Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First Principles Assessment on Phase Stability and Transition Mechanisms of Designated Crystal Structures of Pristine and Janus Transition Metal Dichalcogenides

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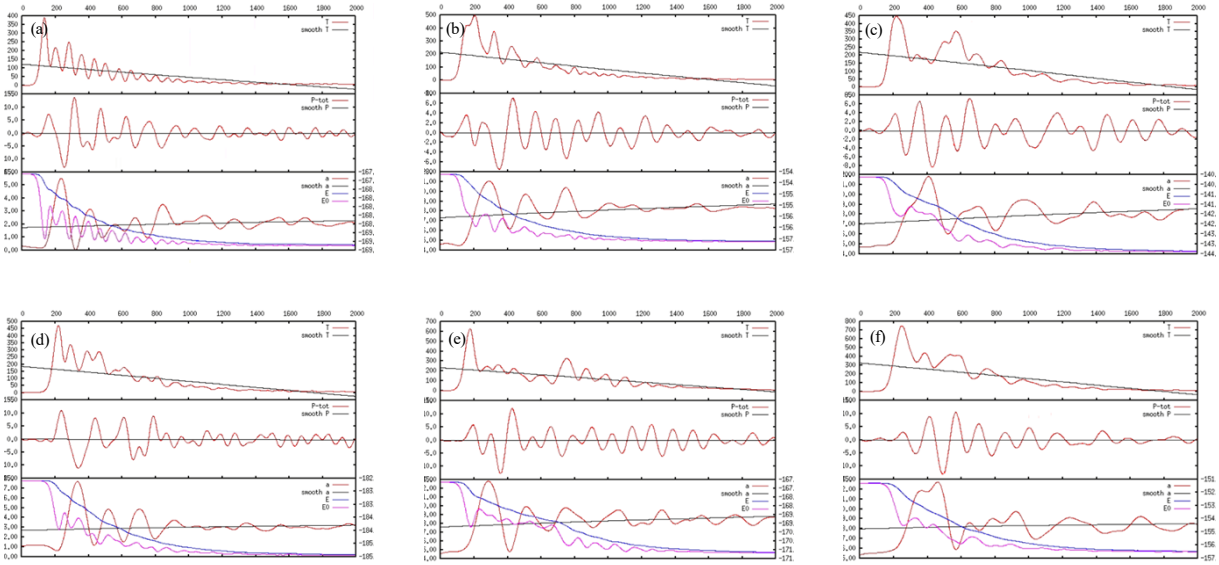
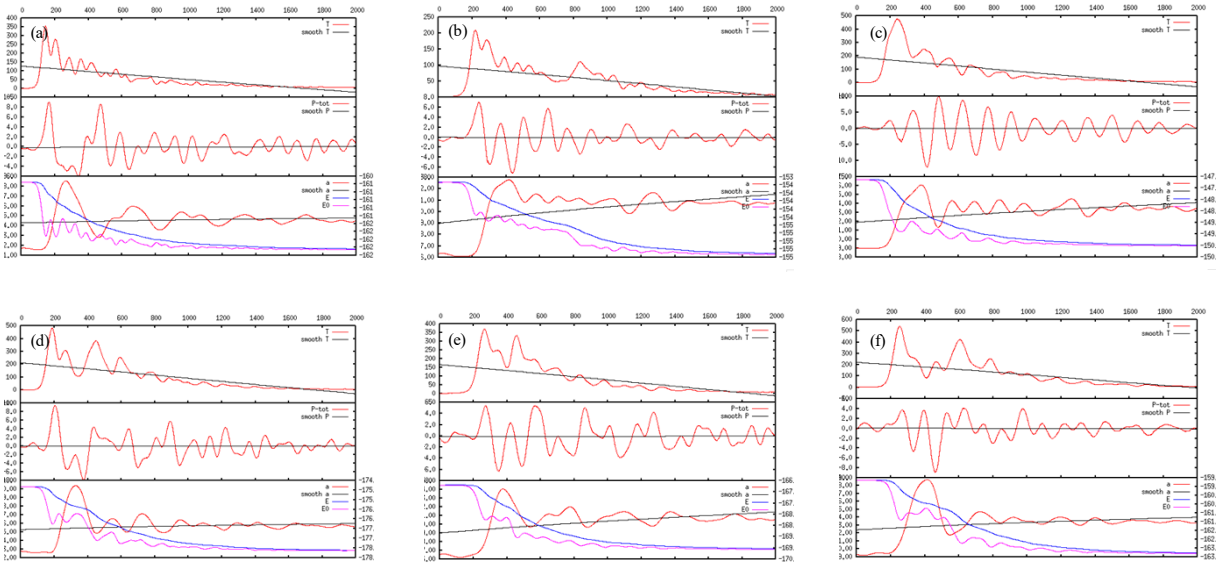
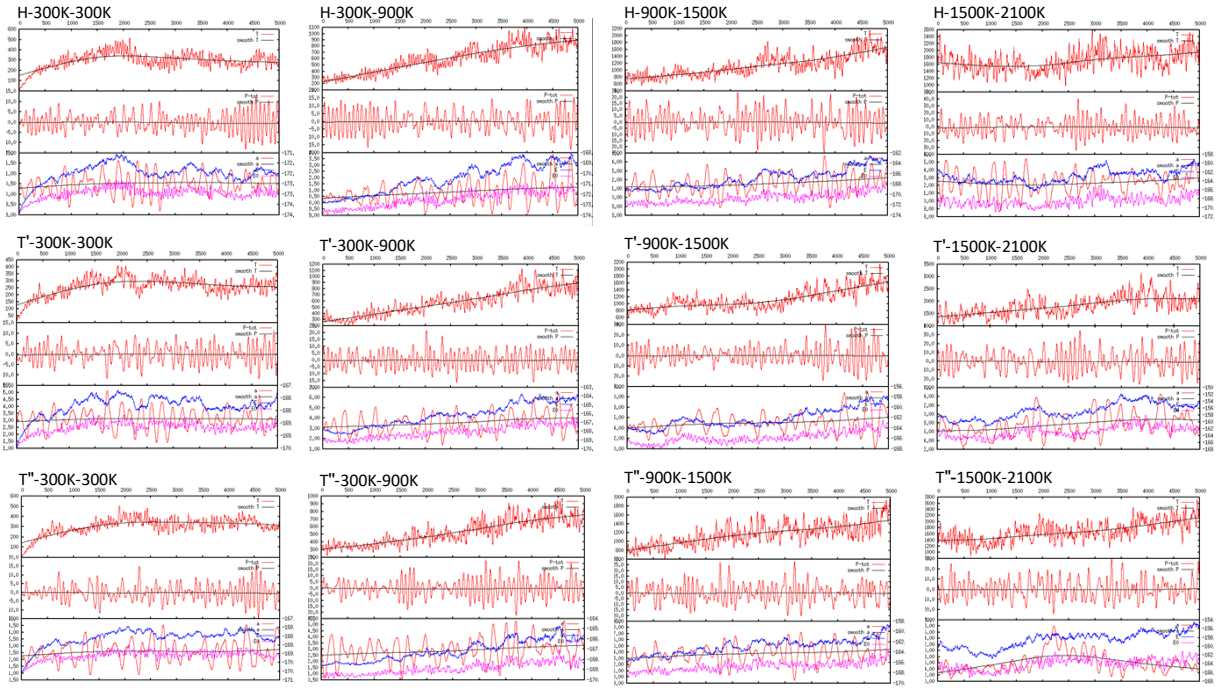
S1) 5K AIMD simulations of pristine TMDs: (a) MoS_2, (b) $MoSe_2$, (c) $MoTe_2$, (d) WS_2, (e) WSe_2, (f) WTe_2.



