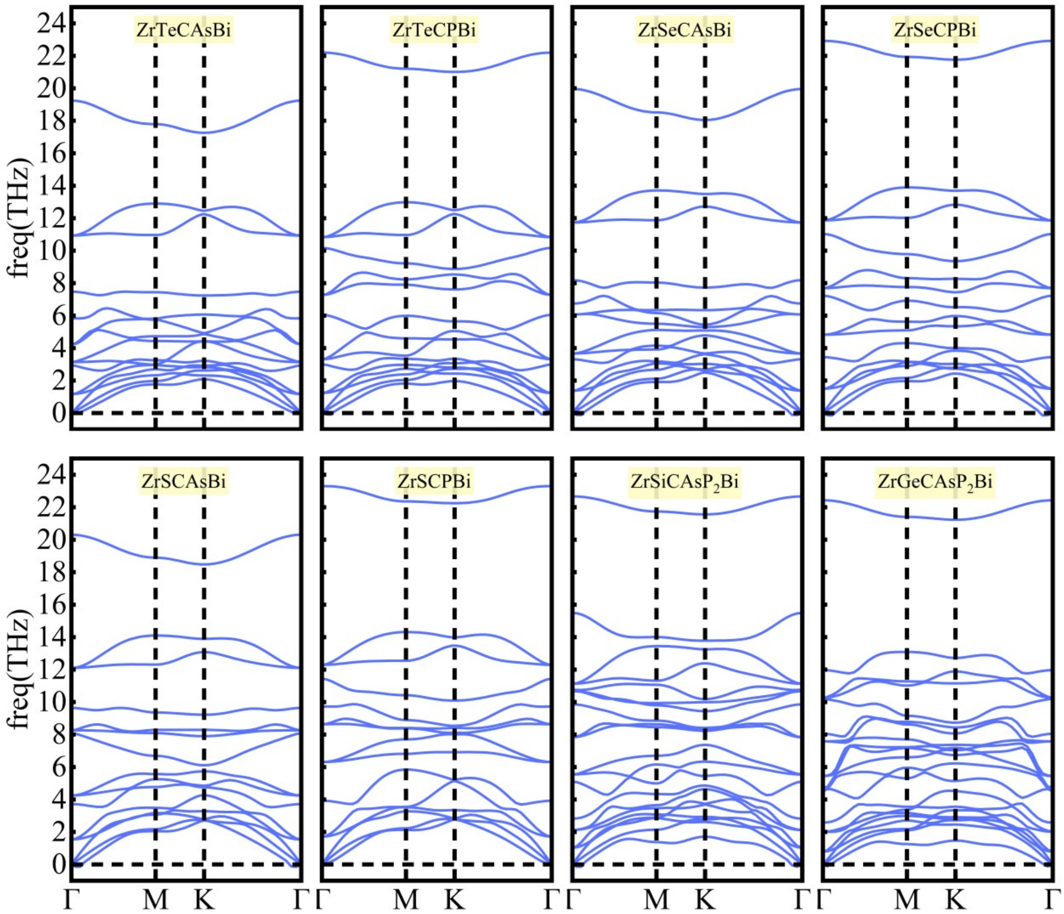
