Supplementary Information

Enhancing Valley Splitting and Anomalous Valley Hall Effect in V-Doped Janus MoSeTe monolayer

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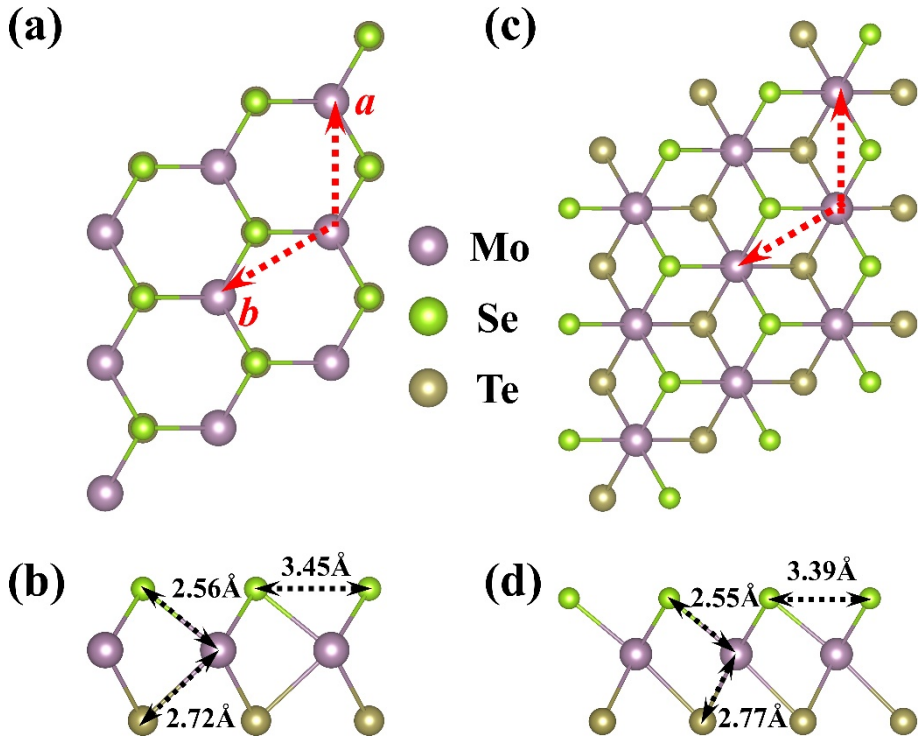

Fig S1 (a) (c) Crystal structure of pristine 2H-MoSeTe and 1T- MoSeTe. (b) (d) Coordination environment of the Mo atom.

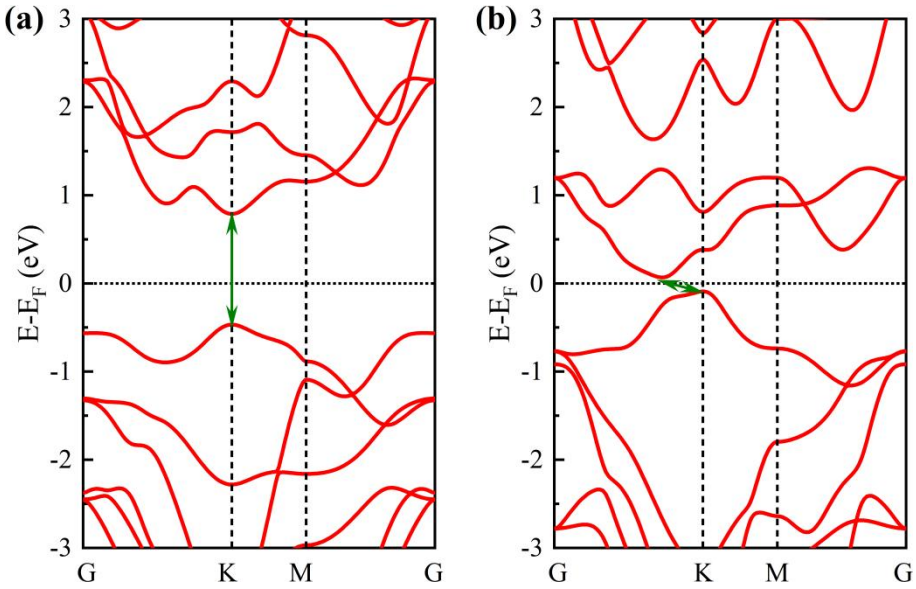

Fig. S2 Band structure of pristine (a) 2H-MoSeTe and (b) 1T- MoSeTe without SOC.

