The Janus-structures of transition metal dichalcogenides with low enthalpy and new crystallchemistry

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Table 1: Calculated enthalpies of MoS_2, $MoSe_2$, VS_2, and VSe_2 structures.

Phase	Enthalpy (eV/f.u.)				Relative ΔH (eV/f.u.)			
	MoS_2	$MoSe_2$	VS_2	VSe_2	MoS_2	$MoSe_2$	VS_2	VSe_2
1H	-21.7979	-19.9729	-16.6216	-14.9782	0.0000	0.0000	0.1225	0.2131
1T	-20.9517	-19.2645	-16.6942	-15.0745	0.8462	0.7085	0.0498	0.1168
1T'	-21.2477	-19.6420	-16.7440	-15.1913	0.5502	0.3309	0.0000	0.0000
fes	-20.9388	-19.2431	-16.1391	-14.5743	0.8591	0.7298	0.6049	0.6170
fxt	-20.8984	-19.2573	-16.0501	-14.5298	0.8996	0.7156	0.6939	0.6615
test-1	-20.5707	-19.0322	-15.9051	-14.5779	1.2272	0.9408	0.8389	0.6134
test-2	-21.0693	-19.4797	-16.1932	-14.7373	0.7287	0.4932	0.5509	0.4540
test-3	-20.7775	-19.2060	-16.3075	-14.7683	1.0205	0.7669	0.4365	0.4230
H-hor	-20.9226	-19.2149	-16.4369	-15.0158	0.8753	0.7581	0.3071	0.1755
T-hor	-21.1194	-19.5238	-16.7402	-15.1292	0.6785	0.4491	0.0038	0.0621
airss-1	-21.0882	-19.4064	-16.4716	-14.8615	0.7098	0.5665	0.2724	0.3298
airss-3	-20.4745	-18.7452	-16.4849	-14.8839	1.3234	1.2278	0.2592	0.3074

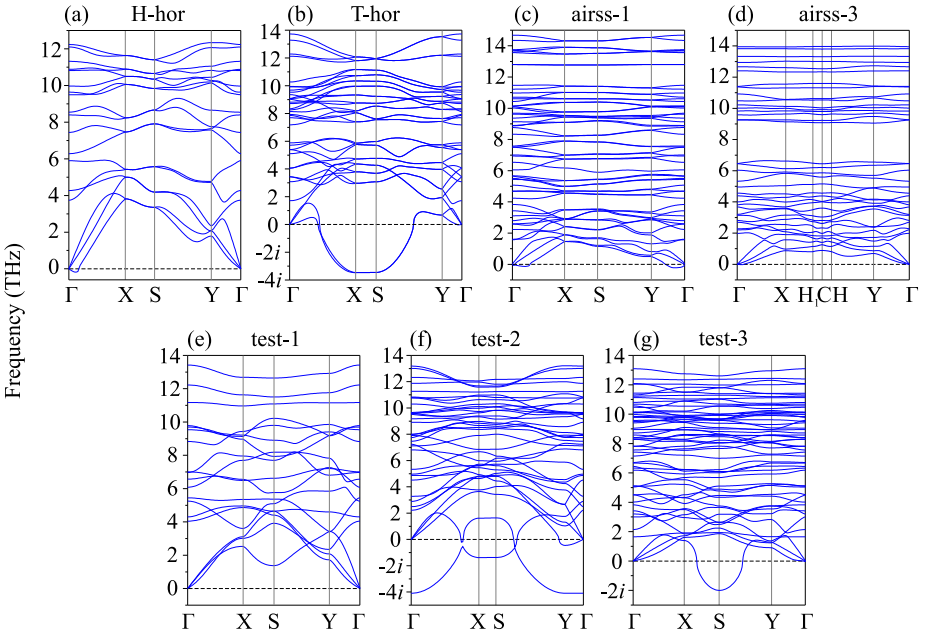

Figure 1: Phonon dispersion curves of MoS_2 structures.