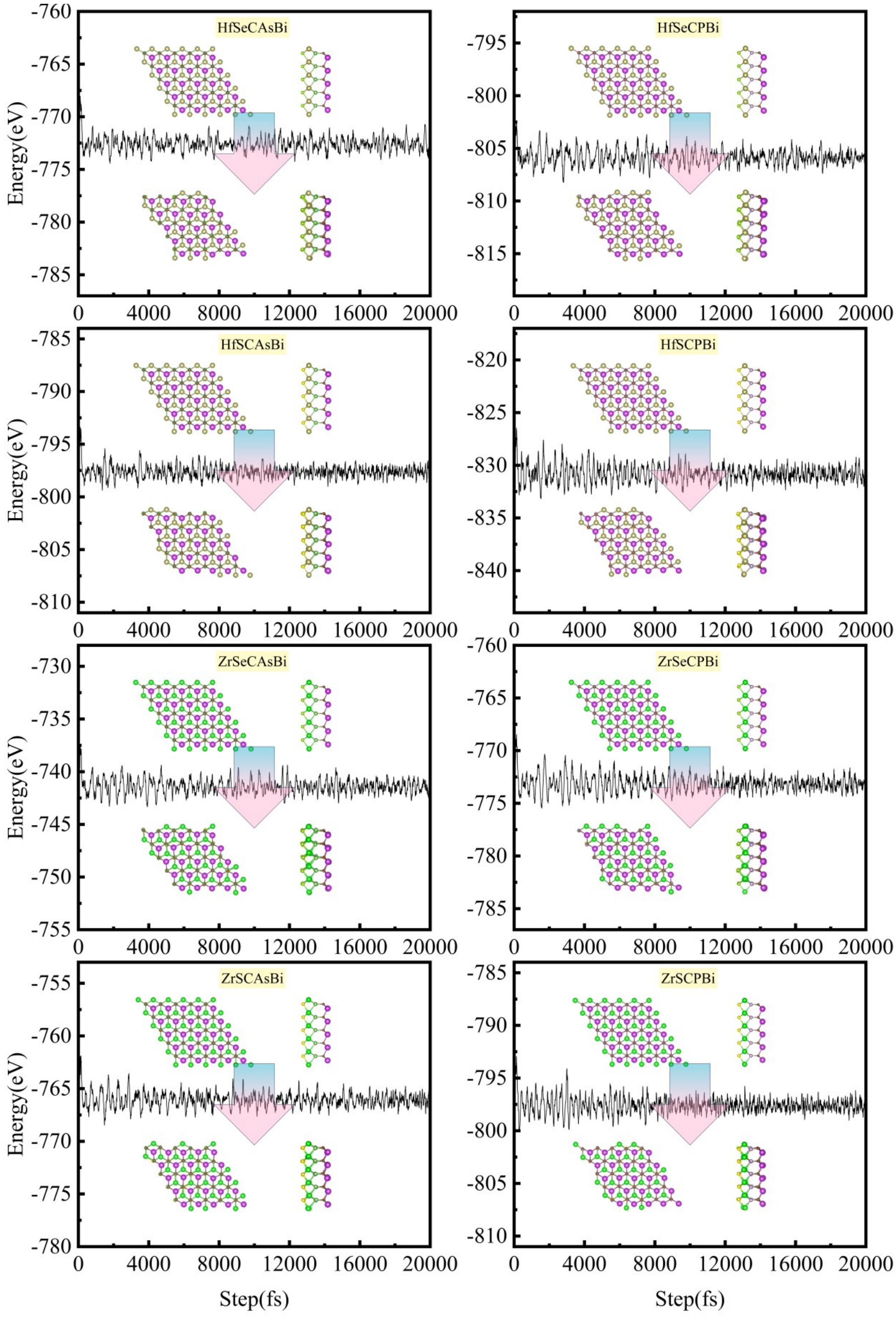



