Supporting Information

Novel non-Janus MoSF Monolayer

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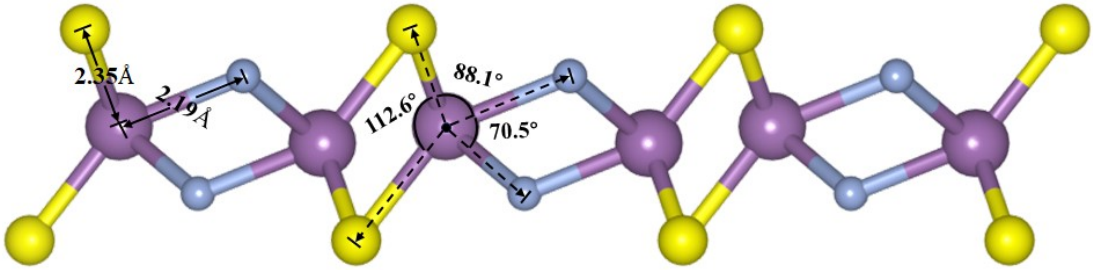

Figure S1. Schematic illustration of the distances and bond angles between Mo, S, and F atoms. The unit cell parameters are a = 3.28 Å, b = 5.34 Å, c = 27.26 Å.

Table S1. Elastic constants of Hybrid 1T'-MoSF monolayer under biaxial strain, in the unit of GPa.

Strain	C_{11}	C_{12}	C_{22}	C_{66}	Stability
1%	31.7	11.9	38.9	-2.8	NO
2%	29.7	11.6	37.4	-0.9	NO
3%	26.4	10.6	35.8	-2.1	NO
4%	24.1	10.3	34.2	-2.7	NO
5%	21.4	9.9	31.9	-3.2	NO
-1%	37.4	12.9	41.8	-1.5	NO
-2%	47.3	7.3	47.9	0.5	NO
-3%	18.3	24.4	40.4	-0.1	NO
-4%	18.7	35.4	32.5	-0.3	NO
-5%	12.1	41.8	30.4	-0.2	NO

