Supporting Information

Functionalized Sc_2N as Ohmic contacted electrodes for Monolayer $PtSe_2$: An *ab initio* Study

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Table S1. The lattice mismatch, interlayer distance (d), binding energy (E_b), band gap (E_g), vertical Schottky barriers ($\Phi_n^{\perp}/\Phi_p^{\perp}$), and lateral Schottky barriers ($\Phi_n^{//}/\Phi_p^{//}$) of the $PtSe_2/Sc_2N$ and $PtSe_2/Sc_2NX_2$ (X = F, O, and OH) vertical heterojunctions with supercells of $(\sqrt{3}\times\sqrt{3})/(2\times2)$.

	mismatch	d (Å)	E_b (meV/Å^2)	E_g (eV)	$\Phi_n^{\perp}/\Phi_p^{\perp}$ (eV)	$\Phi_n^{//}/\Phi_p^{//}$ (eV)
$PtSe_2/Sc_2N$	1.38%	3.02	-86.76	1.12	-0.32/1.44	-0.32/1.31
$PtSe_2/Sc_2NF_2$	0.97%	2.87	-23.51	1.36	-0.02/1.38	-0.14/1.38
$PtSe_2/Sc_2NO_2$	0.32%	2.55	-49.38	1.55	1.32/0.23	1.43/-0.03
$PtSe_2/Sc_2N(OH)_2$	0.21%	2.03	-62.80	1.32	-0.16/1.48	-0.16/1.48

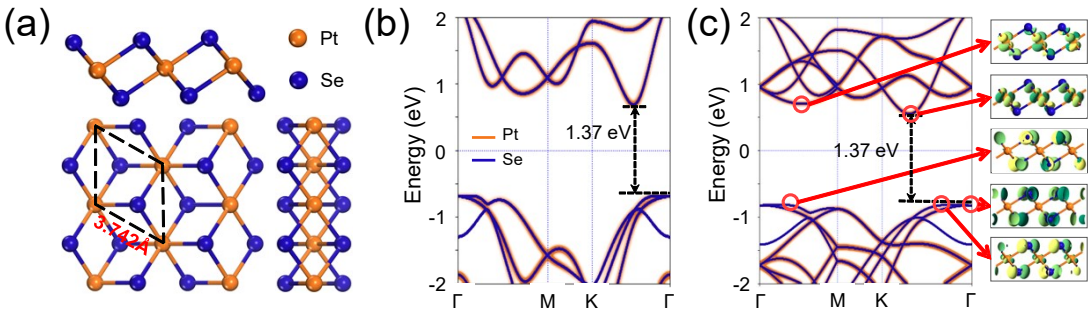

Figure S1. (a) The geometric structure and (b) projected band structure of ML $PtSe_2$. (c) The projected band structure of ML $PtSe_2$ with $\sqrt{3}\times\sqrt{3}$ supercell and Bloch states at specific k point.

