Supplementary Information for

Structural Stability and Intriguing Electronic Properties of Two-dimensional Transition Metal Dichalcogenides Alloys

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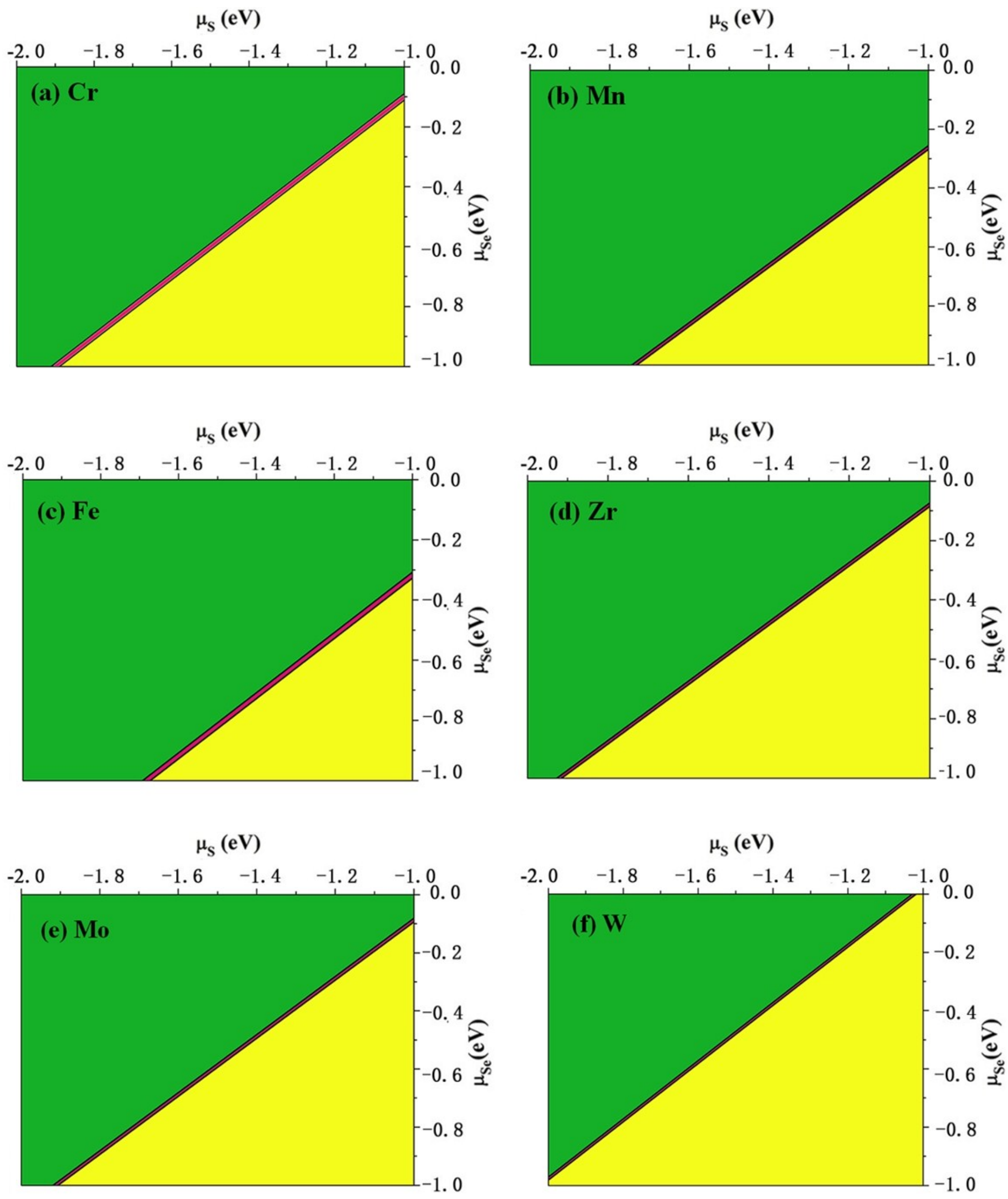
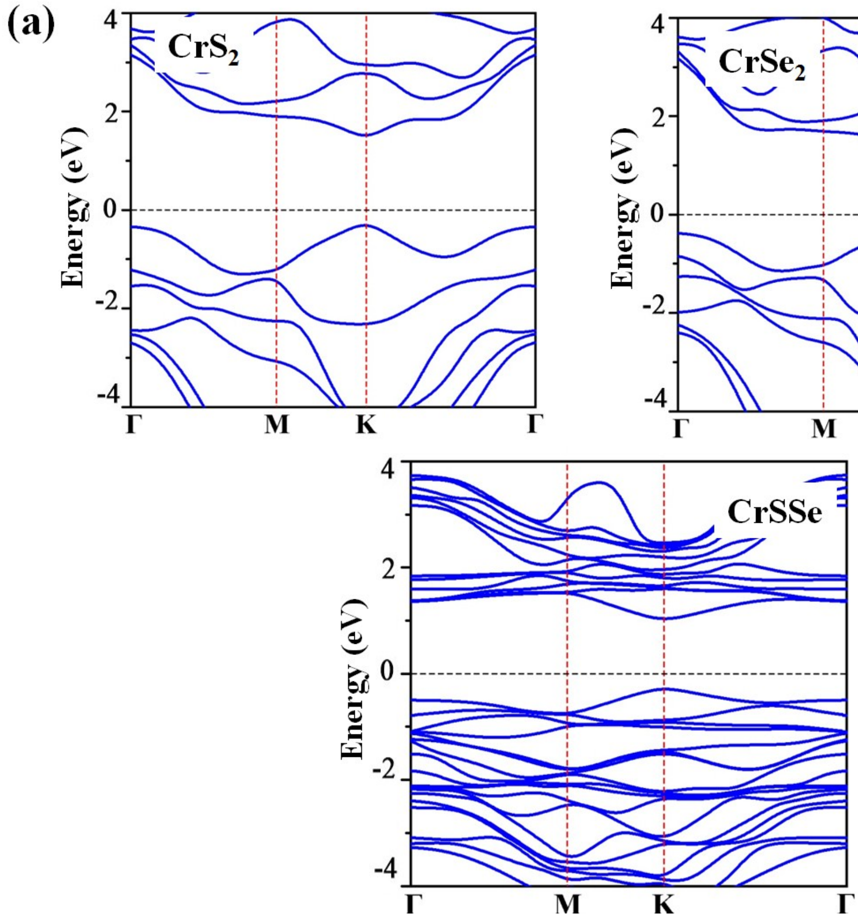
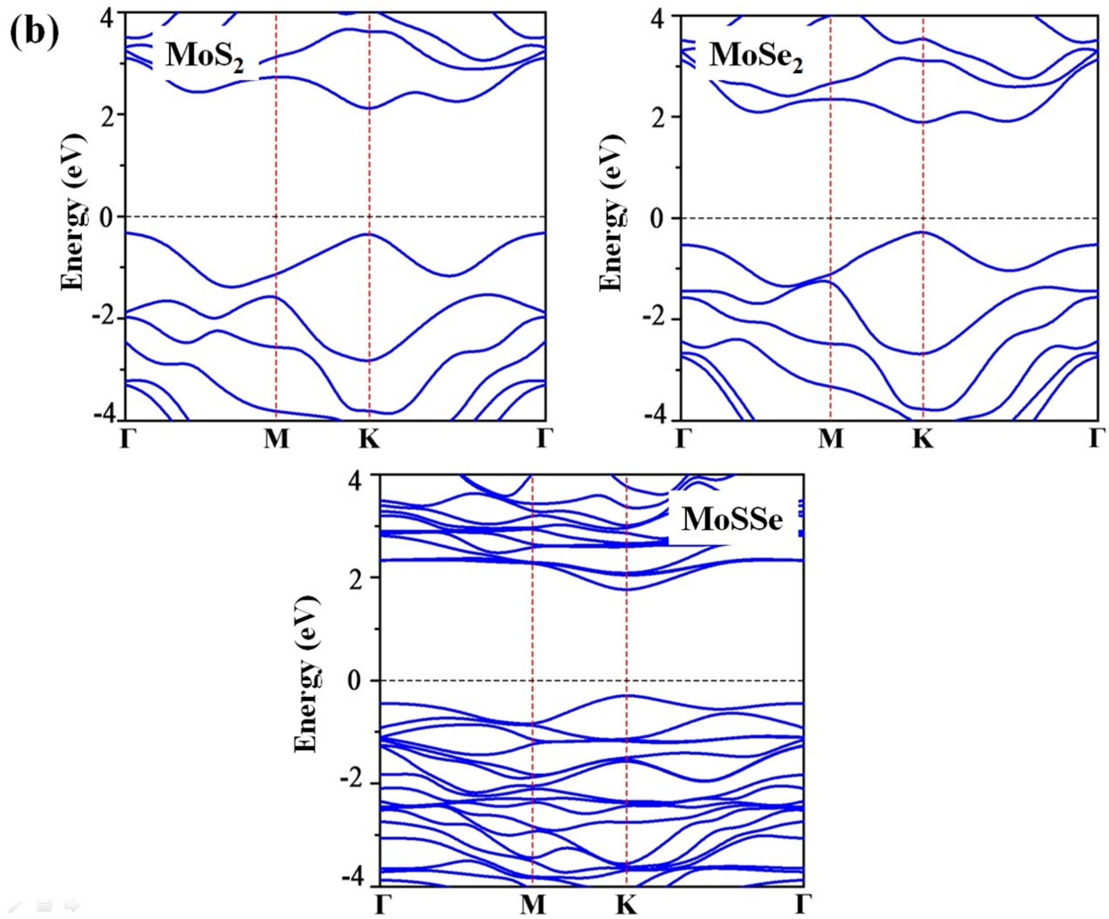