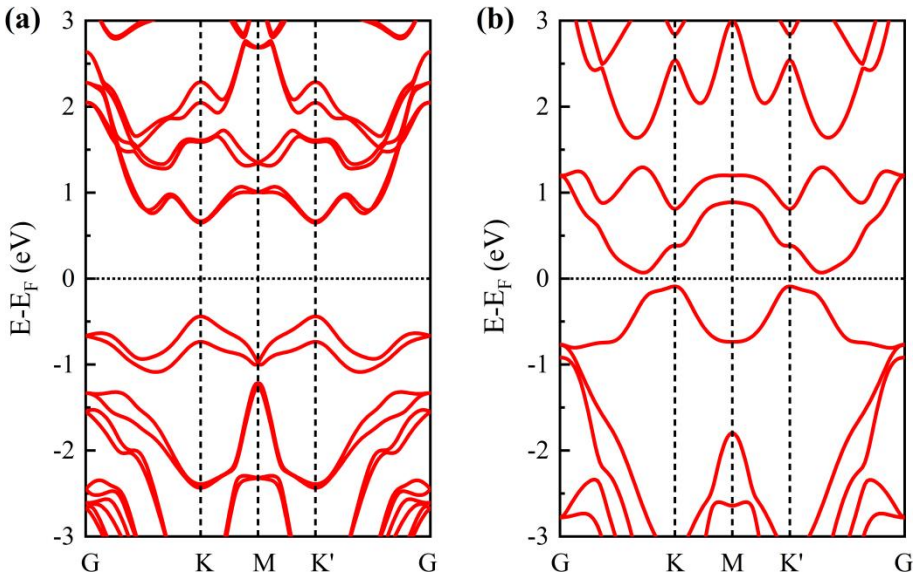

Fig. S3 Band structure of pristine (a) 2H-MoSeTe and (b) 1T- MoSeTe with SOC.