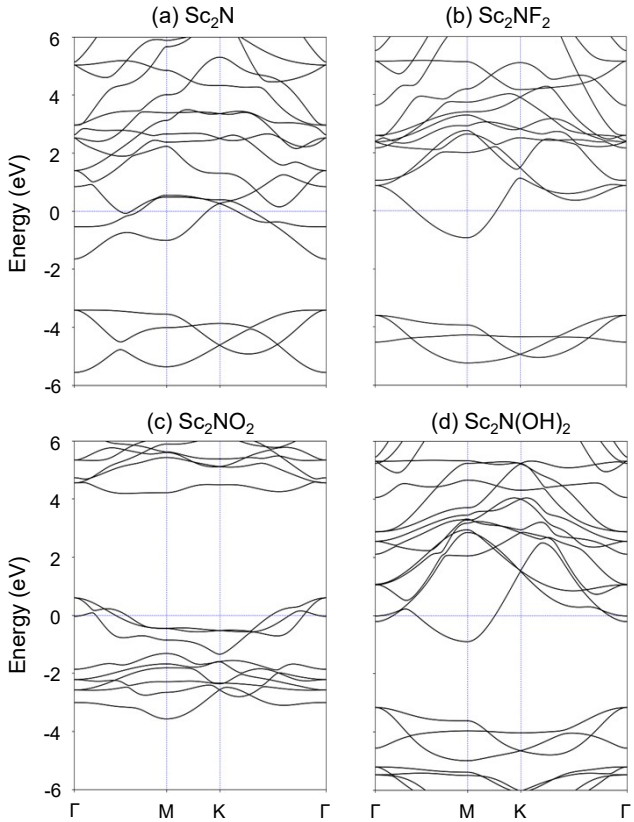

Figure S2. The band structures of ML Sc_2N and functionalized Sc_2NX_2 (X = F, O, and OH).

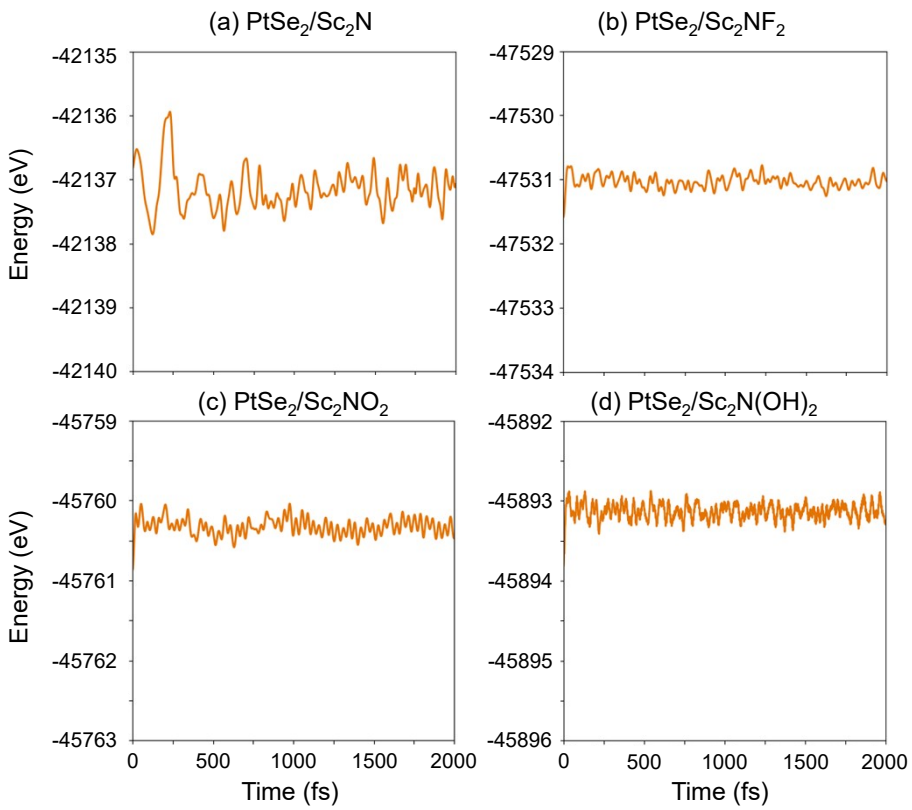

Figure S3. The *ab initio* molecular dynamics (AIMD) simulations of the $PtSe_2/Sc_2NX_2$ (X =null, F, O, and OH) vertical heterojunctions at 300 K for 2000 fs.