Fig.S1. Phase diagrams of transition metal dichalcogenides(Cr, Mn, Fe, Zr, Mn, W). The yellow region and green region indicate the single phases of MS_2 and MSe_2, respectively, and the red region represents the mixed phases of MSSe alloy.



(a)
CrS$_2$
CrSe$_2$
CrSSe
Energy (eV)
Γ M K Γ


(b)
MoS2
MoSe2
MoSSe
Energy (eV)
4
2
0
-2
-4
Γ
M
K
Γ

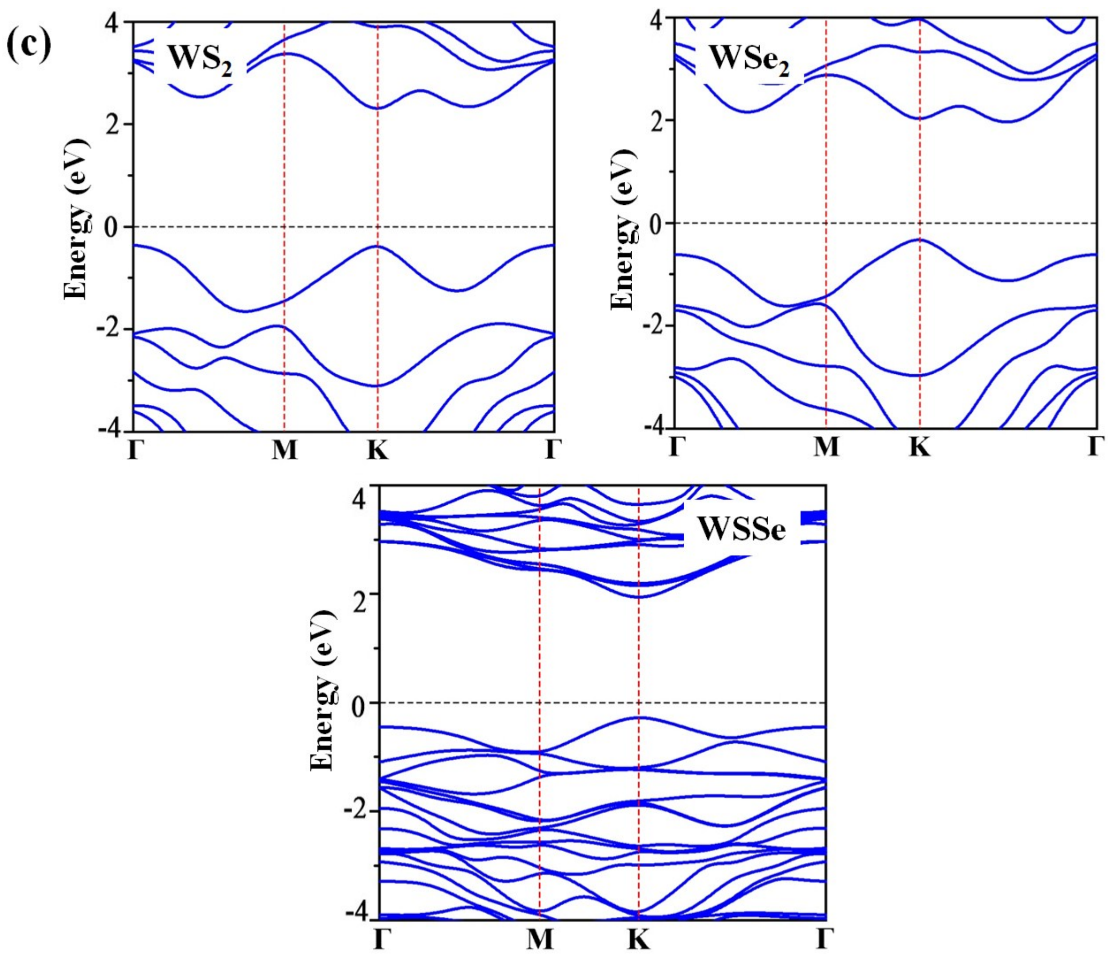


Fig. S2. Band structures of single phases and mixed phases of transition metal dichalcogenides MX_2 with (a) M=Cr, (b) M=Mo and (c) M=W.

