Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Quantifying the composition dependency of the ground-state structure, electronic property and phase transition dynamics in the ternary transition-metal-dichalcogenide monolayers

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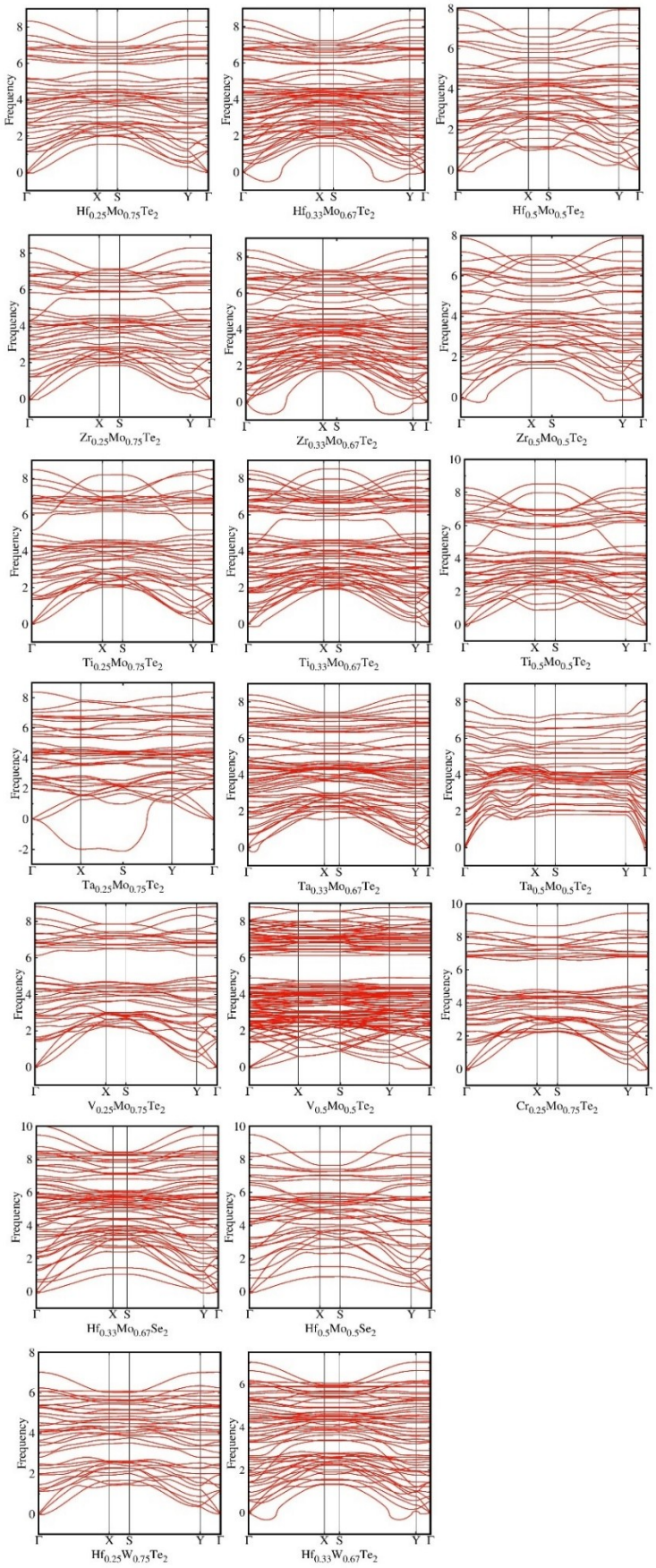