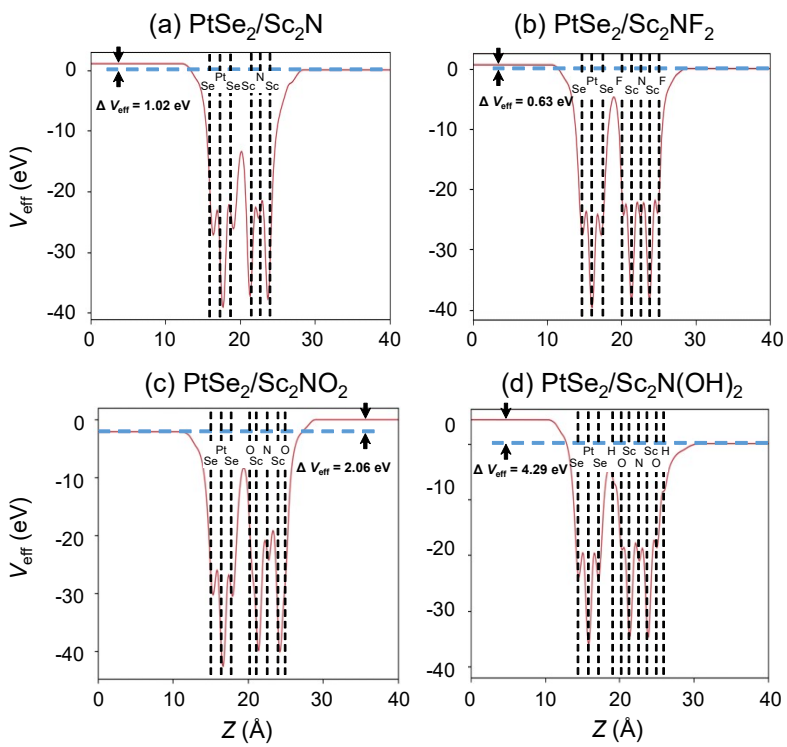

Figure S4. The electrostatic potentials of the $PtSe_2/Sc_2NX_2$ (X =null, F, O, and OH) vertical heterojunctions.