**Figure S5.** Phonon spectra of several materials in $MA_2Z_4$ and $MXAZ_2$.


HfSeCAsBi
HfSeCPBi
HfSCAsBi
HfSCPBi
ZrSeCAsBi
ZrSeCPBi
ZrSCAsBi
ZrSCPBi
Energy(eV)
Step(fs)

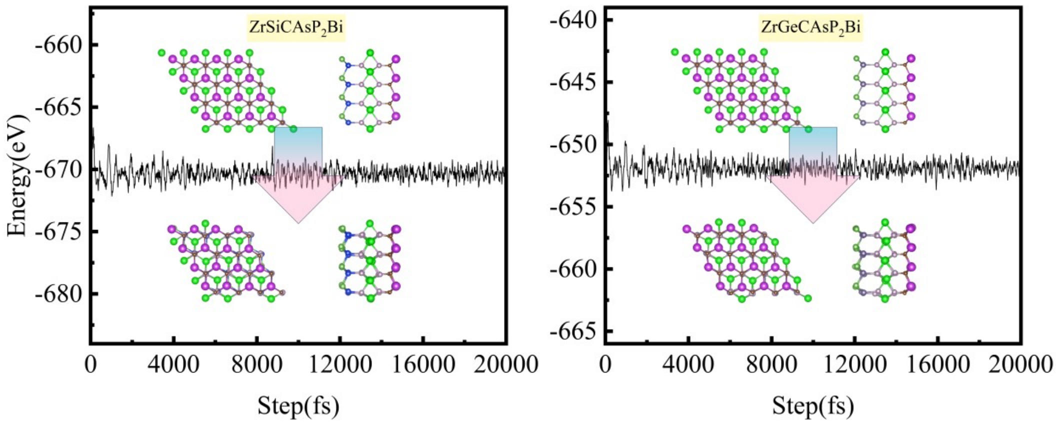



**Figure S6.** Molecular dynamics simulations of several materials in $MA_2Z_4$ and $MXAZ_2$ at 400K.

**TABLE S1. The Rashba strength $\alpha_R$ of various materials, the difference in work function between the two sides of the material ΔΦ, the dipole moment μ within the material, Z represents the sum of atomic numbers, and the electronegativity χ of atoms at different positions.**

| Material | αR(eVÅ) | ΔΦ(V) | μ(eÅ) | Z | χM(kJ/mol) | χX(kJ/mol) | χZ1(kJ/mol) |
|---|---|---|---|---|---|---|---|
| HfTeCAsBi | 2.083 | 1.061 | -0.0739 | 246 | 1.30 | 2.10 | 2.18 |
| HfTeCPBi | 1.775 | 1.268 | -0.0865 | 228 | 1.30 | 2.10 | 2.19 |
| HfSeCAsBi | 1.847 | 1.275 | -0.0851 | 228 | 1.30 | 2.55 | 2.18 |
| HfSeCPBi | 1.380 | 1.487 | -0.0973 | 210 | 1.30 | 2.55 | 2.19 |
| HfSCAsBi | 1.631 | 1.419 | -0.0931 | 210 | 1.30 | 2.58 | 2.18 |
| HfSCPBi | 1.144 | 1.602 | -0.1023 | 192 | 1.30 | 2.58 | 2.19 |
| ZrTeCAsBi | 2.072 | 1.118 | -0.0783 | 214 | 1.33 | 2.10 | 2.18 |
| ZrTeCPBi | 1.749 | 1.322 | -0.0908 | 196 | 1.33 | 2.10 | 2.19 |
| ZrSeCAsBi | 1.849 | 1.348 | -0.0912 | 196 | 1.33 | 2.55 | 2.18 |
| ZrSeCPBi | 1.346 | 1.494 | -0.0988 | 178 | 1.33 | 2.55 | 2.19 |
| ZrSCAsBi | 1.668 | 1.429 | -0.0942 | 178 | 1.33 | 2.58 | 2.18 |
| ZrSCPBi | 1.133 | 1.609 | -0.1040 | 160 | 1.33 | 2.58 | 2.19 |
| TiTeCAsBi | 1.667 | 1.19 | -0.0780 | 196 | 1.54 | 2.10 | 2.18 |
| TiTeCPBi | 1.360 | 1.341 | -0.0860 | 178 | 1.54 | 2.10 | 2.19 |
| TiSeCAsBi | 1.253 | 1.384 | -0.0869 | 178 | 1.54 | 2.55 | 2.18 |
| TiSeCPBi | 0.781 | 1.591 | -0.0983 | 160 | 1.54 | 2.55 | 2.19 |
| TiSCAsBi | 1.030 | 1.623 | -0.0994 | 160 | 1.54 | 2.58 | 2.18 |
| TiSCPBi | 0.552 | 1.788 | -0.1073 | 142 | 1.54 | 2.58 | 2.19 |

