Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Tunable anisotropic Rashba spin-orbit coupling effect in Pb-adsorbed Janus monolayer WSeTe

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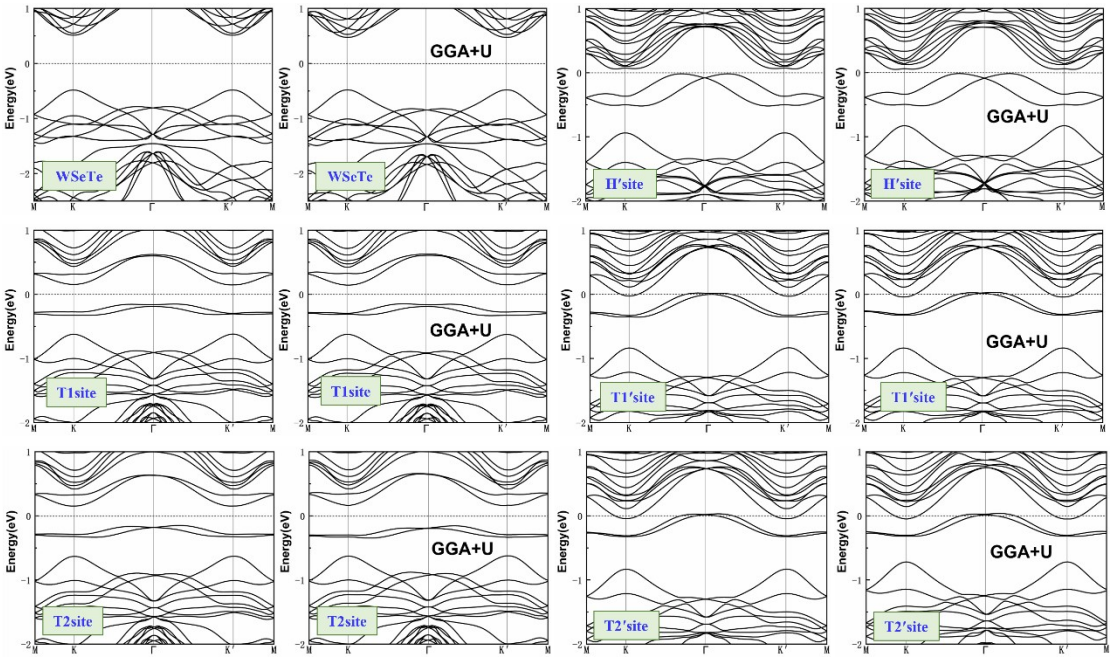

Fig. S1 Band structures of WSeTe ML and Pb-WSeTe system with SOC using PBE/GGA+U functional.

Table S1 Calculated E_R, K_R and Rashba parameters α_R with different adsorption distance calculated according to DFT.

system	WSeTe ML	T1	T2	H	T1′	T2′	H′
E_g^{PBE} (eV)	0.99	0.303	0.302	0.288	/	/	0.075
E_g^{GGA+U} (eV)	0.95	0.290	0.287	0.272	/	/	0.064
α_R^{PBE}(eV·Å)	0.43	0.48	0.60	0.51	0.53	0.52	0.75
α_R^{GGA+U}(eV·Å)	0.443	0.477	0.613	0.513	0.535	0.522	0.757