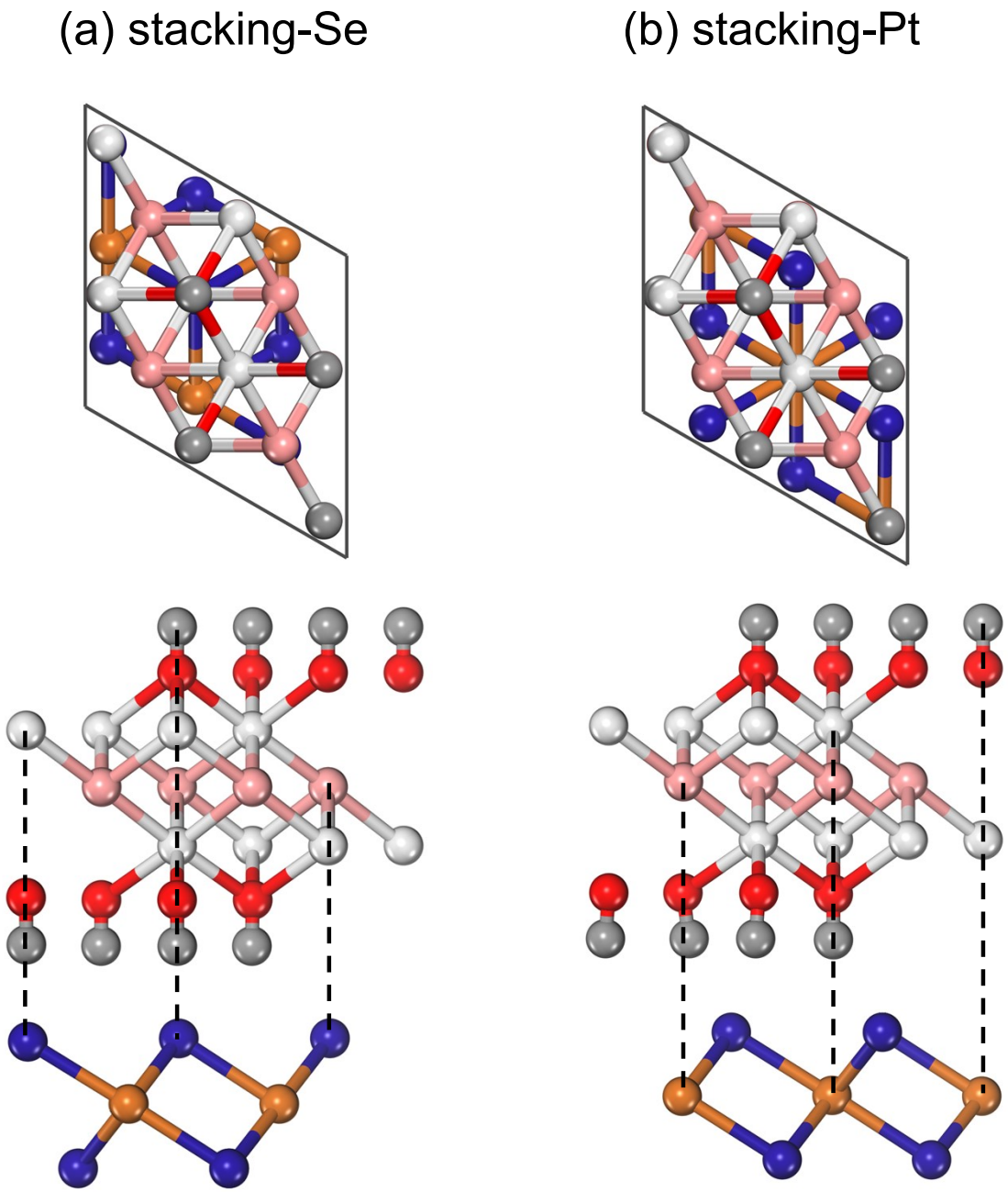

Figure S5. Side and top views of two more considered stacking patterns of the $PtSe_2/Sc_2NX_2$ (X =null, F, O, and OH) vertical heterojunctions with $Sc_2N(OH)_2$ metal as representative.