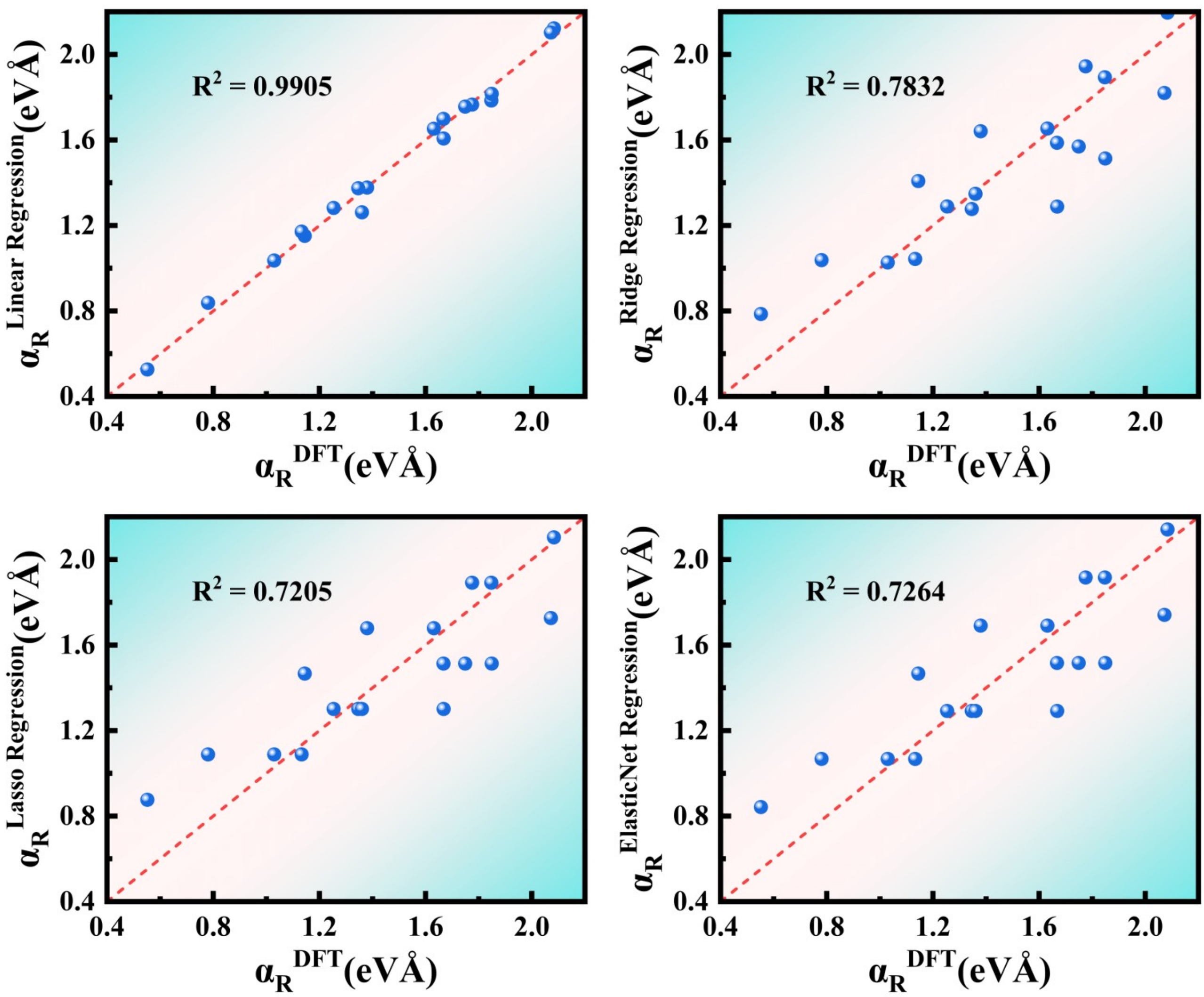



**Figure S7.** The comparison between the calculated values of Rashba spin-orbit coupling strength $\alpha_R$ obtained from different models and the results calculated by DFT method.