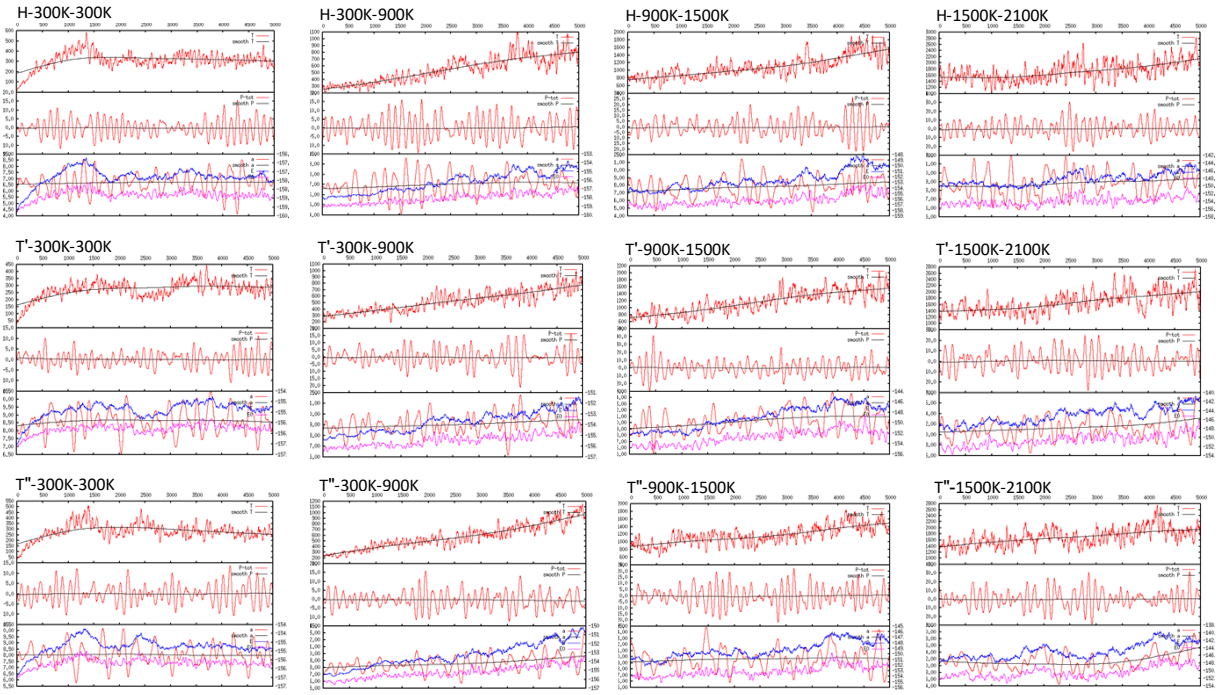
S2) 5K AIMD simulations of Janus TMDs: (a) MoSSe, (b) MoSTe, (c) MoSeTe, (d) WSSe, (e) WSTe, (f) WSeTe.



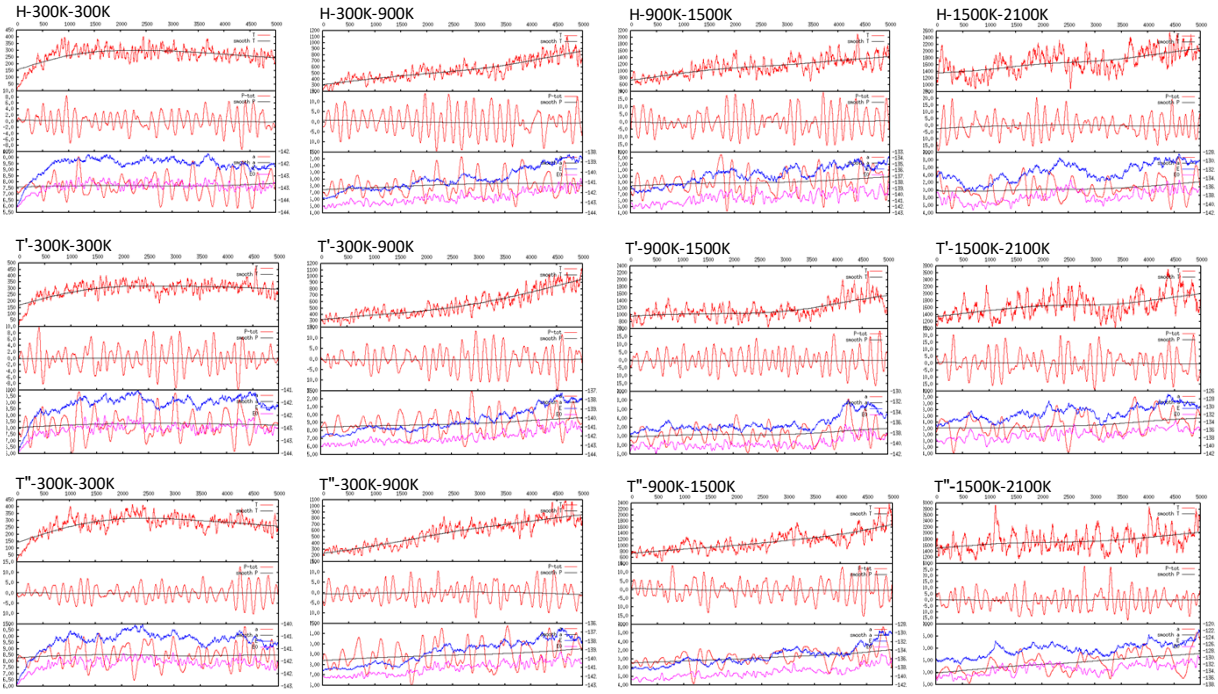
S3) 300K-2100K AIMD simulations for H, T' and T'' phases of MoS_2



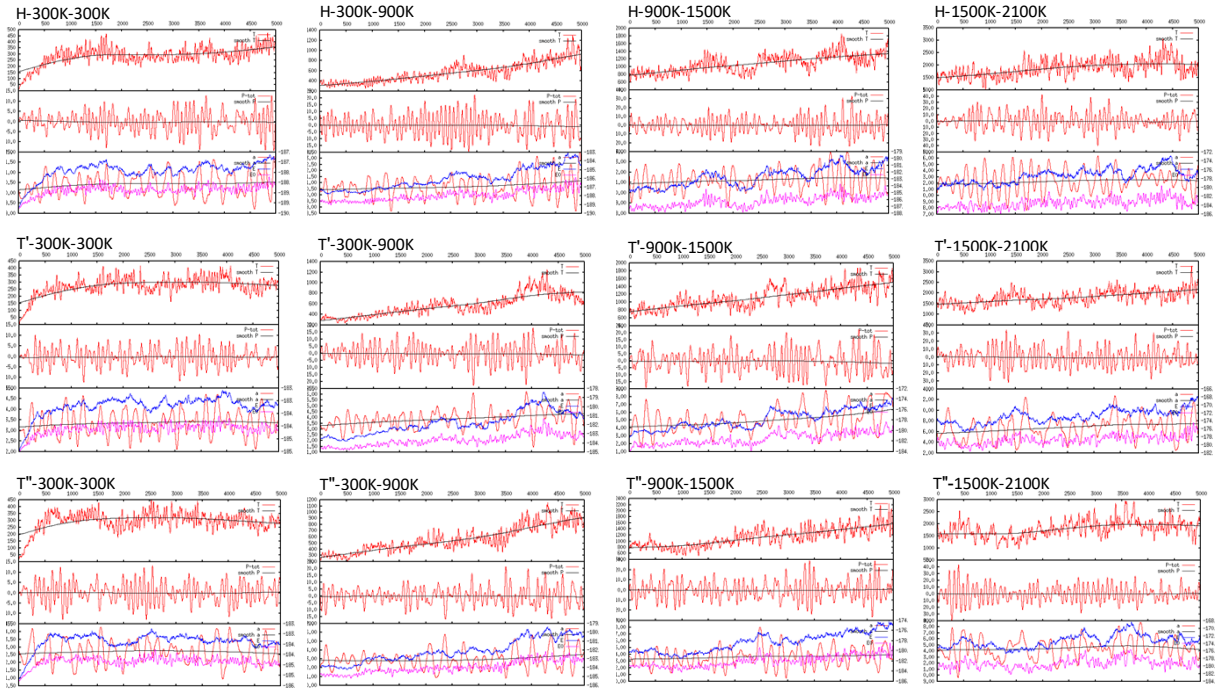
S4) 300K-2100K AIMD simulations for H, T' and T'' phases of $MoSe_2$