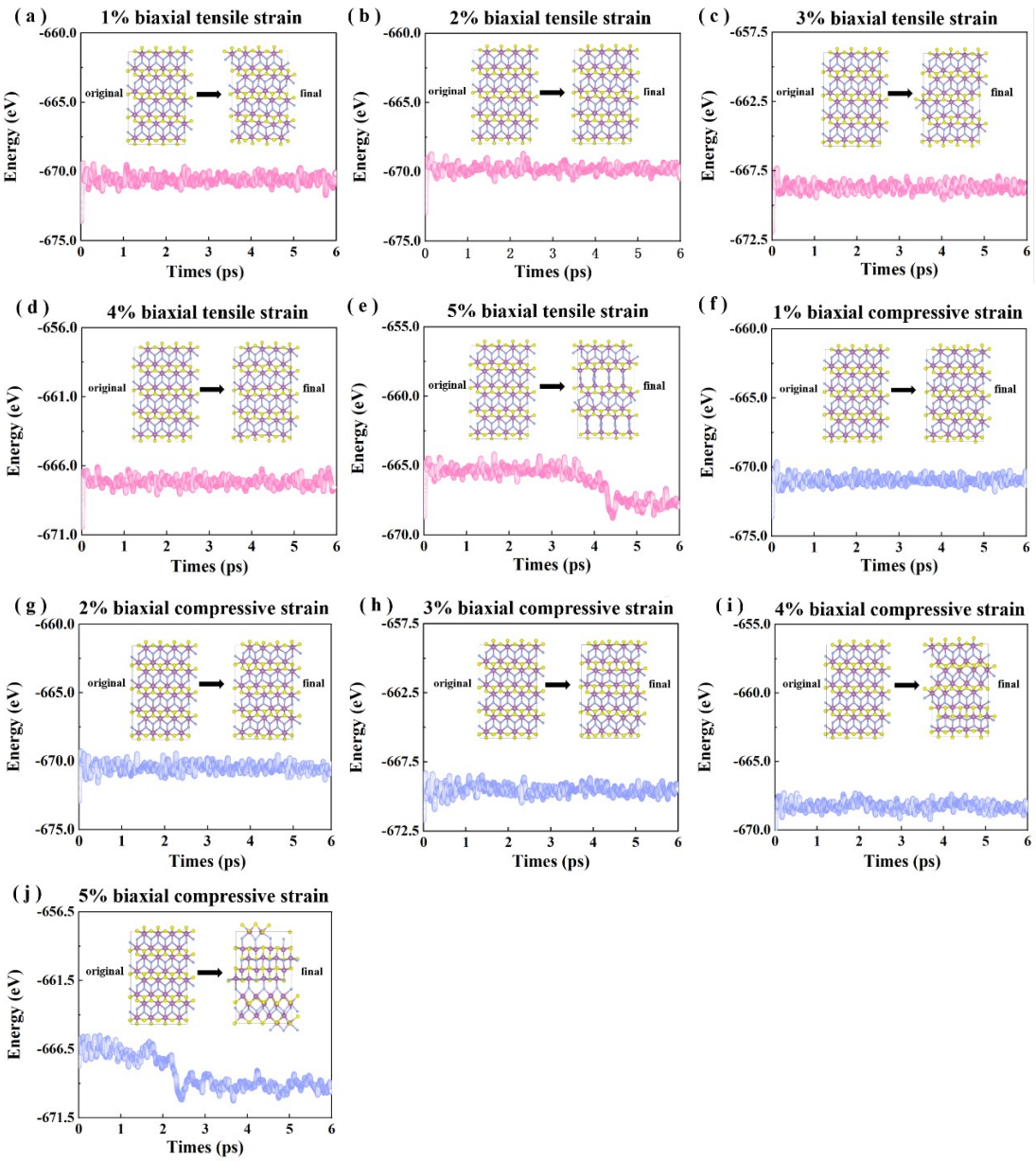

Figure S2. The AIMD simulations at 300K for Hybrid 1T'-MoSF monolayer under biaxial strain.

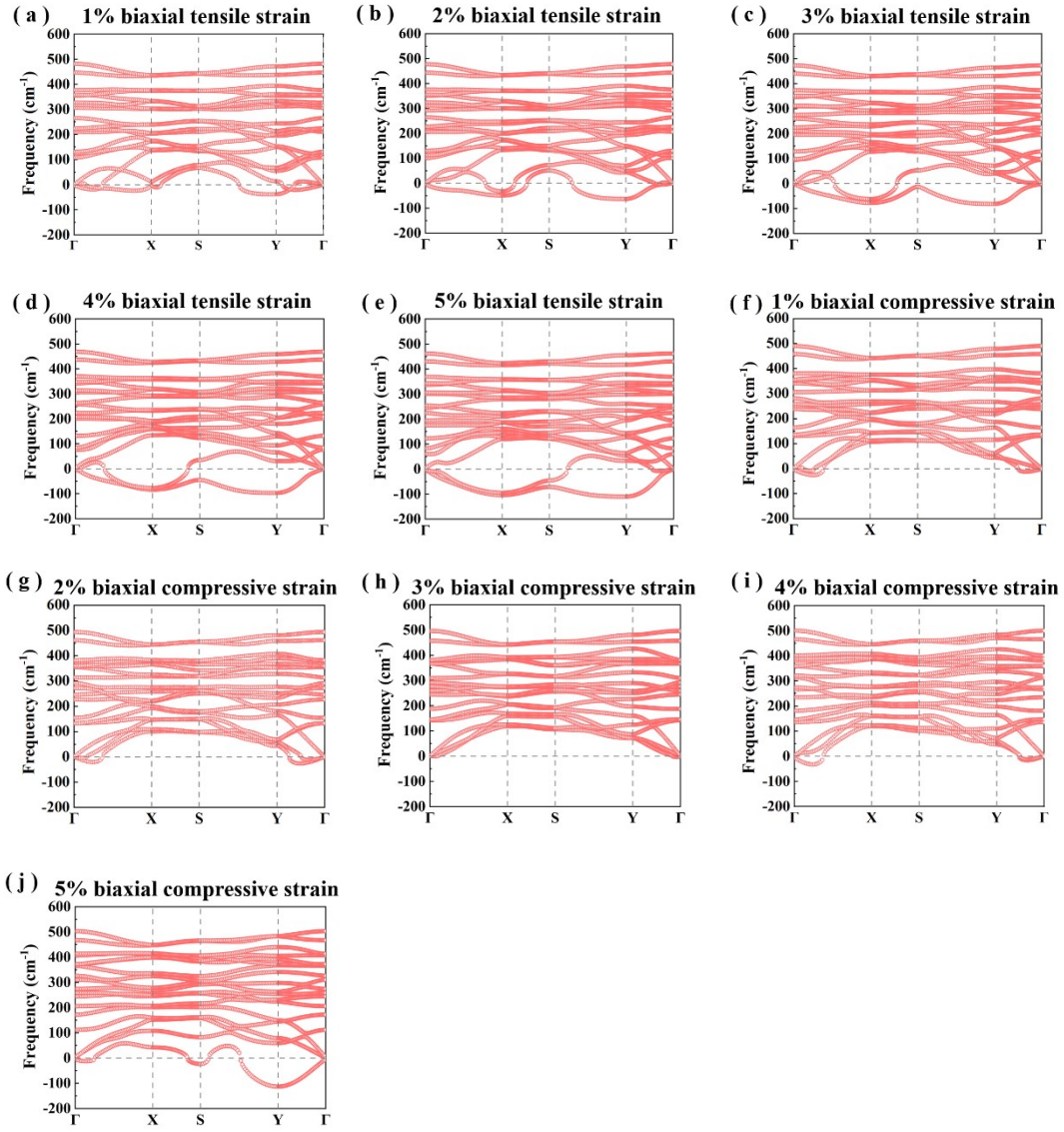

Figure S3. The phonon dispersion of Hybrid 1T'-MoSF monolayer under biaxial strain.