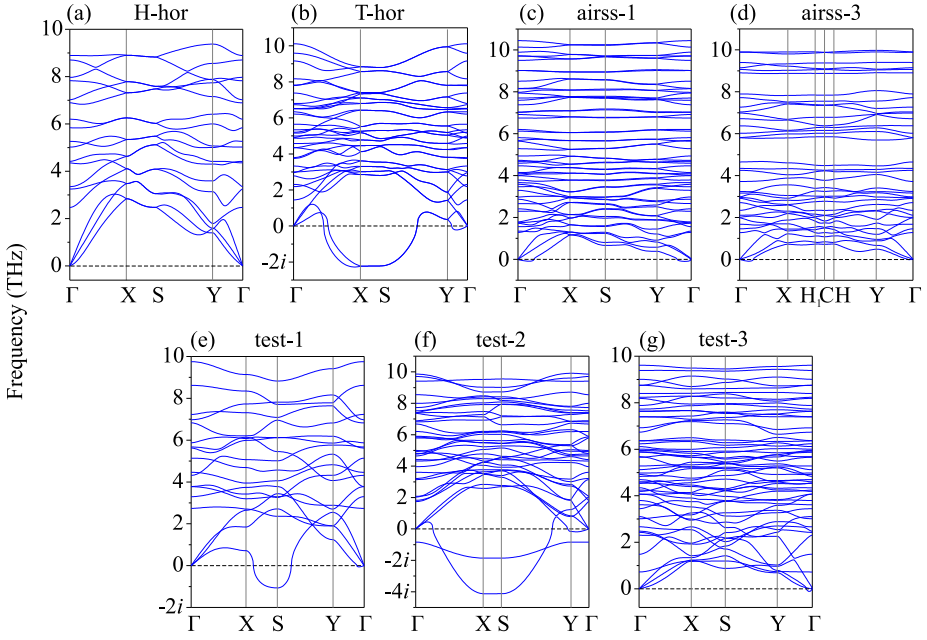

Figure 2: Phonon dispersion curves of $MoSe_2$ structures.

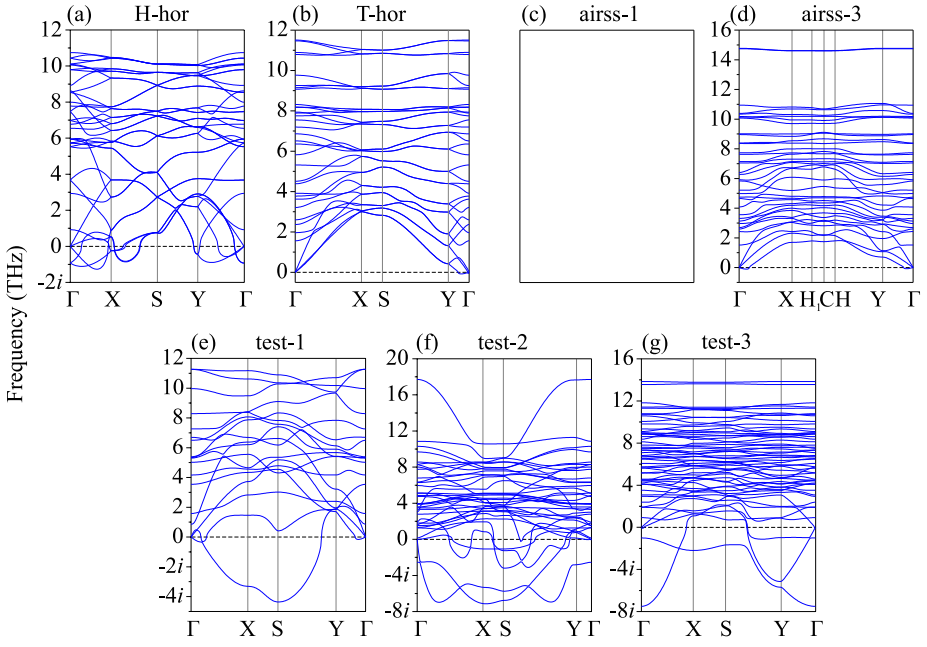

Figure 3: Phonon dispersion curves of VS_2 structures.

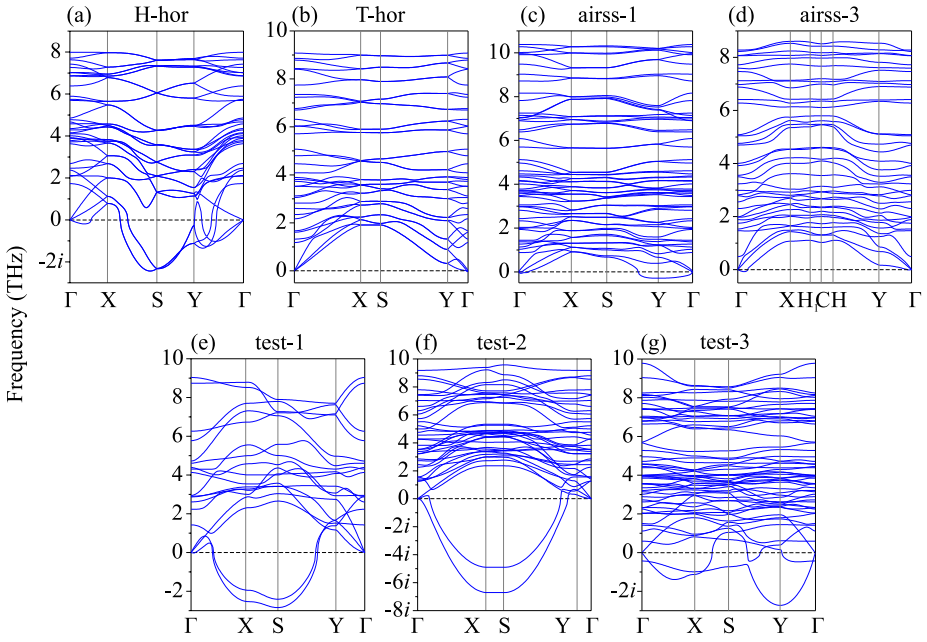

Figure 4: Phonon dispersion curves of VSe_2 structures.