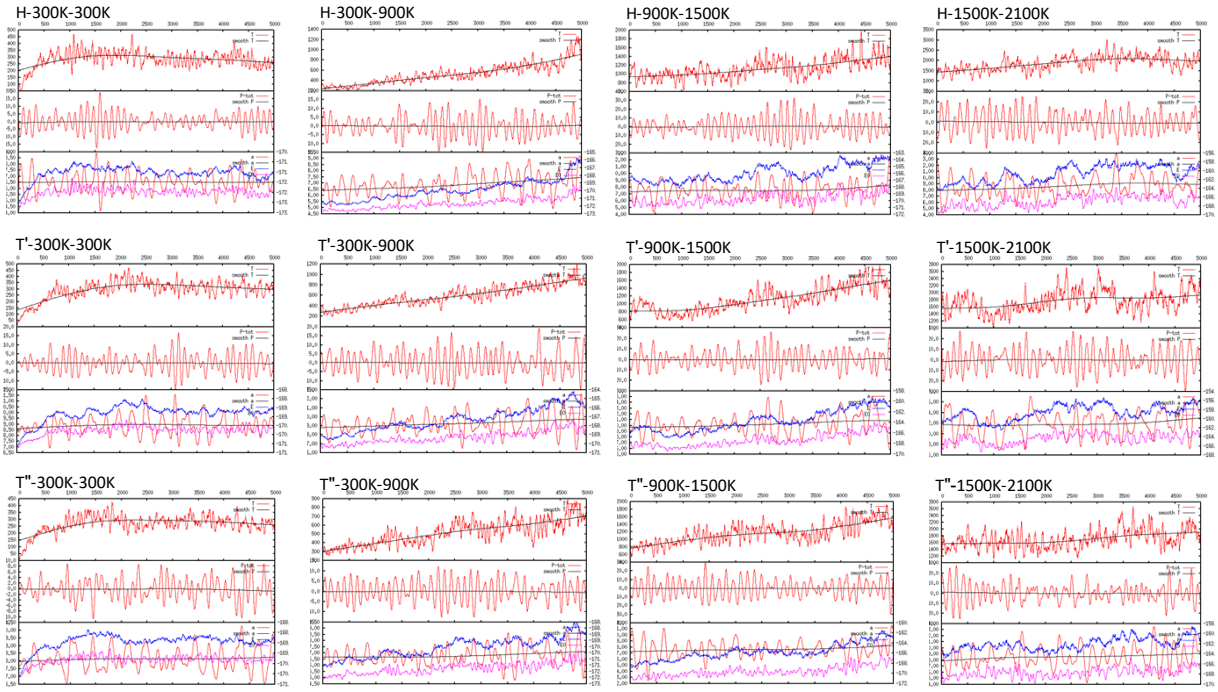
S5) 300K-2100K AIMD simulations for H, T' and T'' phases of $MoTe_2$



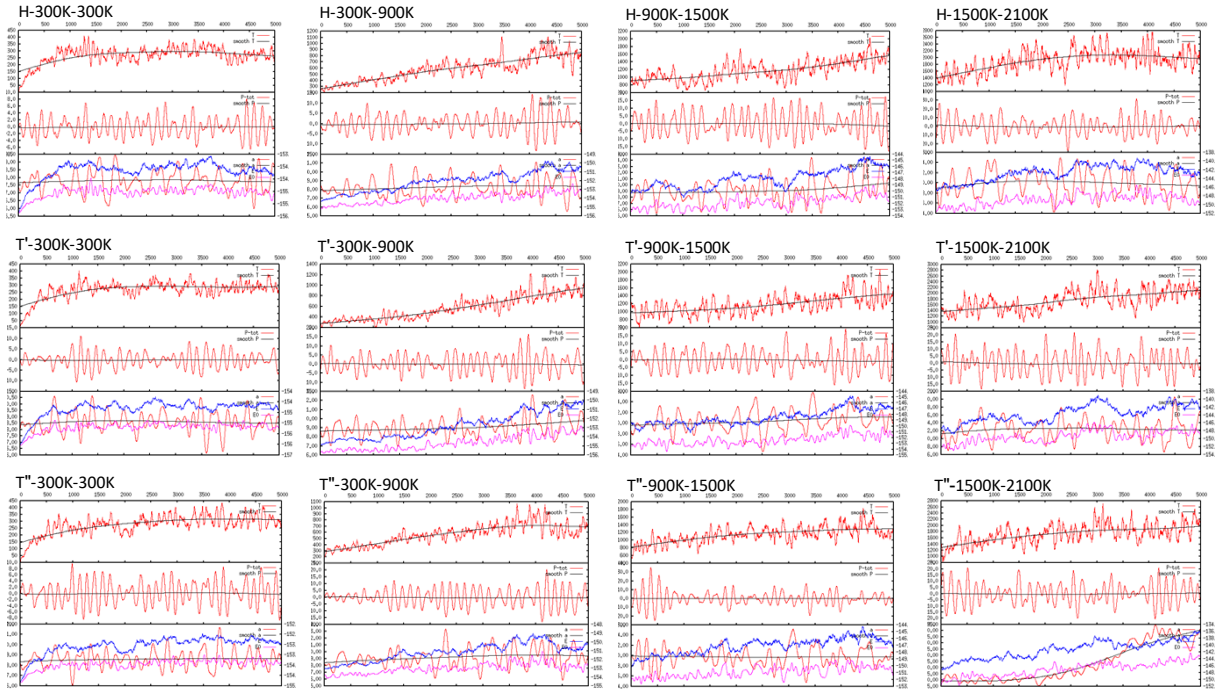
S6) 300K-2100K AIMD simulations for H, T' and T'' phases of WS_2