Fig. S1 Phonon spectrums of H phases of the ternary TMDs

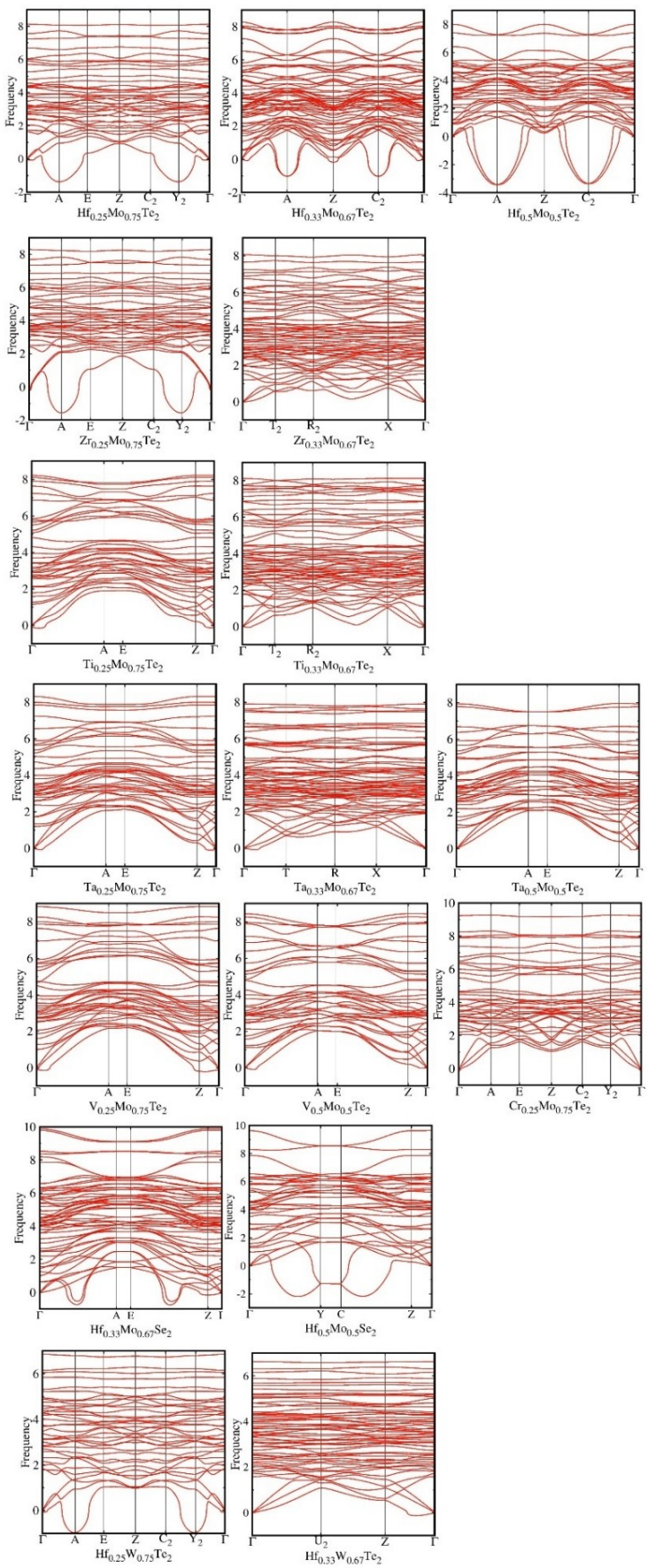

Fig. S2 Phonon spectrums of T’ phases of the ternary TMDs

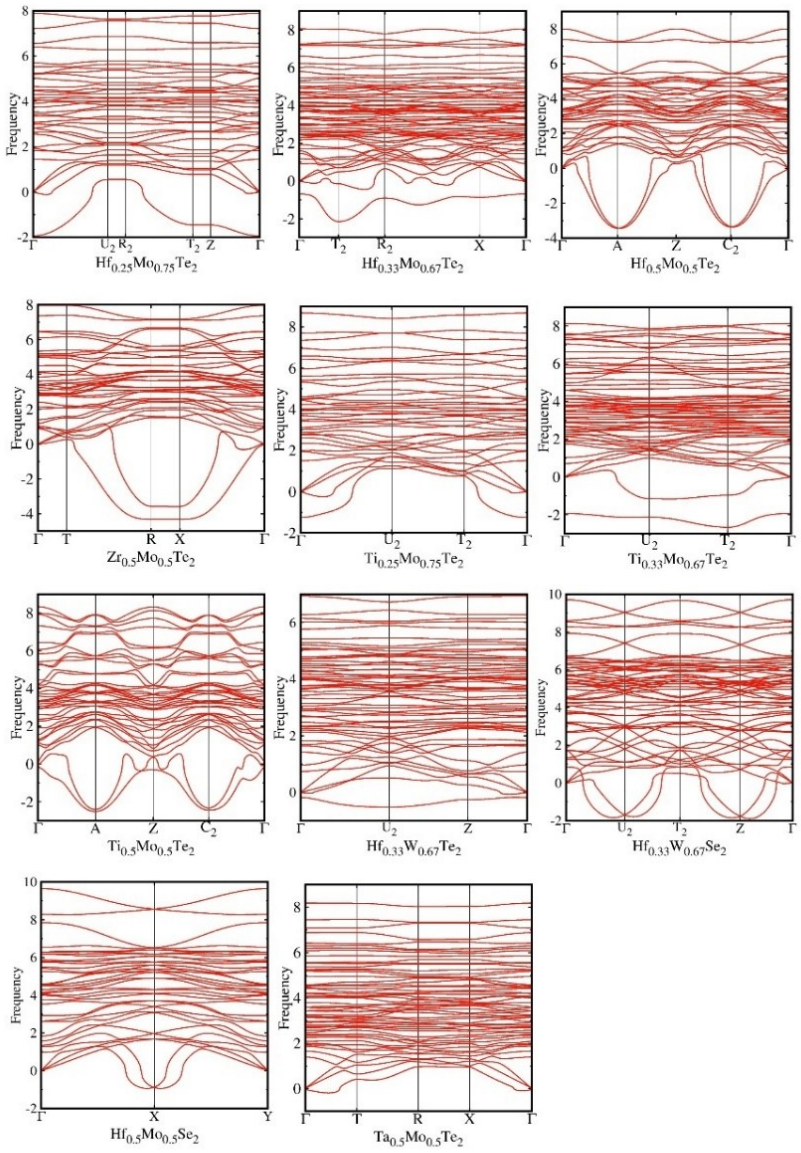

Fig. S3 Phonon spectrums of the T phases of the ternary TMDs