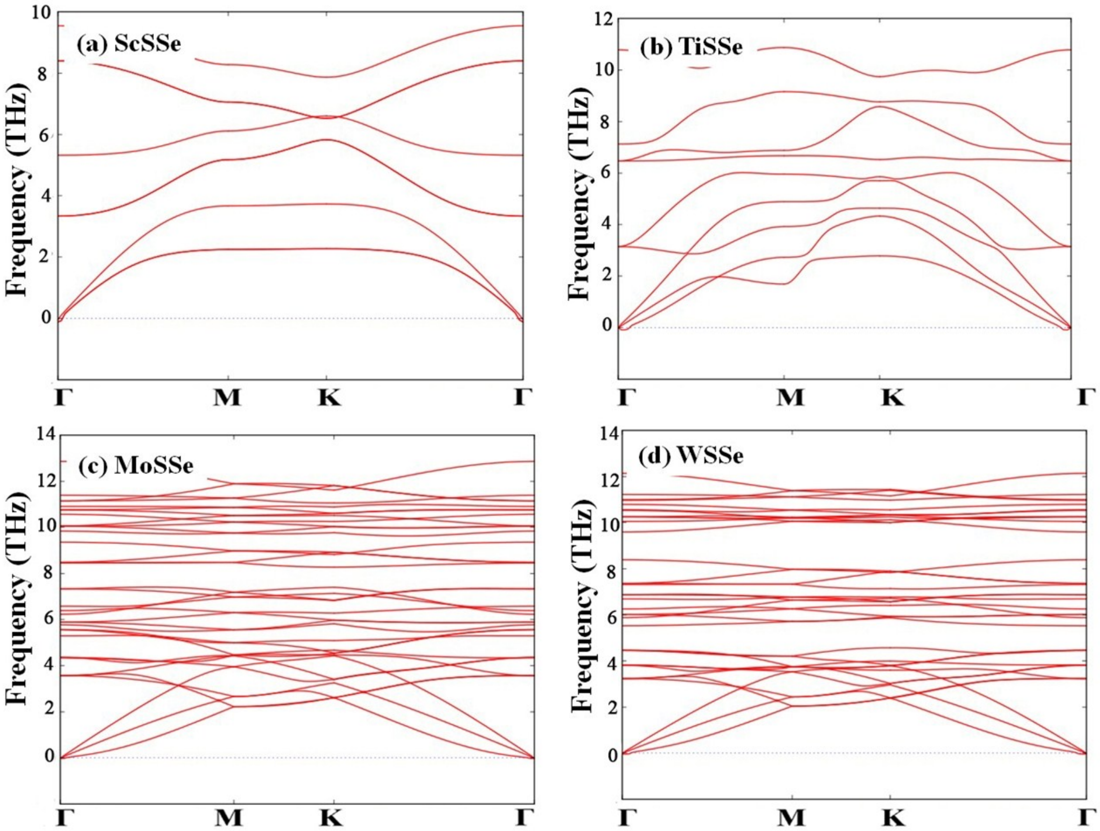


Fig S3. Phonon spectra of mixed phases with the wave vector from Γ, M, K to Γ.

Table S1. Parameter lattices (Å) and bond lengths (Å) for the single phases and mixed phases of transition metal dichalcogenides.

	structure	lattice	d(M-S)	d(M-Se)	d(S-S)	d(Se-Se)	d(S-Se)
ScS_2	1T	3.719	2.545		3.475		
$ScSe_2$	1T	3.610		2.689		3.985	
ScSSe heterolayer	1T	3.560	2.463	2.828			3.888
ScSSe alternating	1T	7.120	2.505(2.529)	2.710(2.755)			
TiS_2	1T	3.398	2.426		3.462		
$TiSe_2$	1T	3.528		2.560		3.712	
TiSSe heterolayer	1T	3.467	2.409	2.579			3.580
TiSSe alternating	1T	6.934	2.408(2.427)	2.562(2.580)			
VS_2	2H	3.174	2.362		2.982		
VSe_2	1T	3.342		2.490		3.693	
VSSe heterolayer	1T	3.269	2.345	2.502			3.573
VSSe alternating	1T	6.538	2.327(2.345)	2.498(2.525)			
CrS_2	2H	3.041	2.289		2.938		
$CrSe_2$	2H	3.209		2.429		3.141	
CrSSe heterolayer	2H	3.125	2.300	2.421			3.041
CrSSe alternating	2H	6.250	2.290(2.291)	2.429(2.431)			
CrSSe separating	2H	6.250	2.285(2.301)	2.420(2.432)	2.911	3.171	
MnS_2	1T	3.346	2.377		3.264		