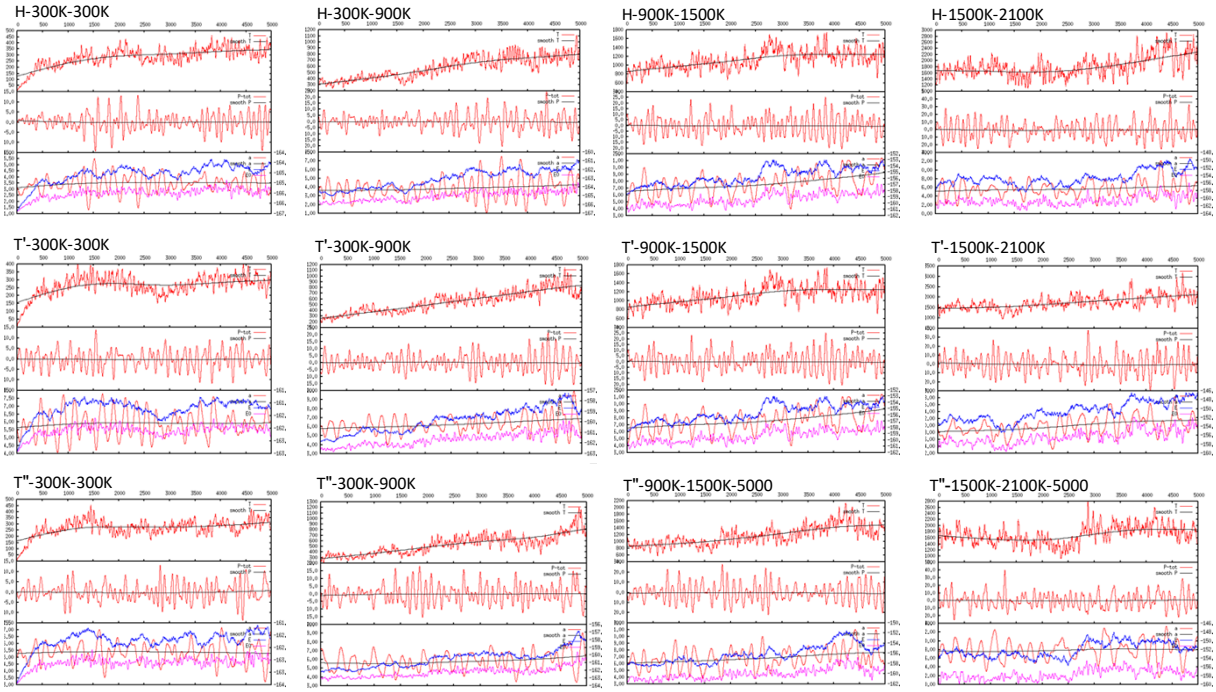
S7) 300K-2100K AIMD simulations for H, T' and T'' phases of WSe_2



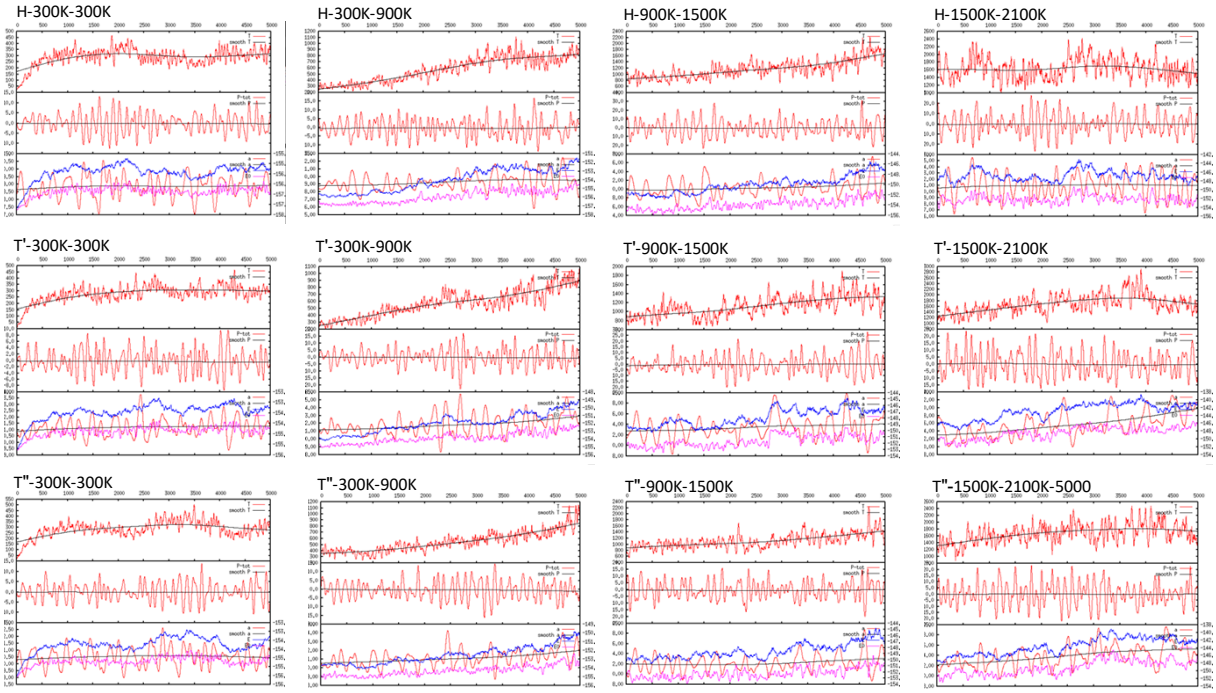
S8) 300K-2100K AIMD simulations for H, T' and T'' phases of WTe_2



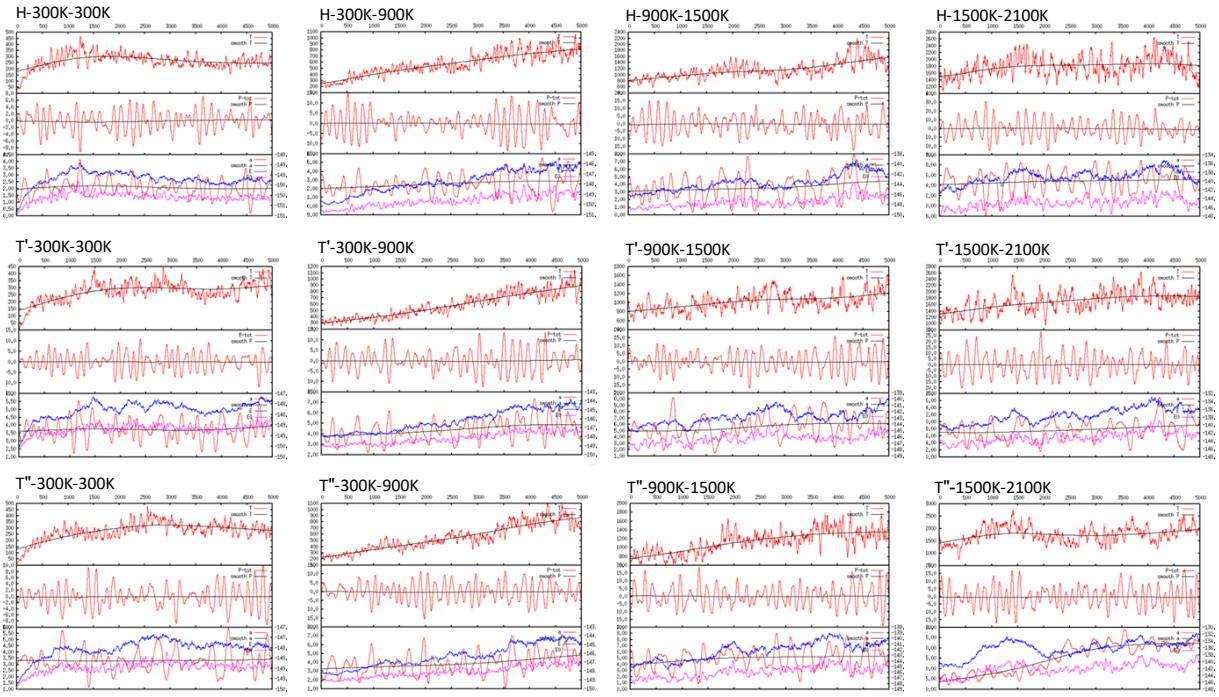
S9) 300K-2100K AIMD simulations for H, T' and T'' phases of MoSSe