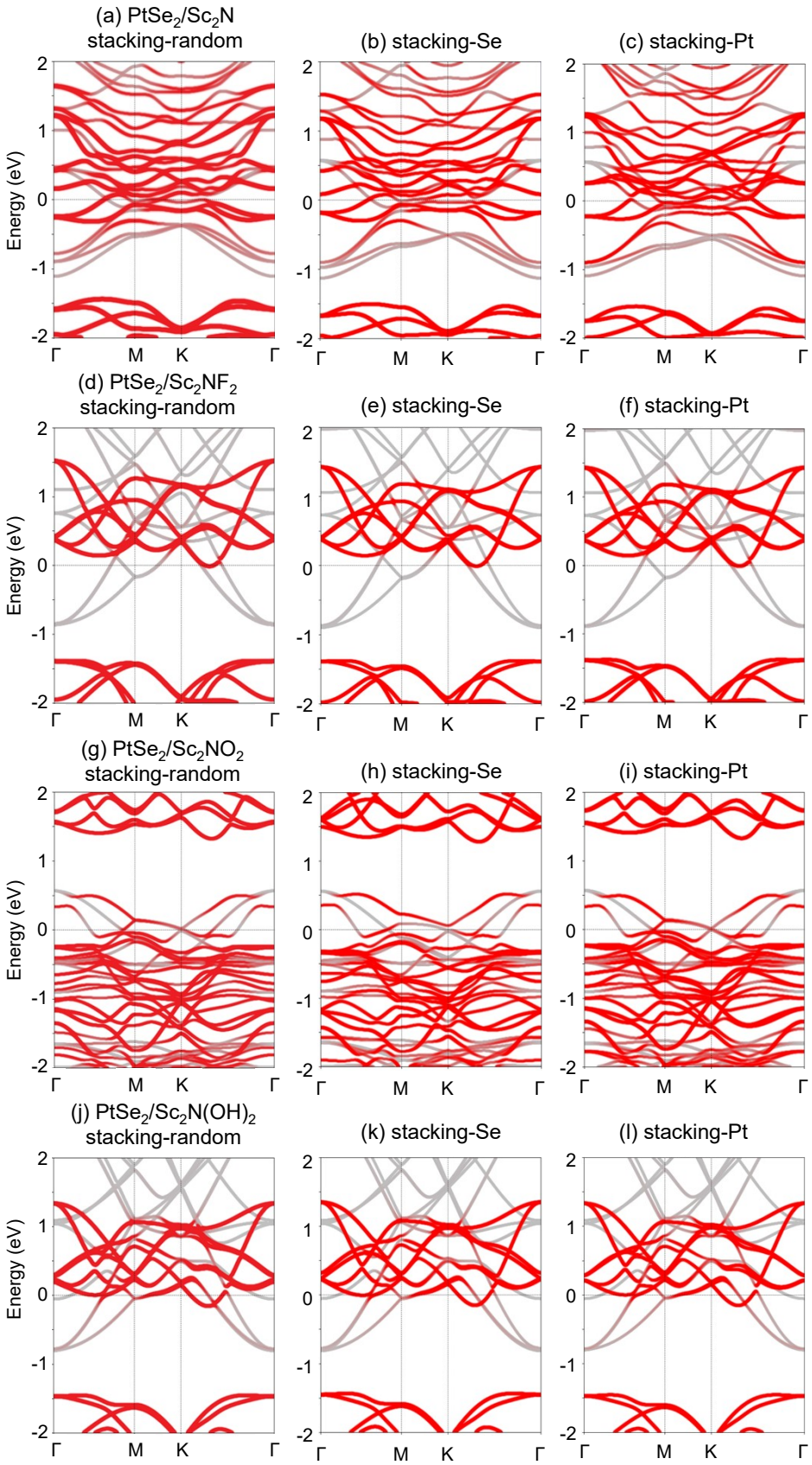

Figure S6. Comparison of projected band structures of the $PtSe_2/Sc_2NX_2$ (X =null, F, O, and OH) vertical heterojunctions with stacking patterns.

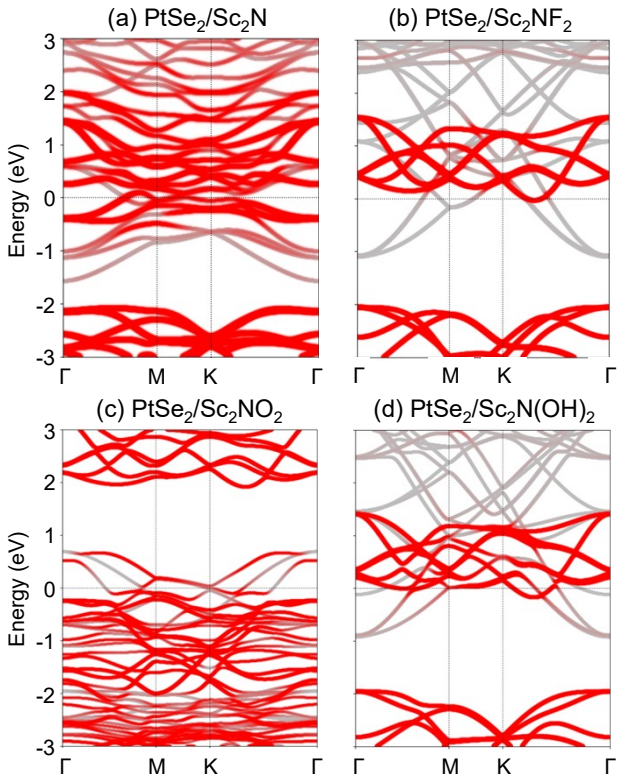

Figure S7. The projected band structures of the $PtSe_2/Sc_2NX_2$ (X =null, F, O, and OH) vertical heterojunctions at HSE06 level.