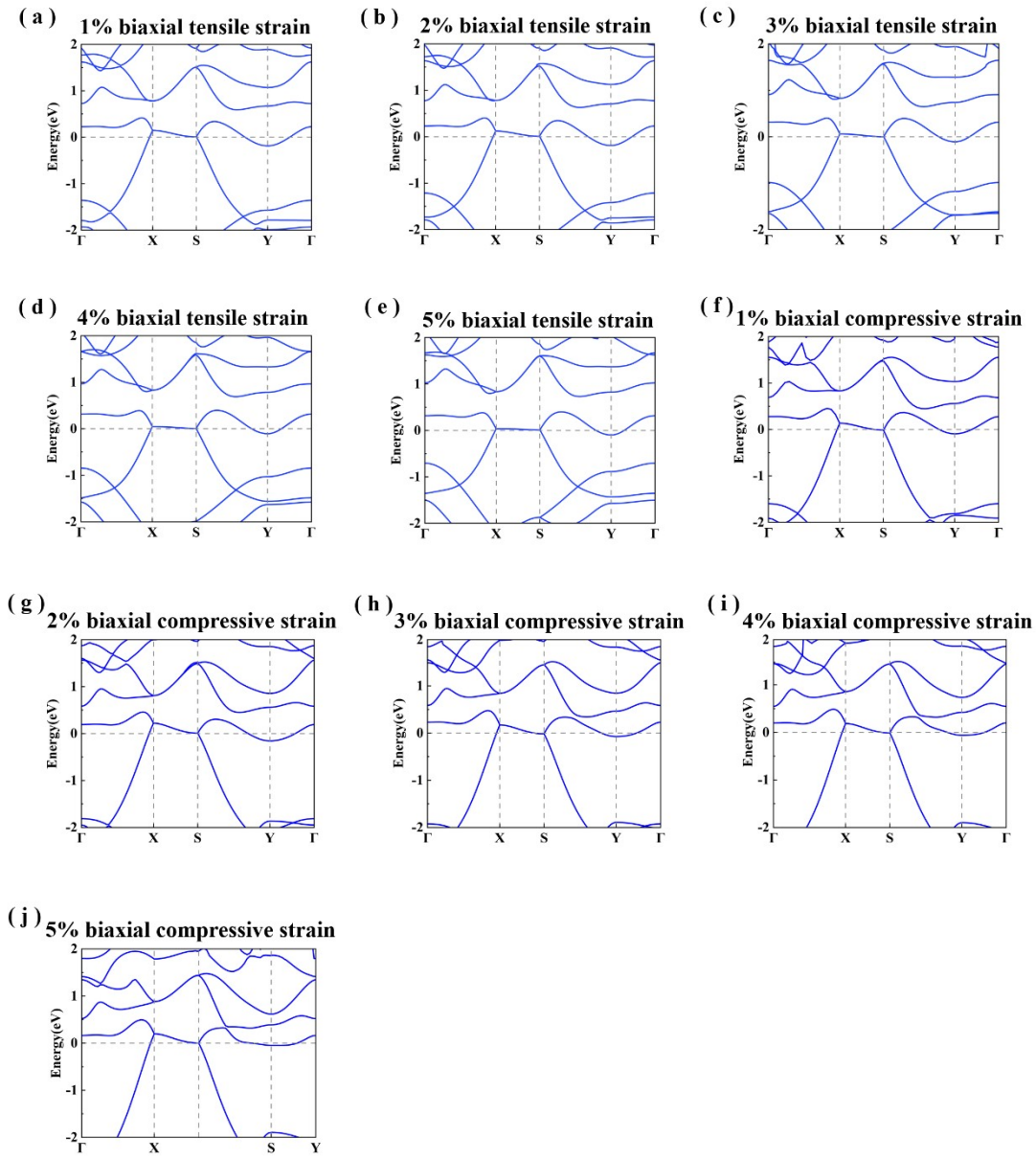

Figure S4. Band structure of Hybrid 1T'-MoSF monolayer under biaxial strain.