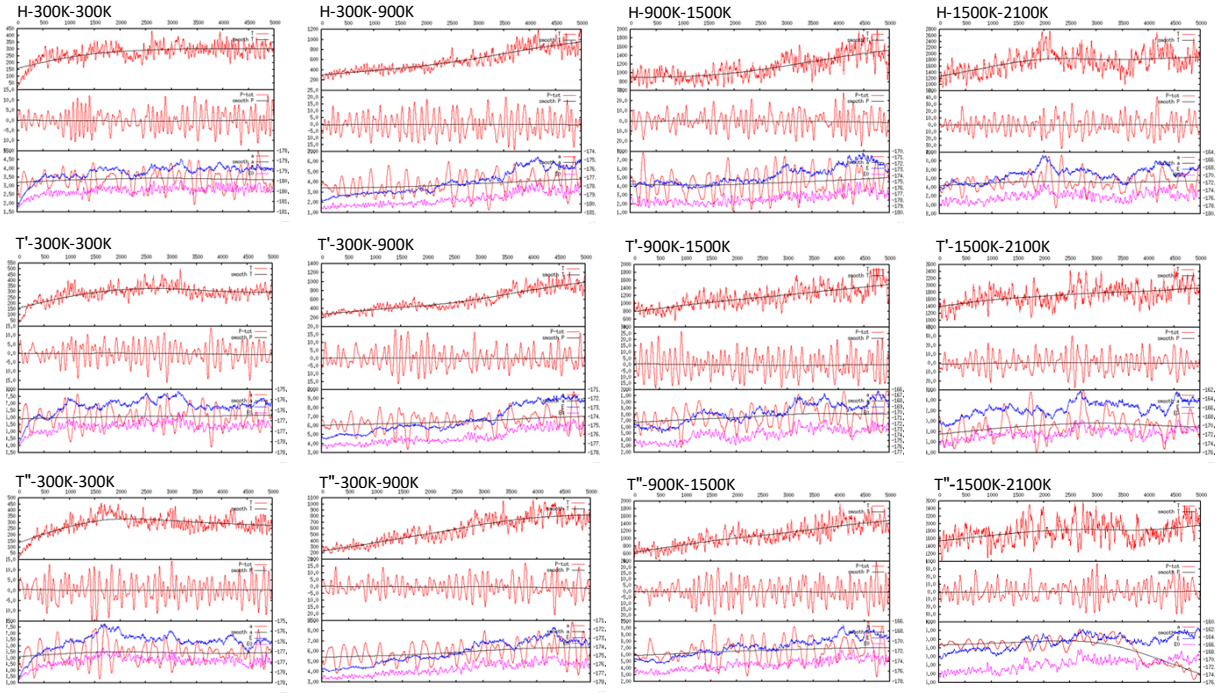
S10) 300K-2100K AIMD simulations for H, T' and T'' phases of MoSTe



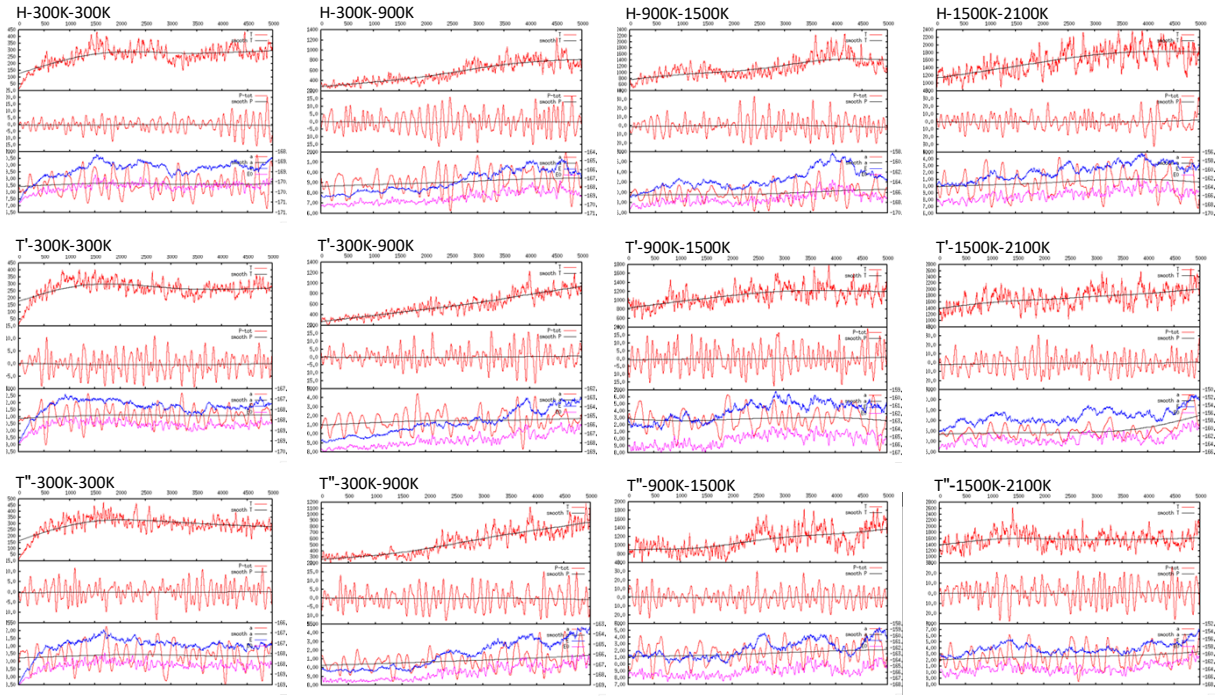
S11) 300K-2100K AIMD simulations for H, T' and T'' phases of MoSeTe



