# Large valleys splitting under biaxial strain in Janus $SHfAX_2$(A=Si, Ge; X=N, P, As)

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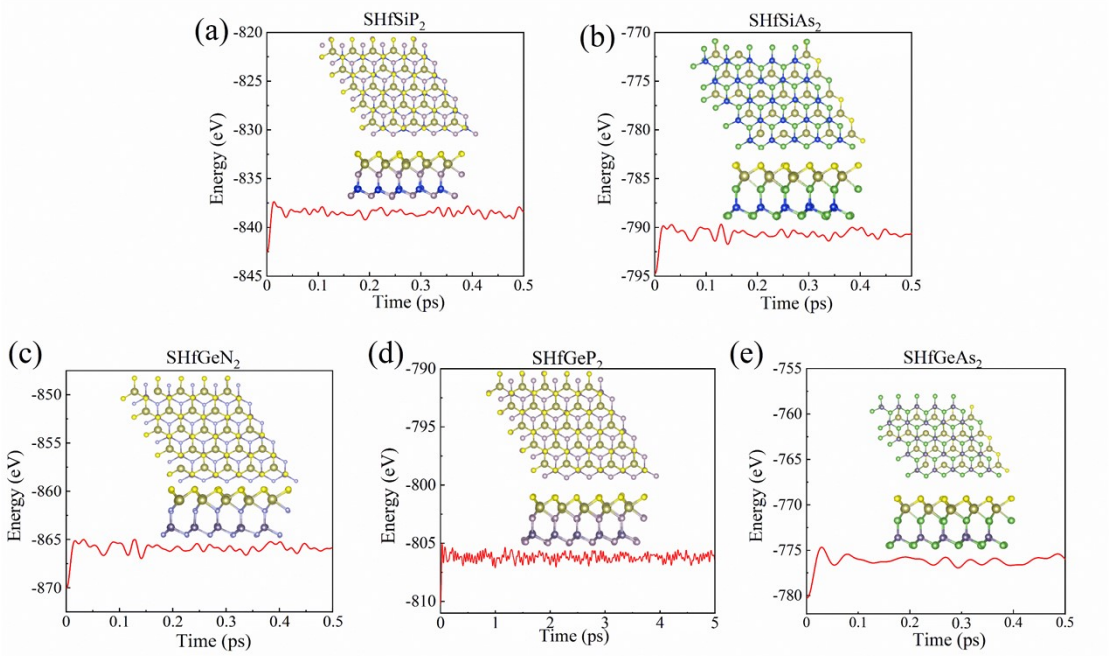


Support **Figure 1.** Variation of the energy as a function of time for the Janus $SHfAX_2$ monolayers at 500K. The insets are the top and side views of the structure at the end of the AIMD simulation.