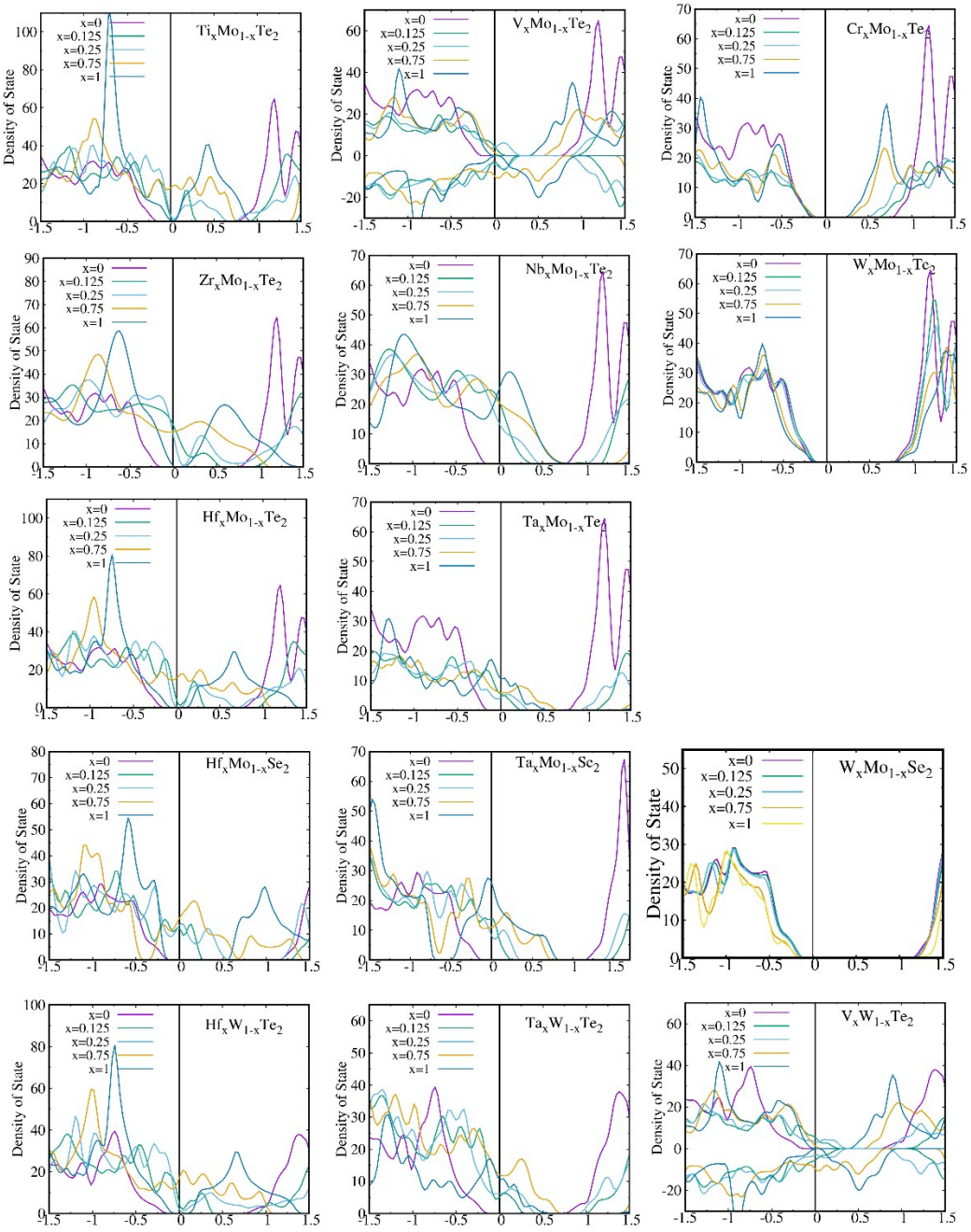

Fig. S4 Density of states calculated by using the GGA-PBE functionals. The value of x varies from 0 to 1. PBE functionals reveal that the pure $HfSe_2$, $HfTe_2$, $ZrTe_2$, and VTe_2 have the semiconducting properties.