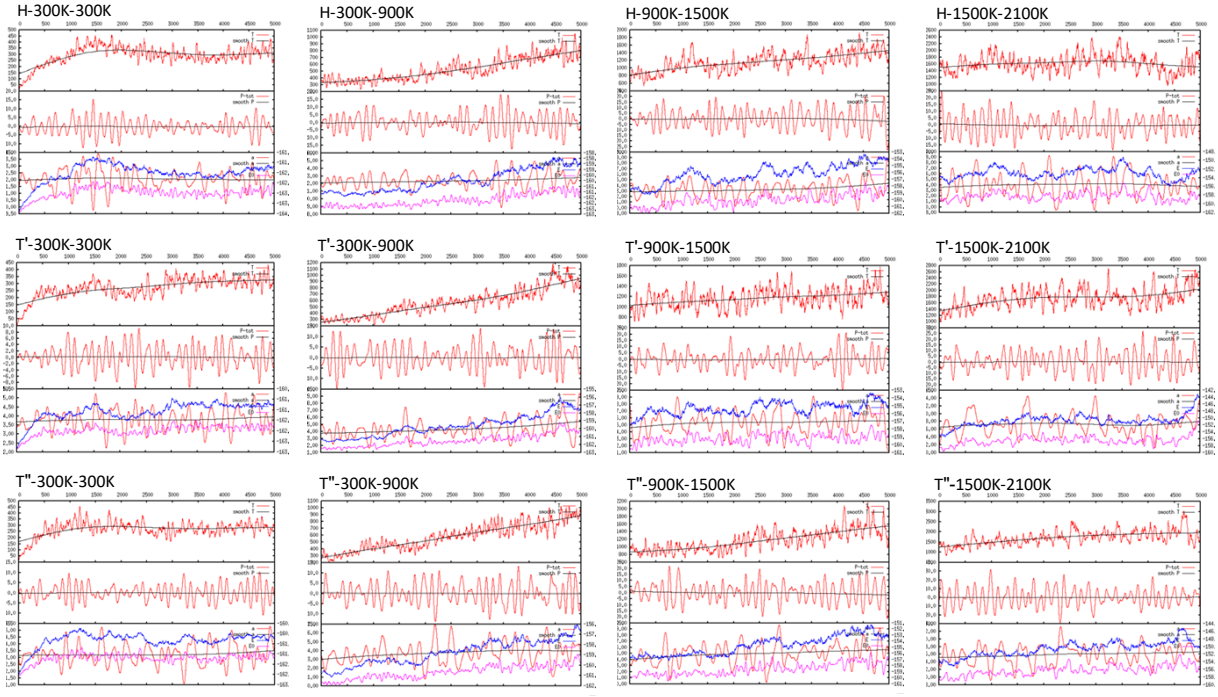
S12) 300K-2100K AIMD simulations for H, T' and T'' phases of WSSe



S13) 300K-2100K AIMD simulations for H, T' and T'' phases of WSTe

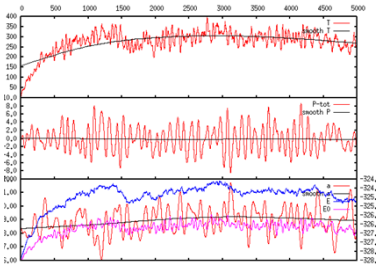


S14) 300K-2100K AIMD simulations for H, T' and T'' phases of WSeTe

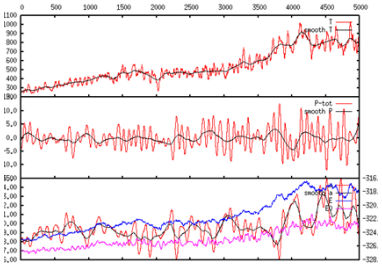


S15) 300K-1500K AIMD Simulations of 2x2 lateral size mixed HT', HT'' and T'T'' phases of MoSSe