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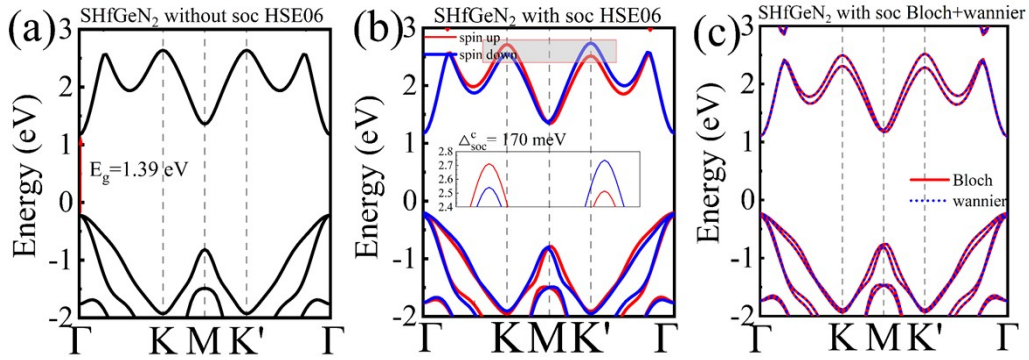
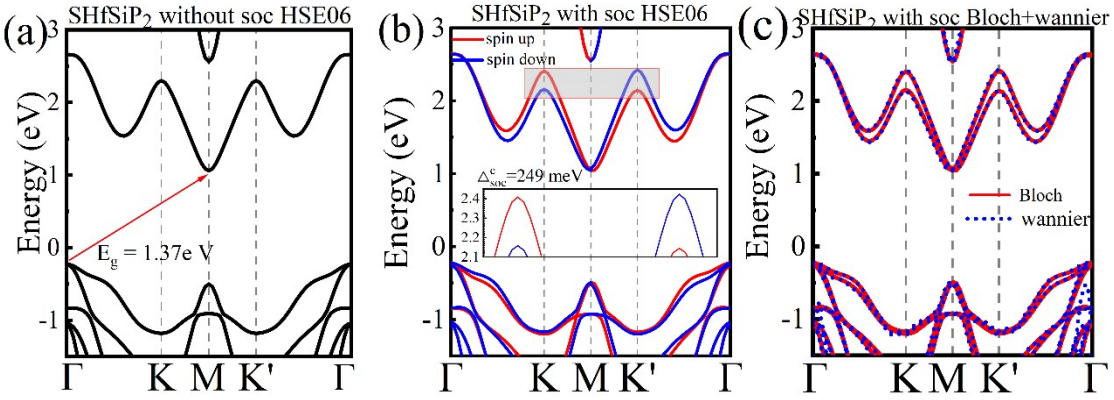
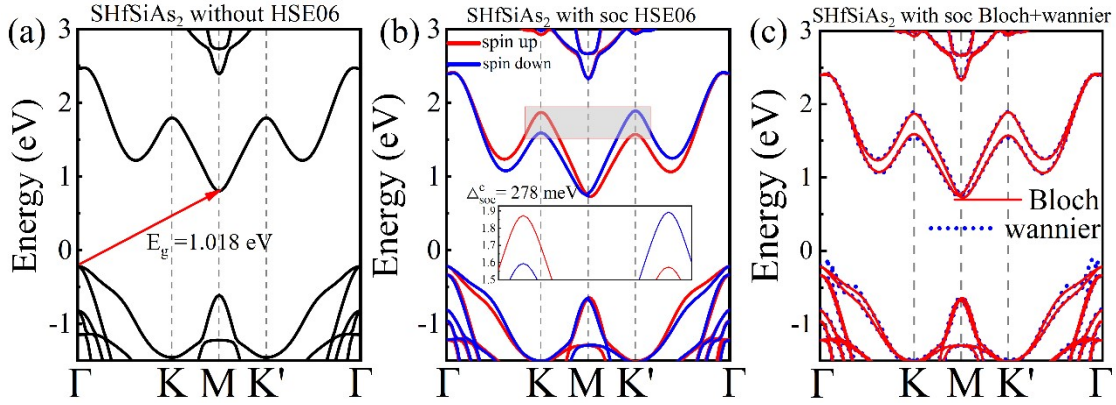


