Supporting Information

Distorted Janus Transition Metal Dichalcogenides: Stable Two Dimensional Materials with Sizable Band Gap and Ultrahigh Carrier Mobility

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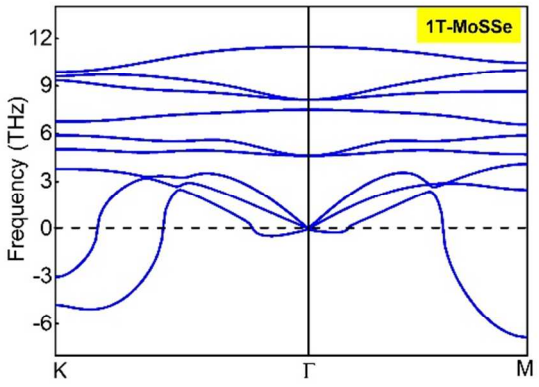

Figure S1. Phonon dispersion of 1T-MoSSe.

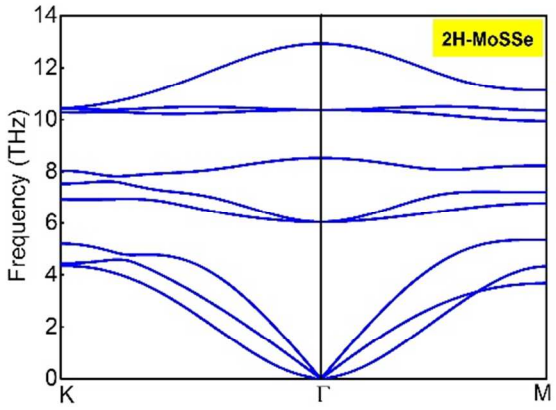

Figure S2. Phonon dispersion of 2H-MoSSe.

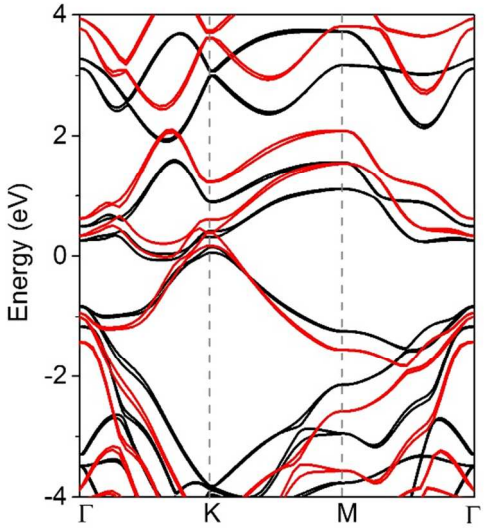

Figure S3. Band structure calculated by PBE(black line) and HSE06 (red line) functionals of 1T-MoSSe. The Fermi level was set to zero.

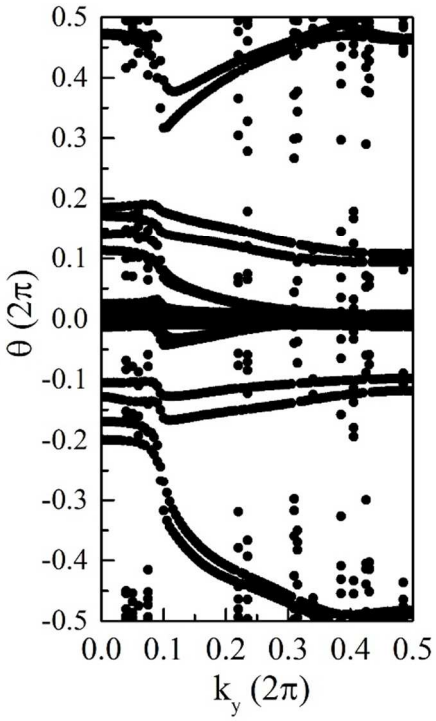

Figure S4. Z_2 index for free standing 1T' MoSSe, it can be seen that the distorted Janus TMD is a trivial semiconductor.