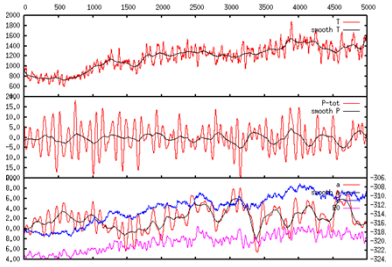
HT'-300K-300K



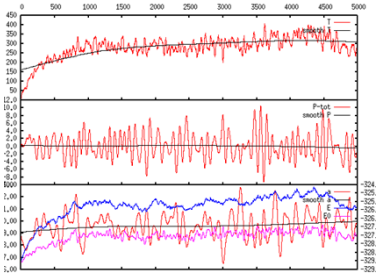
HT'-300K-900K



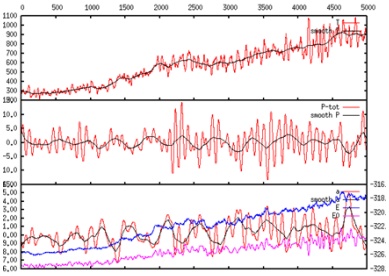
HT'-900K-1500K



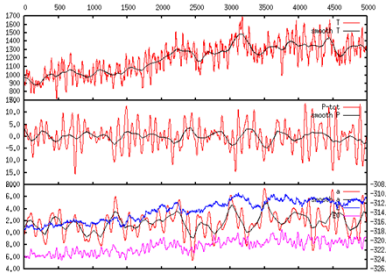
HT"-300K-300K



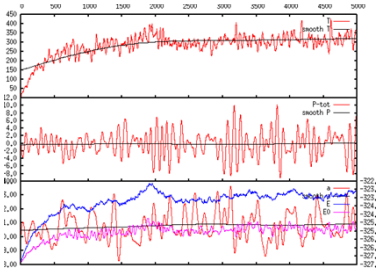
HT"-300K-900K



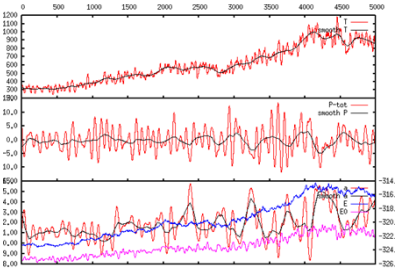
HT"-900K-1500K



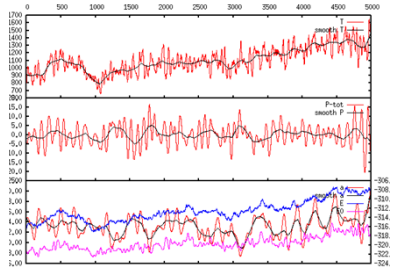
T'T"-300K-300K



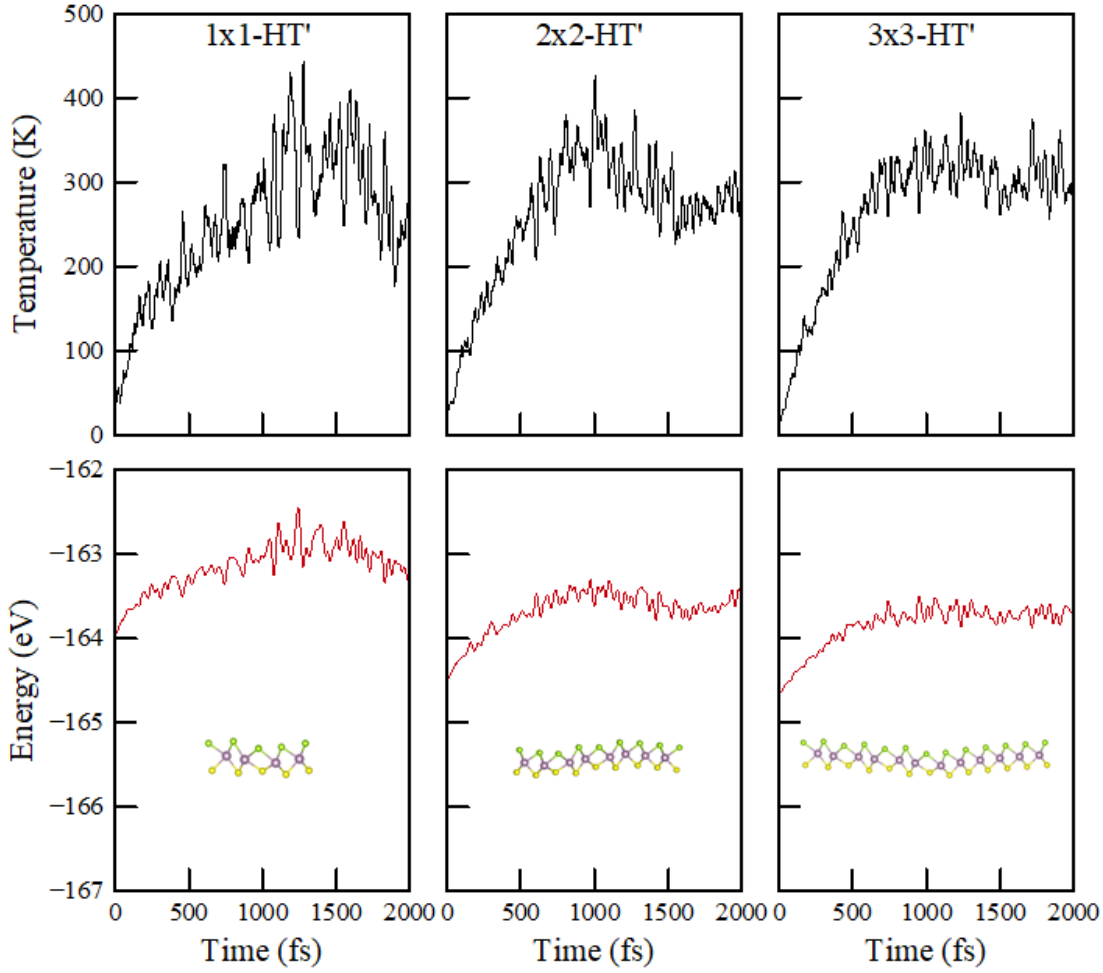
T'T"-300K-900K



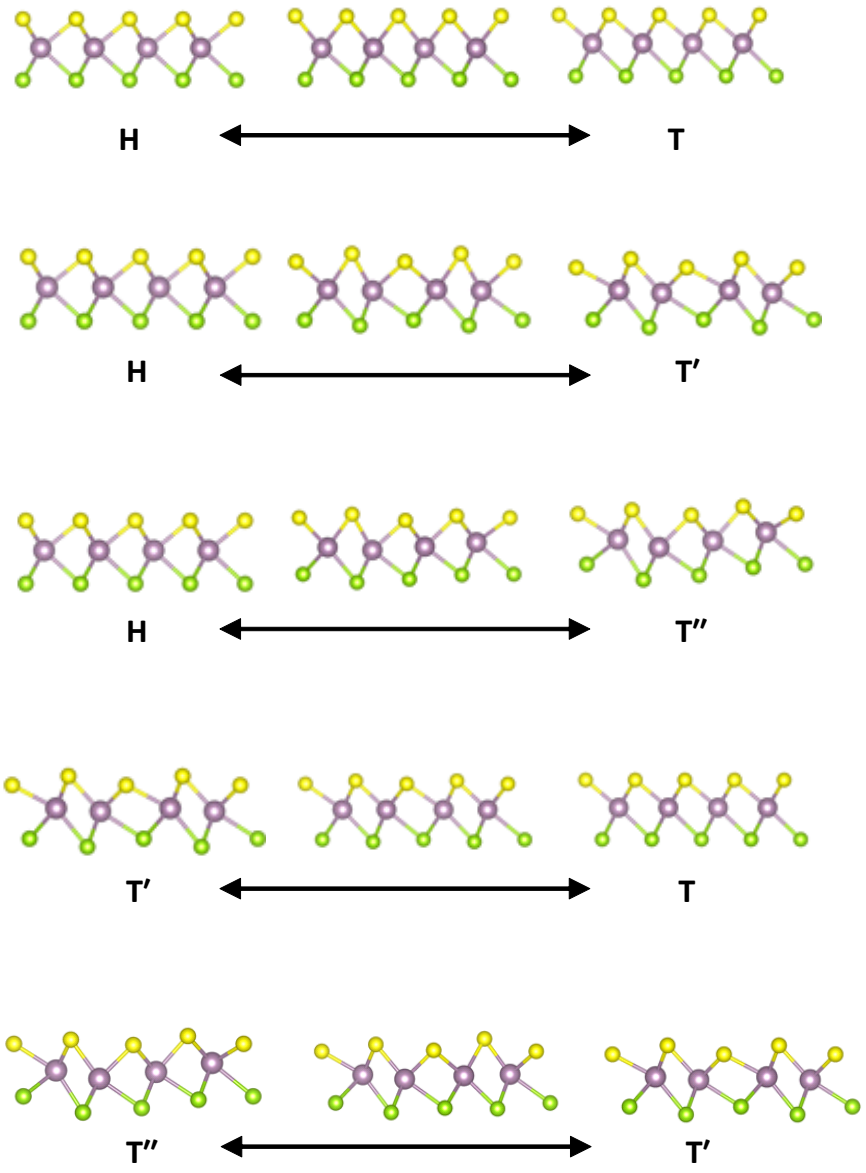
T'T"-900K-1500K



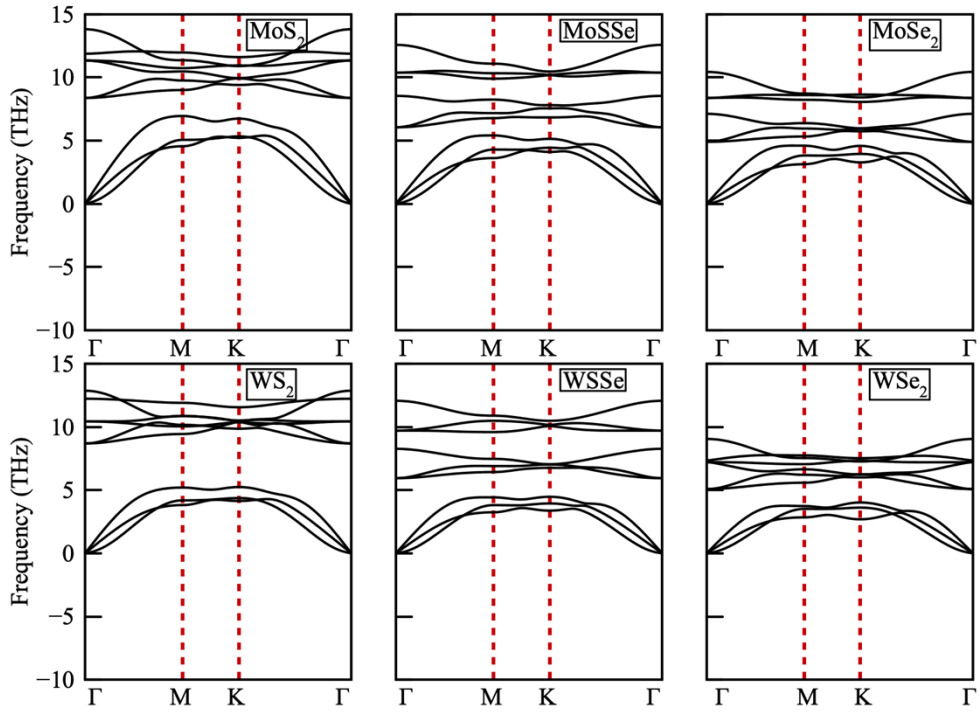
S16) 300K AIMD Simulations of different lateral size mixed HT' phases of MoSSe



S17) Transition state structures between H, T' and T'' phases for MoSSe as an example. All the other materials follow the same transition path.