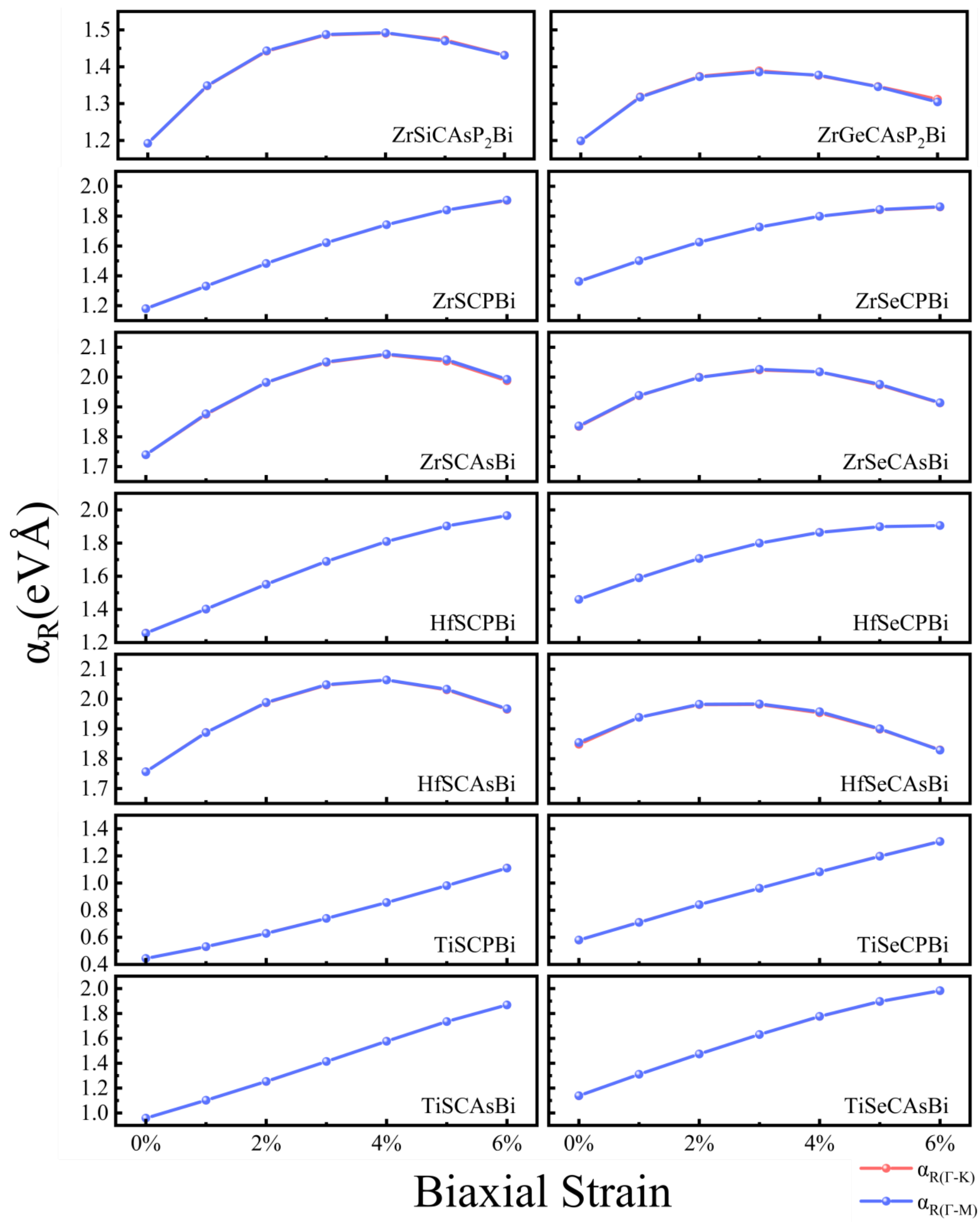



**Figure S8.** The variation of Rashba constant $\alpha_R$ with biaxial strain for several materials in $MA_2Z_4$ and $MXAZ_2$ systems.