$MnSe_2$	1T	3.502		2.474		3.497	
MnSSe heterolayer	1T	3.408	2.334	2.474			3.385
MnSSe alternating	1T	6.816	2.328(2.332)	2.475(2.479)			
FeS_2	2H	3.151	2.267		2.707		
$FeSe_2$	2H	3.272		2.429		3.053	

FeSSe heterolayer	2H	3.218	2.254	2.424			2.833
FeSSe alternating	2H	6.436	2.263	2.406(2.414)			
NiS_2	1T	3.349	2.258		3.028		
$NiSe_2$	1T	3.541		2.390		3.211	
NiSSe heterolayer	1T	3.445	2.284	2.368			3.122
NiSSe alternating	1T	6.890	2.271(2.258)	2.382(2.391)			
ZrS_2	1T	3.684	2.574		3.596		
$ZrSe_2$	1T	3.800		2.706		3.852	
ZrSSe heterlayer	1T	3.742	2.568	2.713			3.721
ZrSSe alternating	1T	7.484	2.558(2.581)	2.701(2.722)			
MoS_2	2H	3.183	2.413		3.127		
$MoSe_2$	2H	3.320		2.541		3.336	
MoSSe heterolayer	2H	3.250	2.420	2.535			3.232
MoSSe alternating	2H	6.500	2.409(2.412)	2.543(2.545)			
MoSSe separating	2H	6.500	2.409(2.419)	2.536(2.544)	3.095	3.372	
WS_2	2H	3.182	2.416		3.139		
WSe_2	2H	3.316		2.545		3.354	
WSSe heterolayer	2H	3.249	2.423	2.540			3.246
WSSe alternating	2H	6.498	2.412(2.415)	2.548(2.551)			
WSSe separating	2H	6.498	2.412(2.422)	2.542(2.549)	3.107	3.387	