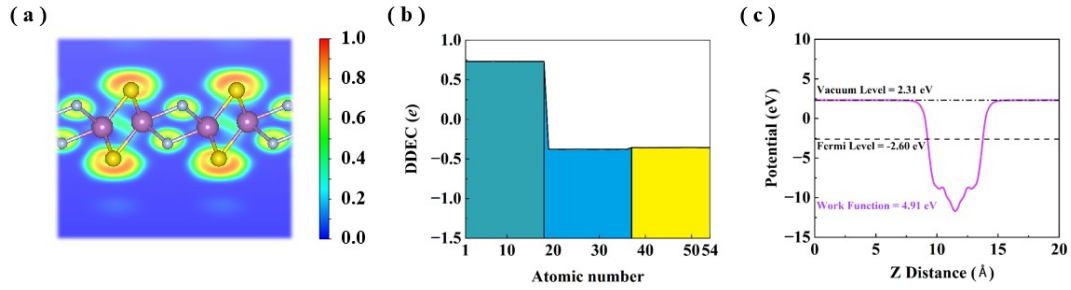

Figure S5. (a) Electron localization function (ELF) of Hybrid 1T'-MoSF, (b) The DDEC charge of Janus monolayer MoSF, (c) Work function.

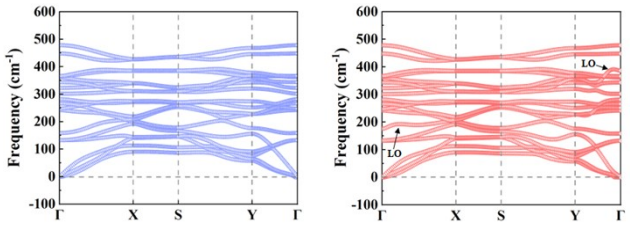

Figure S6. The phonon dispersion of Hybrid 1T'-MoSF monolayer without LO-TO splitting (blue) and with LO-TO splitting (red).

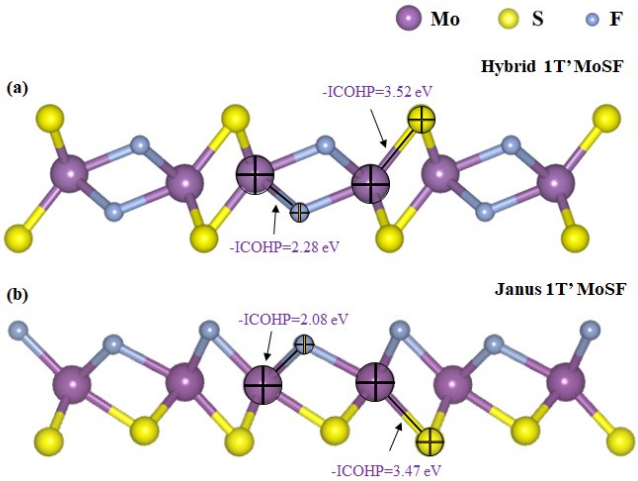

Figure S7. The -ICOHP value of Mo-S and Mo-F bonds for (a) Hybrid 1T'-MoSF and (b) Janus 1T'-MoSF.

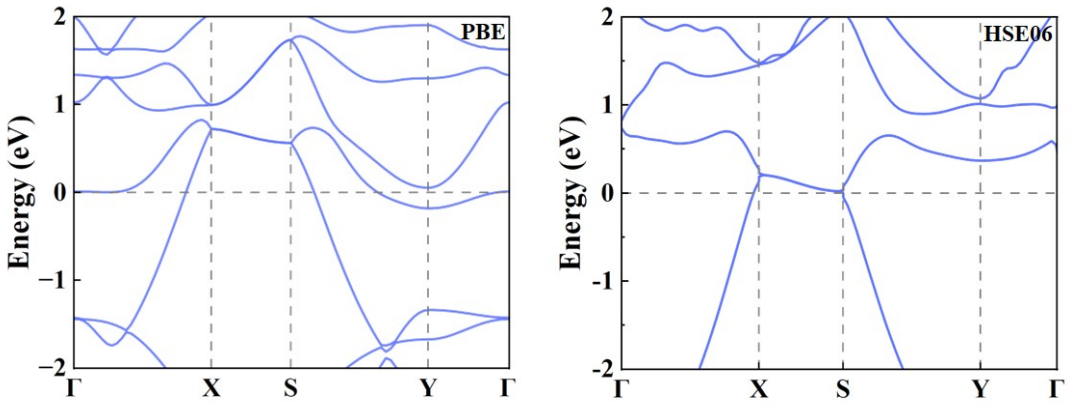

Figure S8. The band structure using PBE and HSE06 exchange-correlation functional.