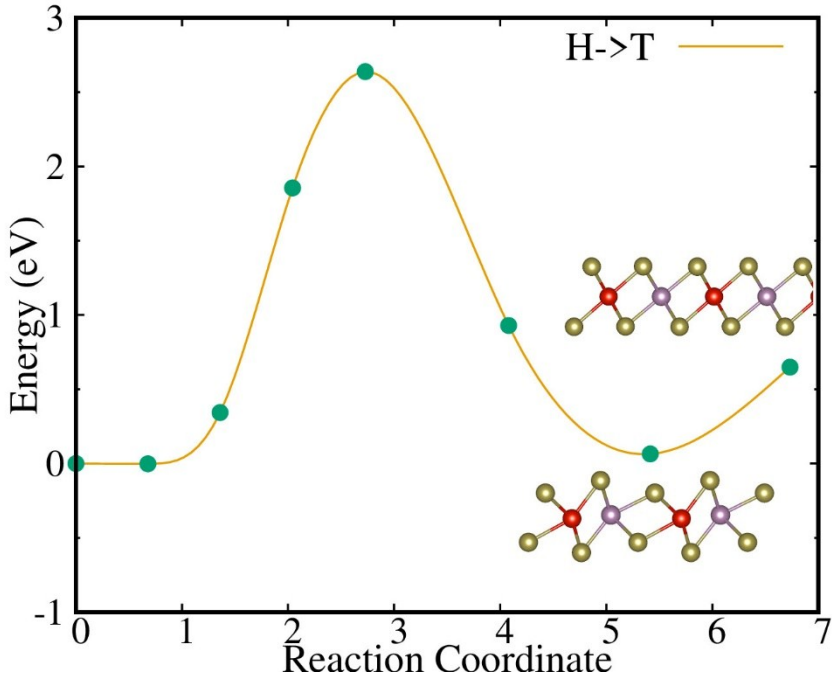

Fig. S5 MEP of the transition between H phase and T phase of $V_xMo_{1-x}Te_2$. It can be seen that the H phase may translate to a distorted structure with lower energy than the T phase in the transition path.