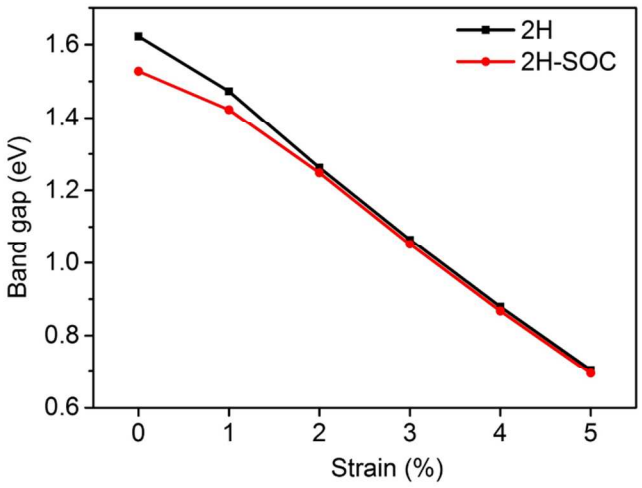

Figure S5. Calculated band gap of 2H-MoSSe as a function of applied strain.

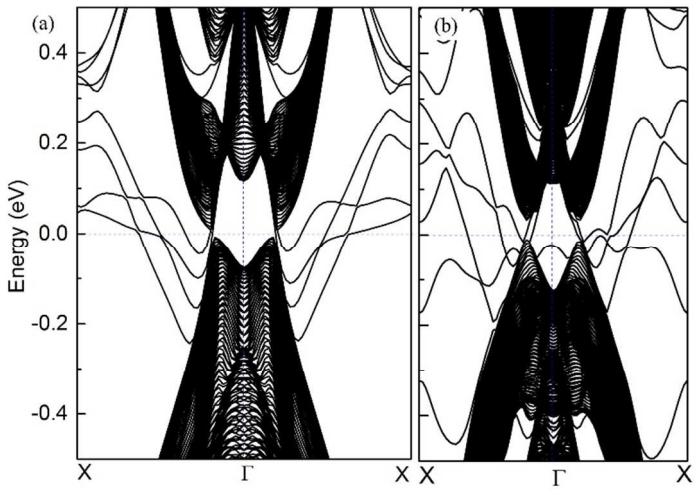

Figure S6. The calculated edge states for 1T'-MoSSe at strain of (a) 0% and (b) 3%.

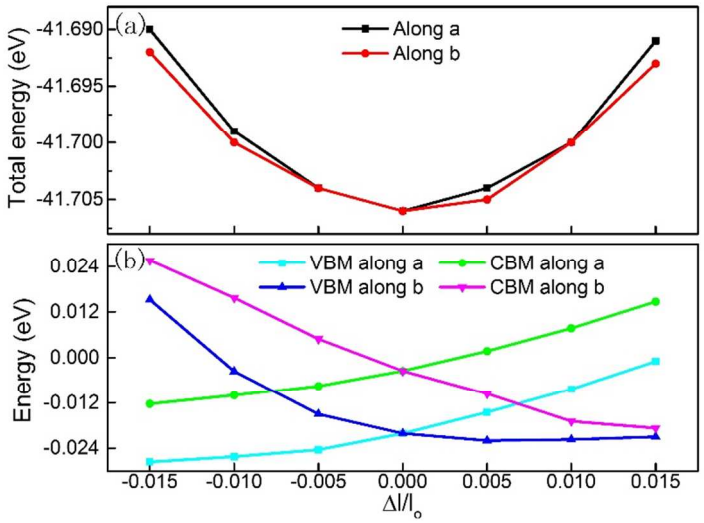

Figure S7. (a) Total energy variation under strain deformation. (b) VBM and CBM energies as a function of applied strain, for carrier mobility calculations.