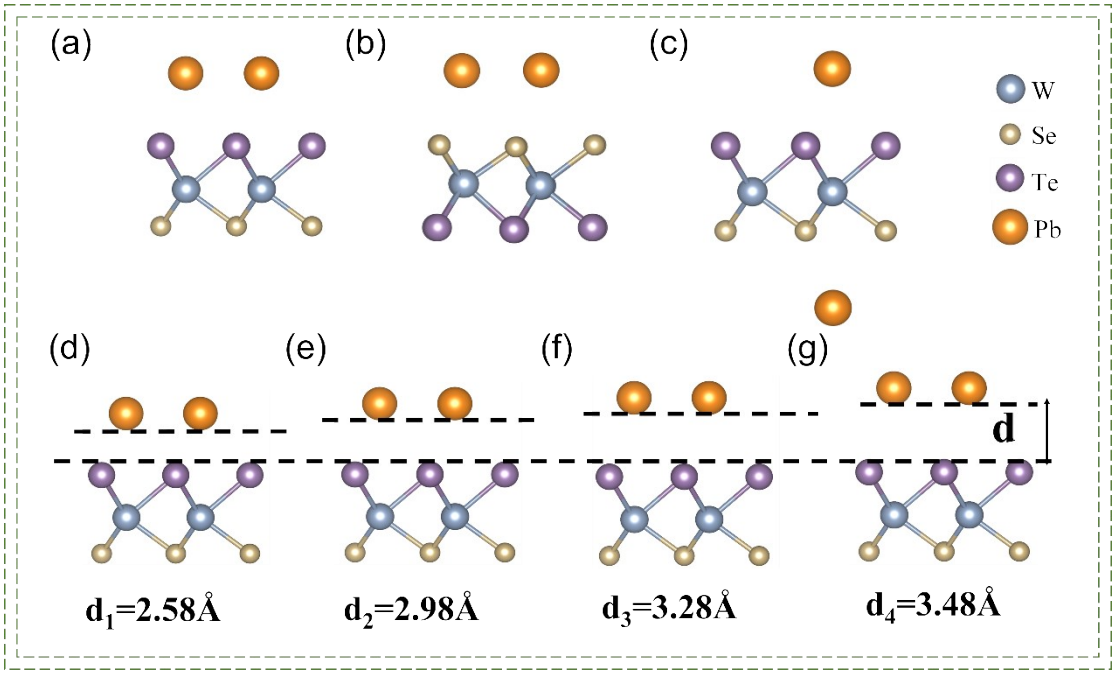

Fig. S2 (a) Te side: two Pb atoms placed parallel to each other above the W atom, (b) Se side: two Pb atoms placed parallel to each other above the W atom, and (c) two Pb atoms placed relative to the W atom. Illustration for four adsorption distances (d) d_1=2.58 Å , (e) d_2=2.98 Å , (f) d_3=3.28 Å and (g) d_4=3.48 Å for the adsorption structure shown in (a).