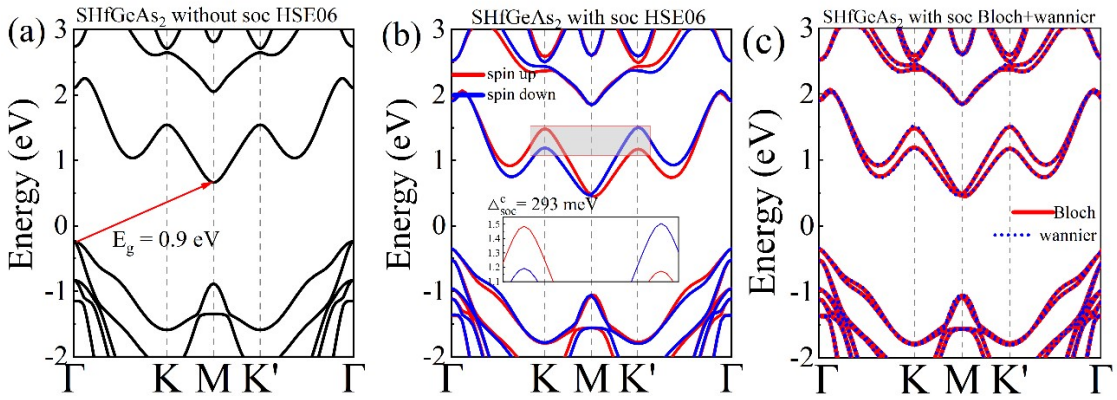

Support **Figure 2.** The electron energy band diagram of 1L $SHfGeN_2$ along the high symmetry point (a) without considering SOC; (b) with considering SOC; (c) The red dashed line obtained from the Bloch, while the blue dashed line is derived from the Wannier functions with considering SOC. the Fermi energy is set to zero.