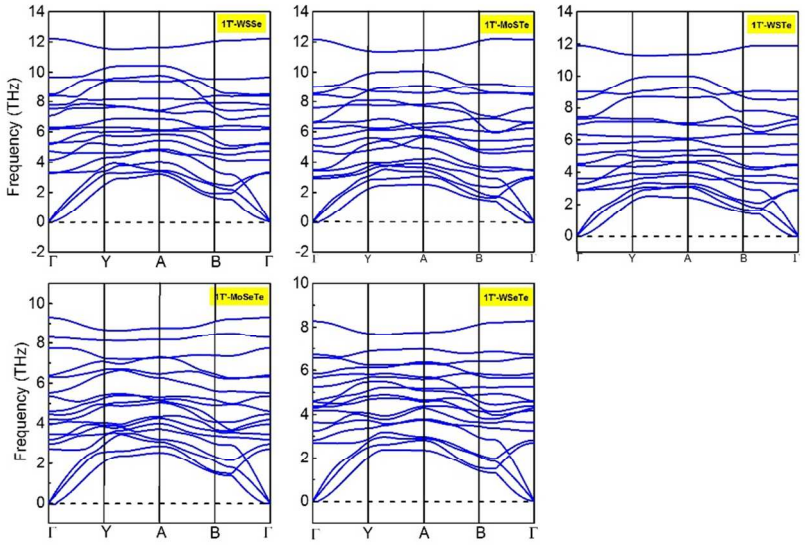

Figure S8. Phonon dispersion curves of Janus 1T'-MXY monolayer. The absence of imaginary frequency presents the structural ability of all 1T'-MXY monolayer.

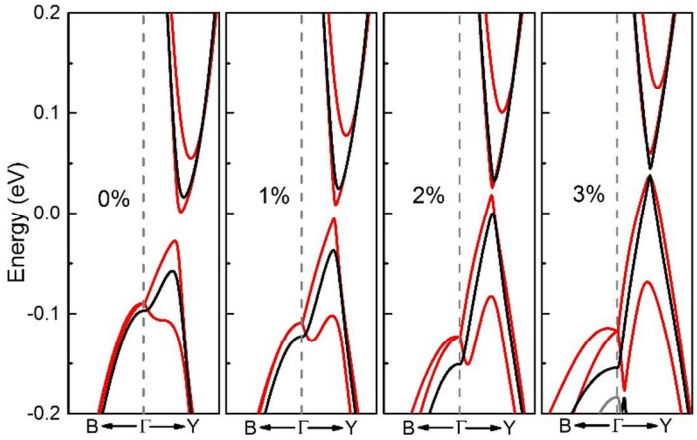

Figure S9. Zoomed band structures of 1T'-WSSe near Γ point under different strain deformation with (red solid line) and without (black solid line) spin-orbital coupling. The Fermi level was set to zero.

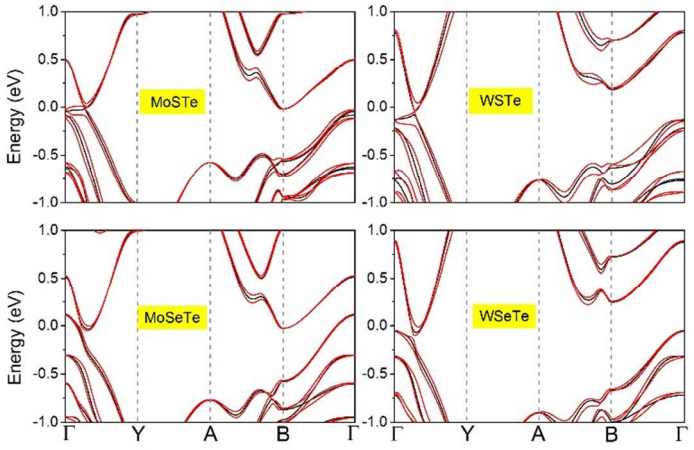

Figure S10. Band structures with (red solid line) and without (black solid line) spin-orbital coupling of other 1T'-MXY monolayer. The Fermi level was set to zero.

Table S1. Band gaps of 1T'-MXY, calculated by HSE06 method including spin-orbit coupling effect (HSE-SOC)

	WSSe	MoSTe	WSTe	MoSeTe	WSeTe
Band gap (eV)	0.09	0.08	0.05	-	0.05

The "-"sign in the table means there is no gap, it is a metal