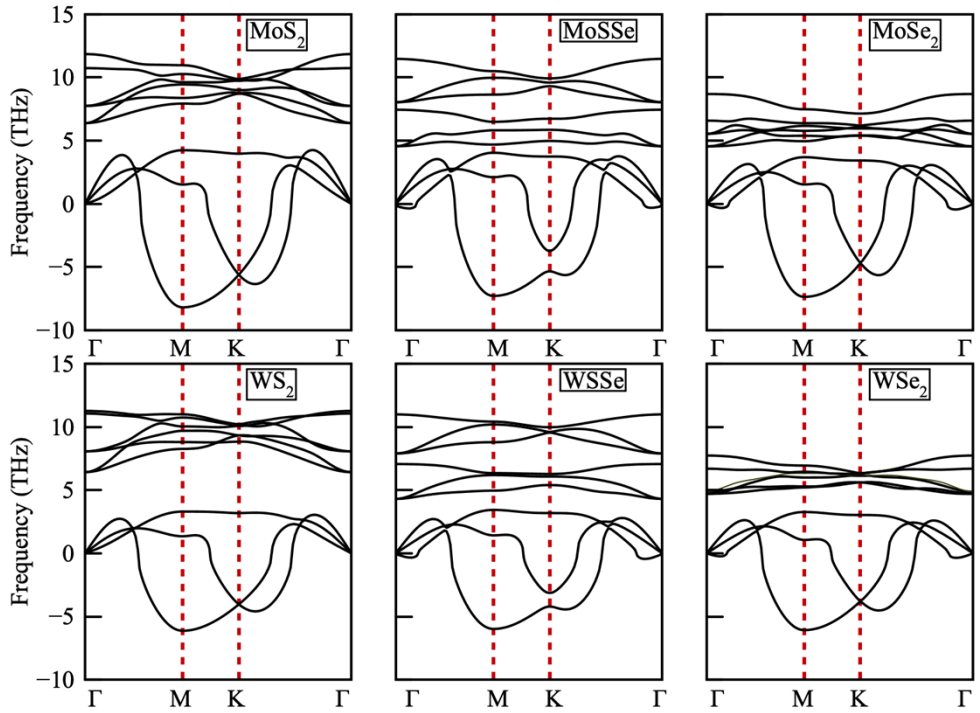


S18) Phonon structures of H phase for MoS_2, MoSSe, $MoSe_2$, WS_2, WSSe, and WSe_2

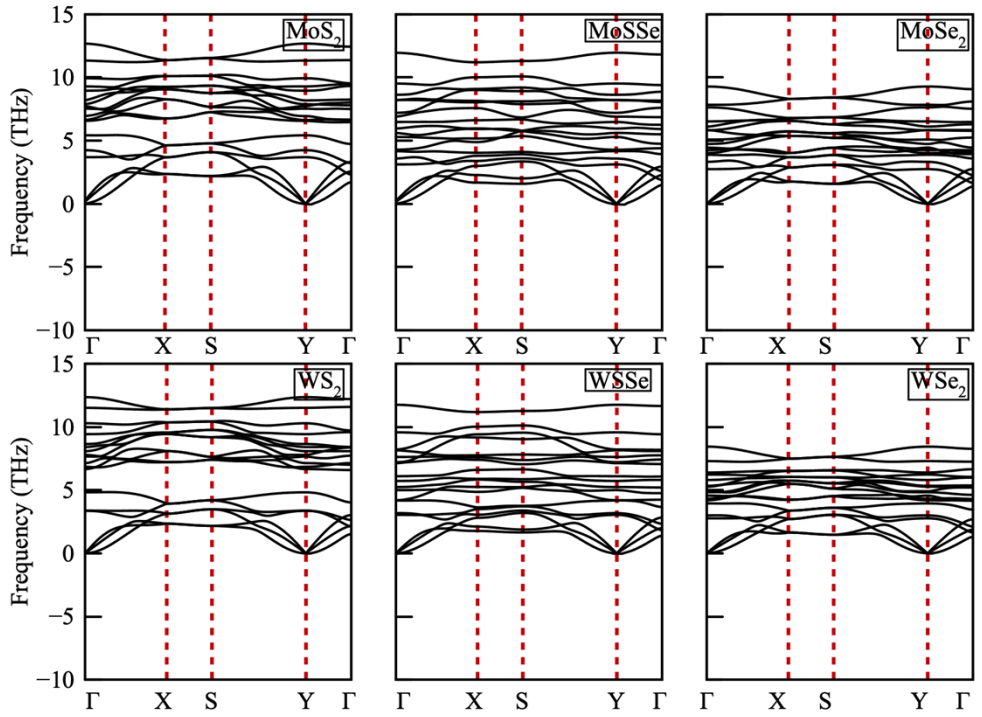


S18)

S19) Phonon structures of T phase for MoS_2, MoSSe, $MoSe_2$, WS_2, WSSe, and WSe_2



S20) Phonon structures of T' phase for MoS_2, MoSSe, $MoSe_2$, WS_2, WSSe, and WSe_2



S21) Phonon structures of T'' phase for MoS_2, MoSSe, $MoSe_2$, WS_2, WSSe, and WSe_2

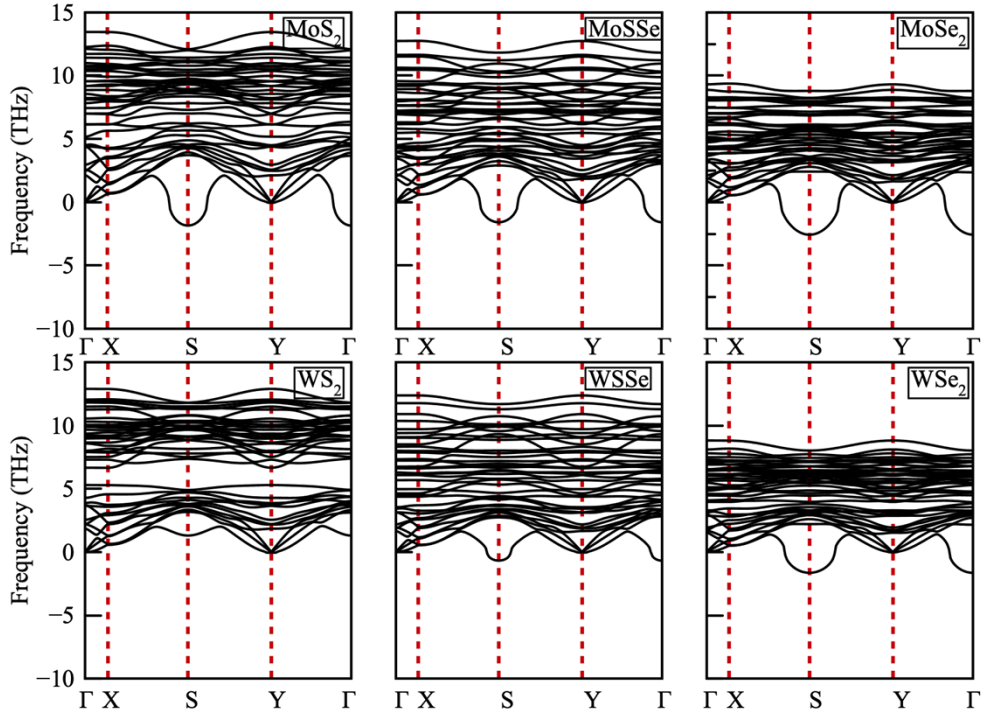


Table 1) Relative energy values of mixed HT' phases of MoSSe for different merging configurations.

	1x1	2x2	3x3
a	-163.40	-164.21	-164.49
b	-163.93	-164.48	-164.65
c	-163.93	-162.95	-163.67
d	-163.40	-163.19	-164.03