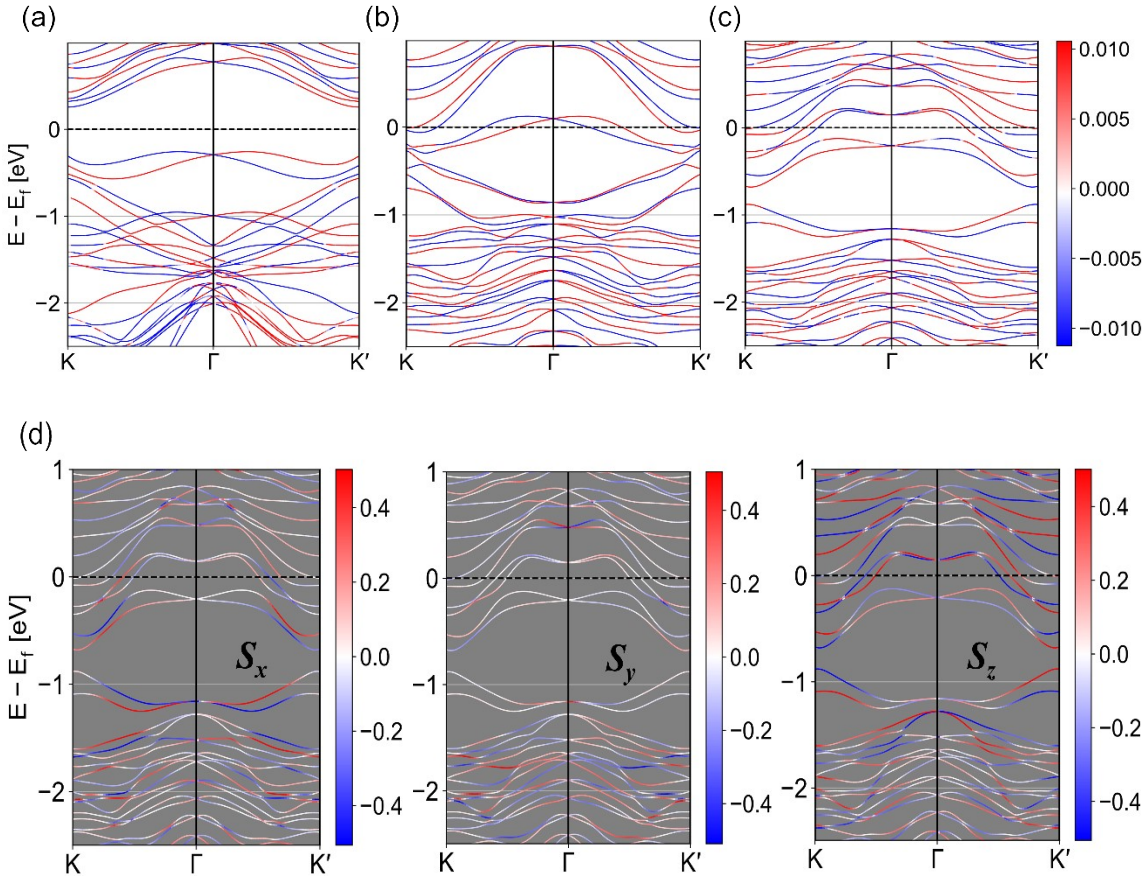

Fig. S3 Spin projected electronic energy bands. (a) Te side：two Pb atoms placed parallel to each other above the W atom, (b) Se side: two Pb atoms placed parallel to each other above the W atom, (c) two Pb atoms placed relative to the W atom, and (d) Spin polarization of two Pb atoms placed relative to the W atom projected to the spin-split bands along the K-Γ-K' line. Color bars represent the expectation values of spin component S_x, S_y, and S_z.