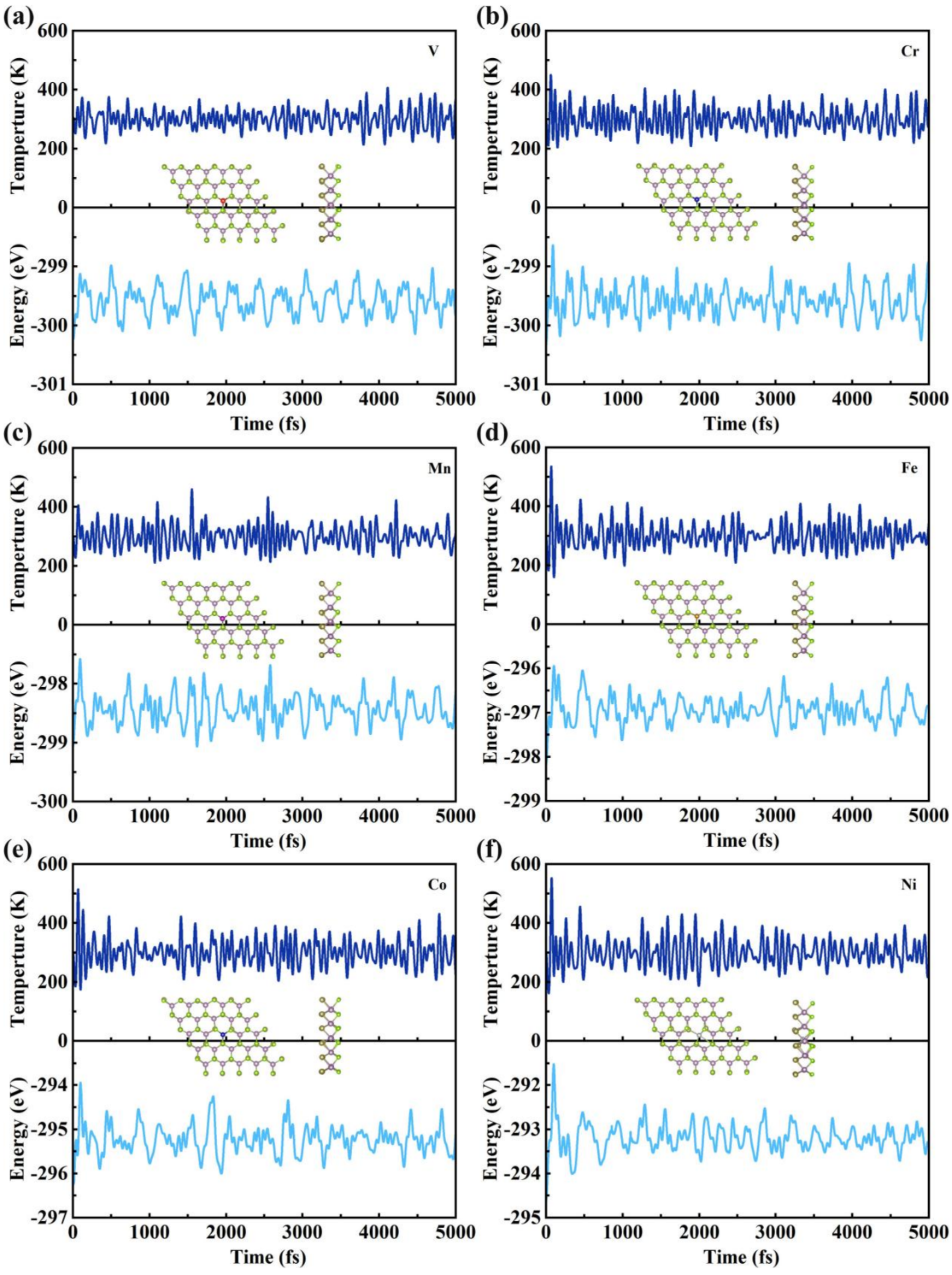

Fig. S4 The fluctuation of (a) V-doped, (b) Cr-doped, (c) Mn-doped, (d) Fe-doped, (e) Co-doped and (f) Ni-doped 4×4×1 2H-MoSeTe superlattice of the total energy during 5 ps AIMD simulation at 300 K. The snapshot of the corresponding structure after the AIMD simulation is given in the inset.

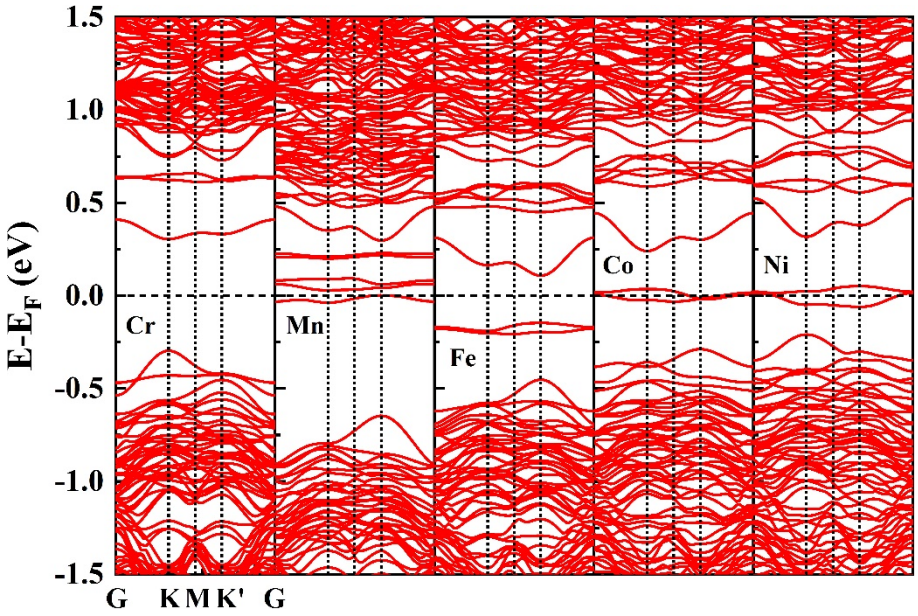

Fig. S5 Band structures of Cr-doped, Mn-doped, Fe-doped, Co-doped and Ni-doped 4×4×1 2H-MoSeTe superlattice with SOC.

TABLE SI. The valley splitting (KK') and formation energy of different dopant TM atoms on the 4×4×1 2H-MoSeTe superlattice.

	Cr	Mn	Fe	Co	Ni
ΔKK' (meV)	123	-147	-125	-70	94
E_F	-5.71	-4.44	-5.78	-7.31	-6.41