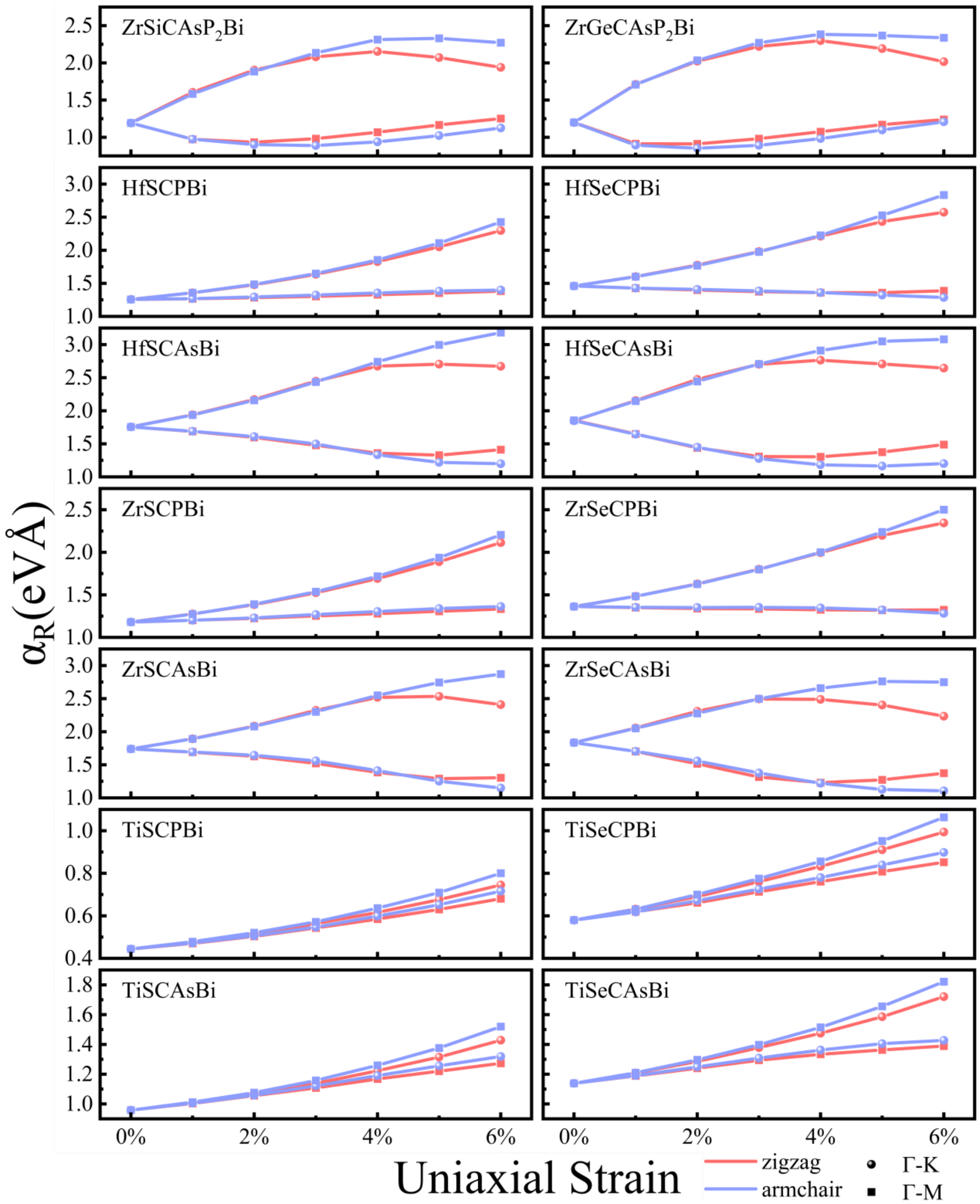



**Figure S9.** The variation of Rashba constant $\alpha_R$ with uniaxial strain for several materials in $MA_2Z_4$ and $MXAZ_2$ systems.