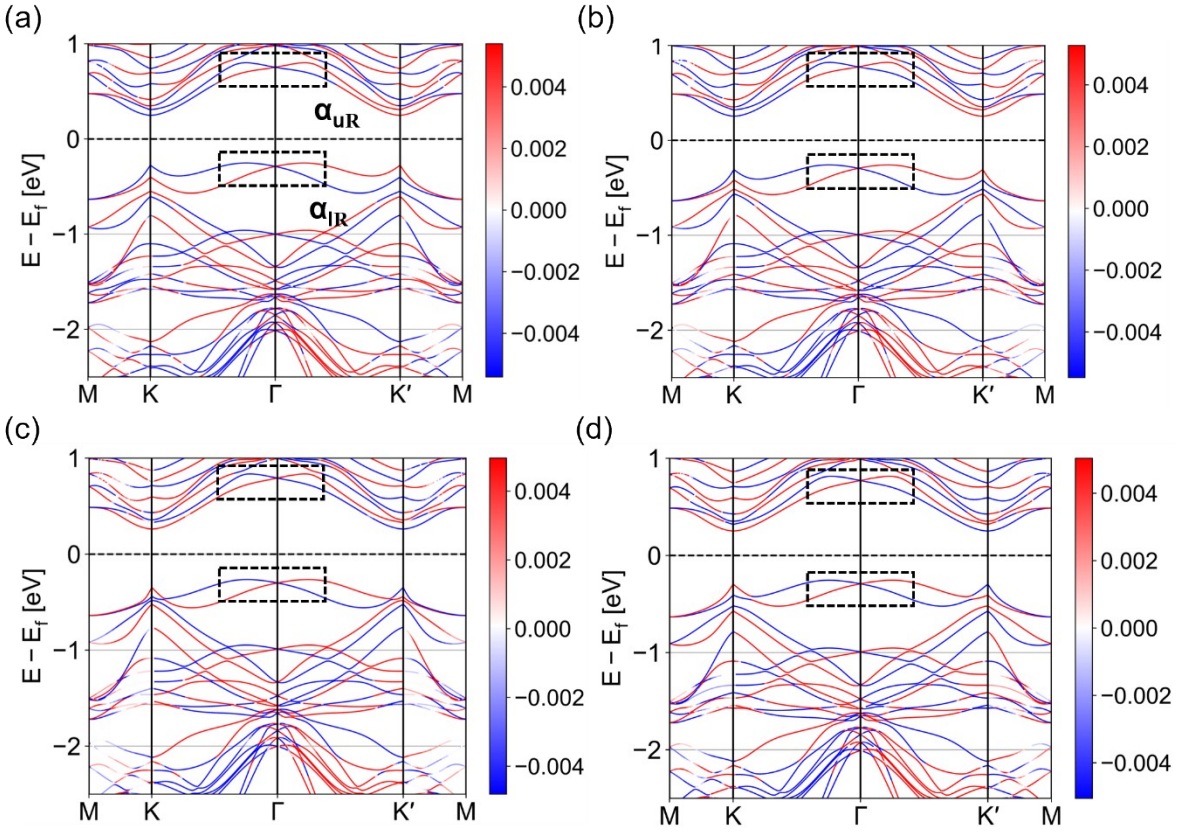

Fig. S4 Spin projected electronic energy band of the adsorption structure shown in S1(a) with four adsorption vertical distances (a) d_1=2.58 Å, (b) d_2=2.98 Å, (c) d_3=3.28 Å and (d) d_4=3.48 Å. The red and blue colors represent opposite spin directions, and the black dashed rectangles indicate Rashba spin splitting.

Table S2 Calculated E_R, K_R and Rashba parameters α_R with different adsorption distance calculated according to DFT.

	d_1 upper	d_1 lower	d_2 upper	d_2 lower	d_3 upper	d_3 lower	d_4 upper	d_4 lower
E_R(eV)	0.0481	0.0368	0.0474	0.0354	0.0425	0.0347	0.0438	0.0395
K_R(Å^{-1})	0.1336	0.1337	0.1336	0.1337	0.1215	0.1336	0.1336	0.1579
α_R(eV·Å)	0.72	0.55	0.71	0.53	0.70	0.52	0.64	0.50

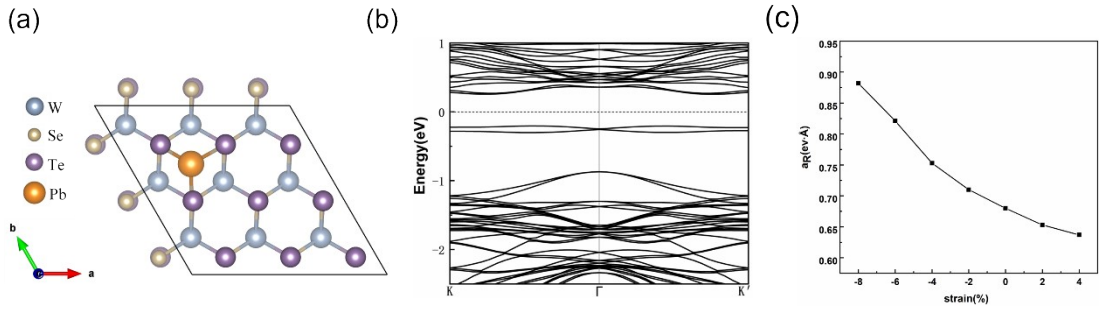

Fig. S5 Pb absorbed 3×3×1 supercell WSeTe of H′ site. (a) Top view, (b) Band structure with SOC, (c) Variation of the Rashba parameters of the Rashba bands close to the neighborhood of the Fermi energy as a function of biaxial strain.