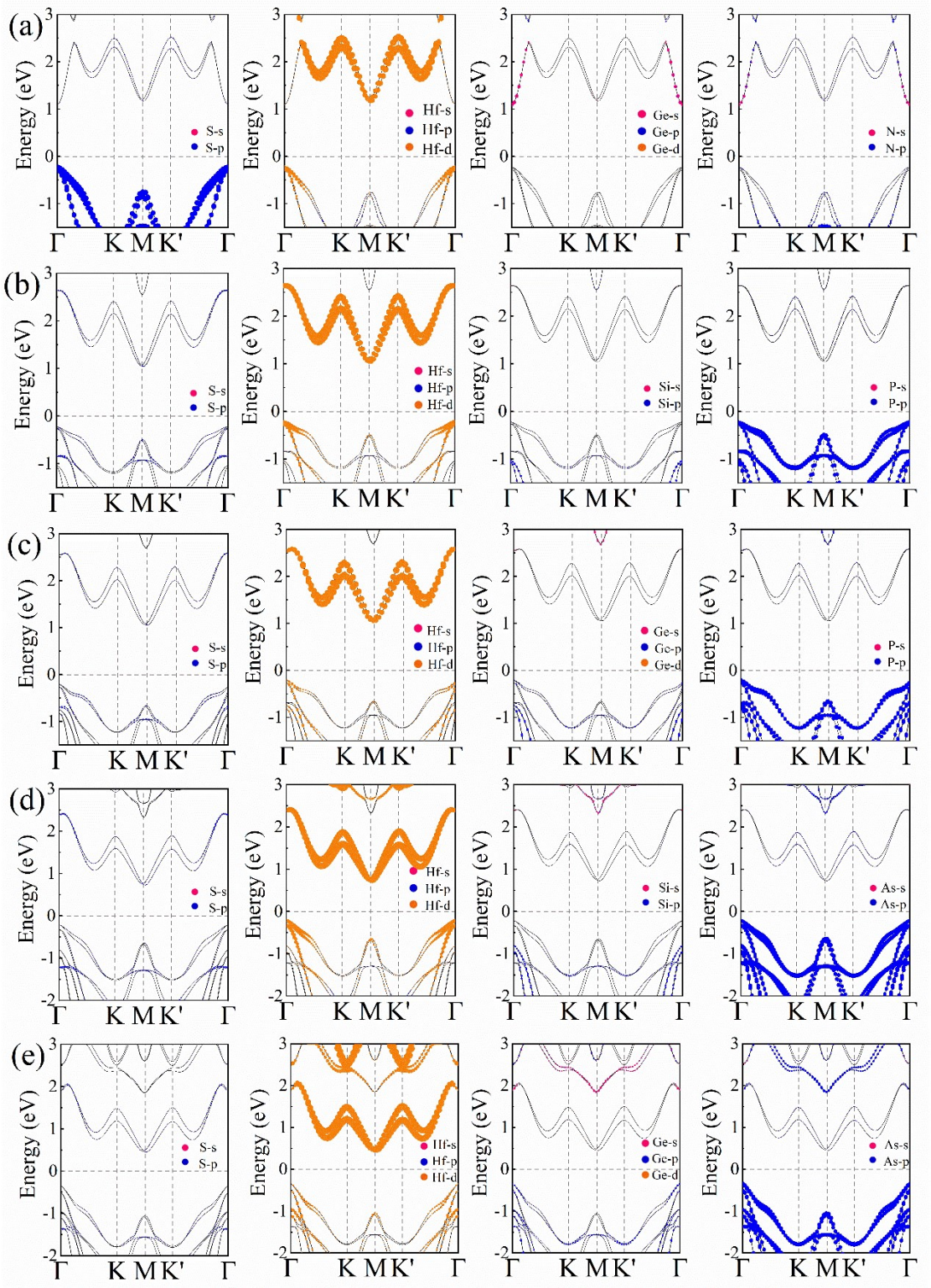

Support **Figure 3.** The electron energy band diagram of 1L $SHfSiP_2$ along the high symmetry point (a) without considering SOC; (b) with considering SOC; (c) The red dashed line obtained from the Bloch, while the blue dashed line is derived from the Wannier functions with considering SOC. the Fermi energy is set to zero.