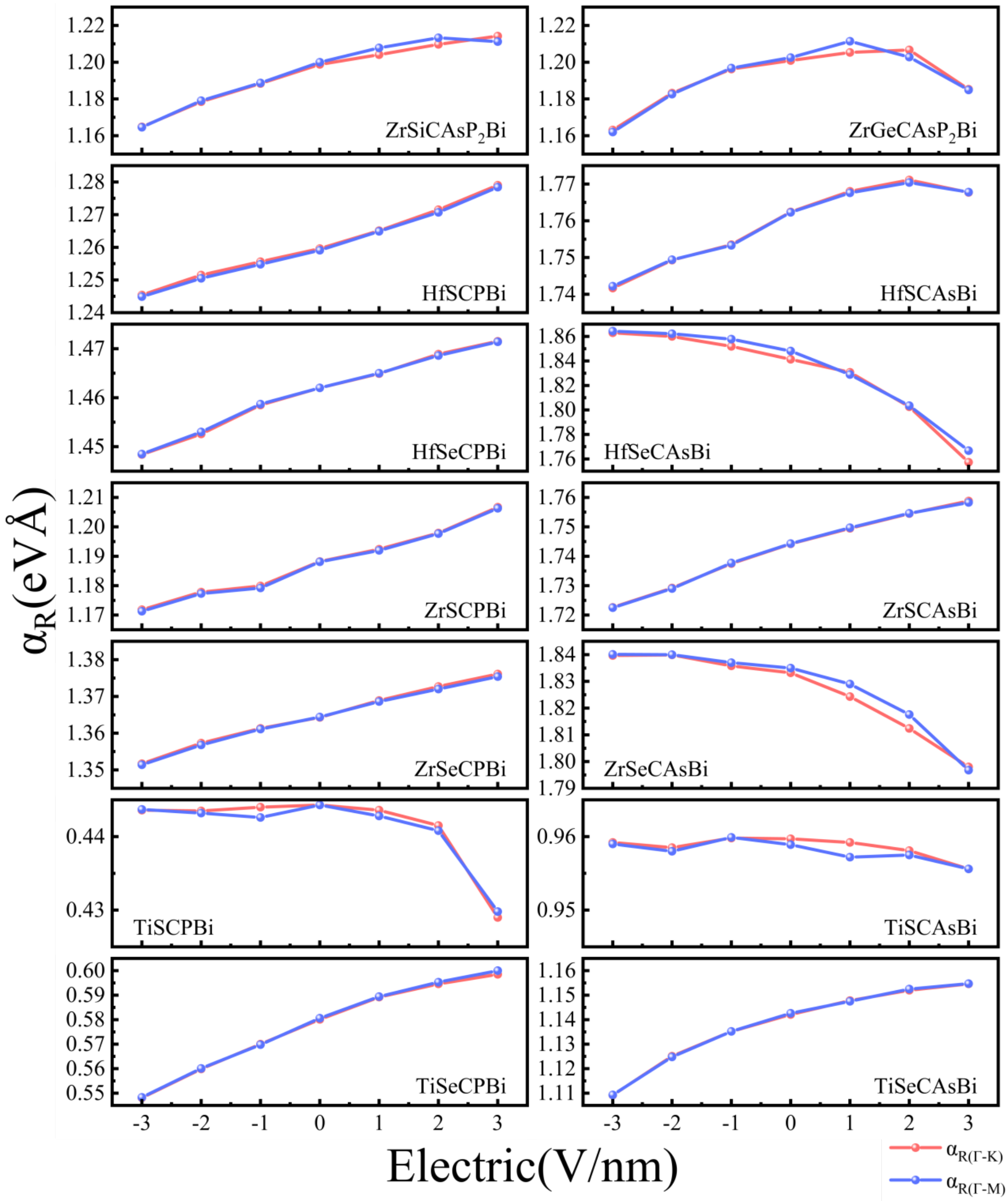



**Figure S10.** The variation of Rashba constant $\alpha_R$ with electric field for several materials in MA2Z4 and $MXAZ_2$ systems.

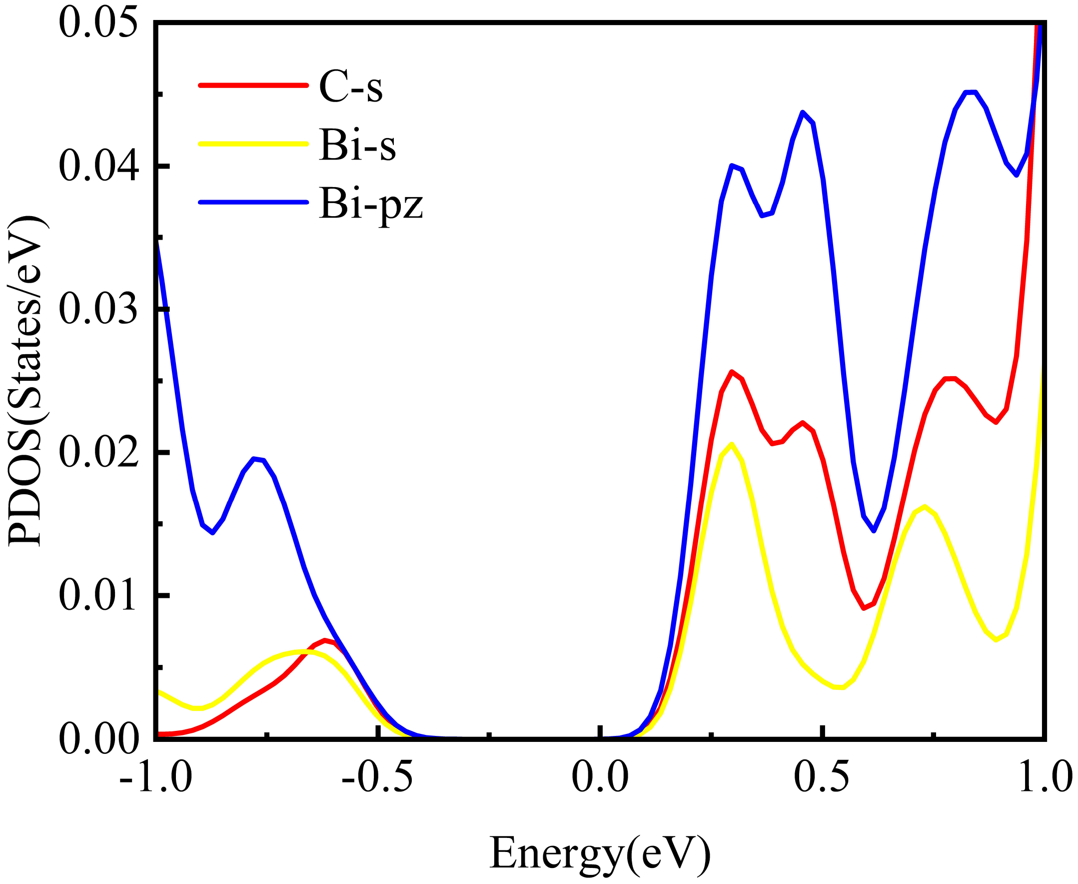



**Figure S11.** PDOS of the constituent atoms within the ZrSeCAsBi system.