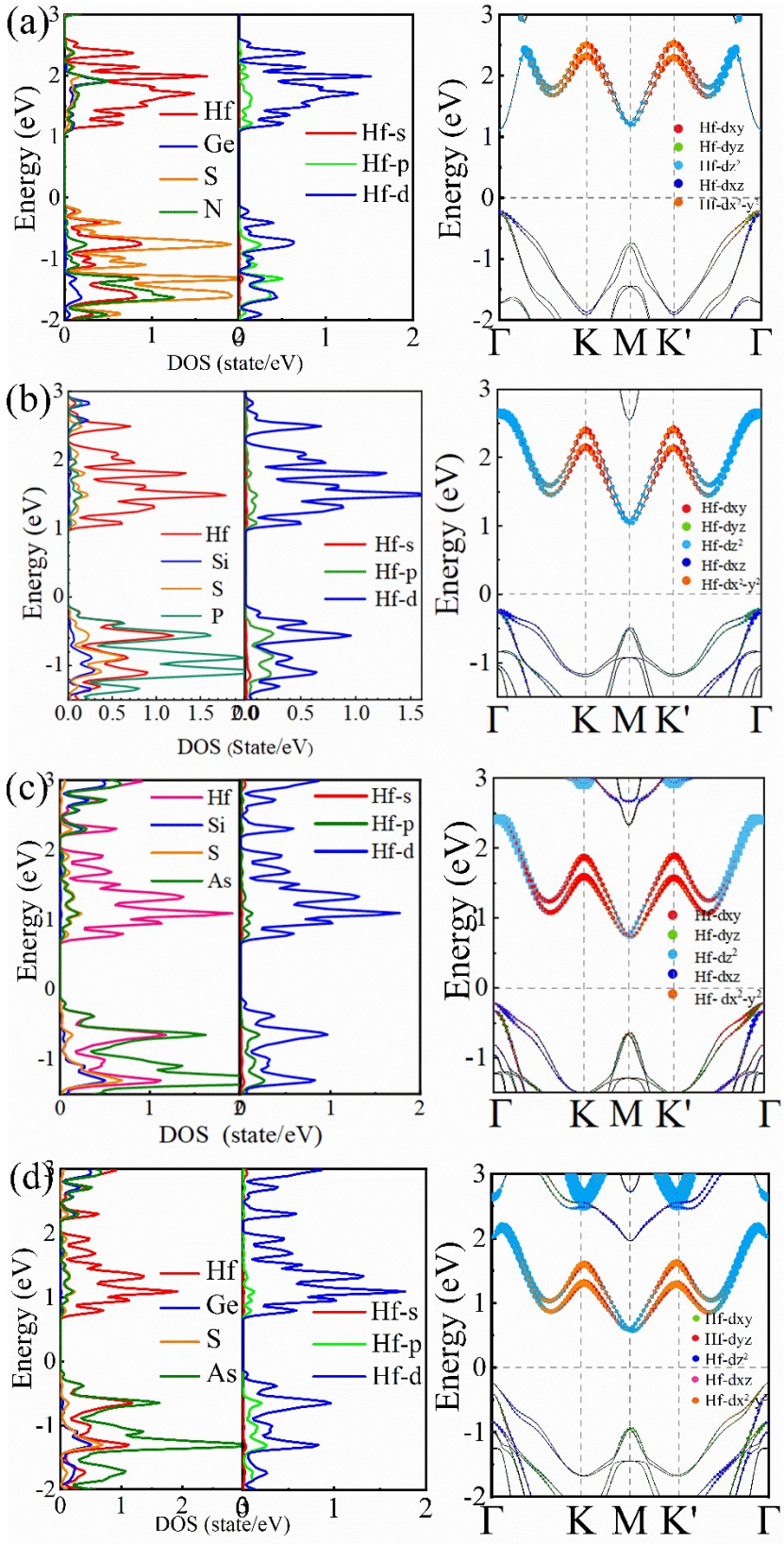

Support **Figure 4.** The electron energy band diagram of 1L $SHfSiAs_2$ along the high symmetry point (a) without considering SOC; (b) with considering SOC; (c) The red dashed line obtained from the Bloch, while the blue dashed line is derived from the Wannier functions with considering SOC. the Fermi energy is set to zero.



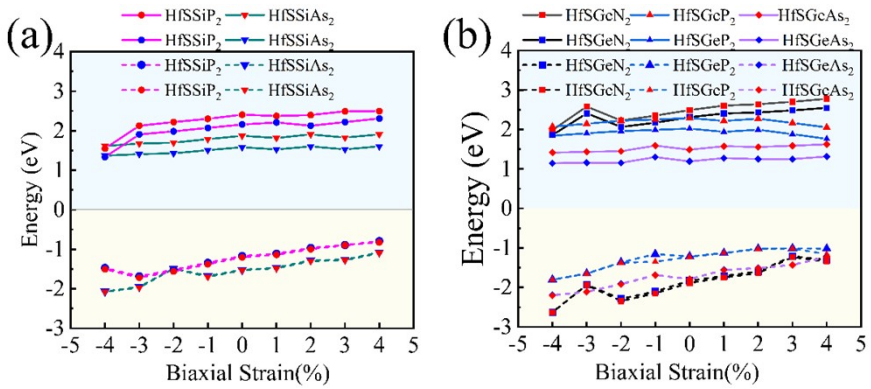

Support **Figure 5.** The electron energy band diagram of 1L $SHfGeAs_2$ along the high symmetry point (a) without considering SOC; (b) with considering SOC; (c) The red dashed line obtained from the Bloch, while the blue dashed line is derived from the Wannier functions with considering SOC. the Fermi energy is set to zero.




Support **Figure 6.** (a-e) The projected energy band diagram of $SHfGeN_2$, $SHfSiP_2$, $SHfGeP_2$, $SHfSiAs_2$ and $SHfGeAs_2$ the S-*s*, S-*p* orbitals; Hf-*s*, Hf-*p*, Hf-*d* orbitals; Ge-*s*, Ge-*p* orbitals; N-*s*, N-*p* orbitals.




Support **Figure 7.** The left is total density of states of each atom of 1L $SHfSiN_2$(a) $SHfSiP_2$ (b), $SHfSiAs_2$(c), $SHfGeAs_2$(d), and the middle projected density of states of the *s*, *p*, *d* orbitals of Hf atom, the right is projected energy band diagram of the d orbitals of the Hf atom in two-dimensional, where the $d_{xy}$, $d_{x2-y2}$, $d_{z2}$, $d_{yz}$, $d_{xz}$ orbitals of Hf is in red, green, light blue, dark blue, orang.




Support **Figure 8.** The actual curves of valence in a and conduction band energies in b at the K point of 1L $SHfAX_2$. And the y-axis is the energy minus the vacuum level. Red dots represent spin-up, blue dots represent spin-down, dashed lines indicate the conduction band, and solid lines indicate the valence band.