Supporting Information for

The mechanical, electronic and optical properties of two-dimensional transition metal chalcogenides MX_2 and M_2X_3 (M= Ni, Pd; X= S, Se, Te) with hexagonal and orthorhombic structures

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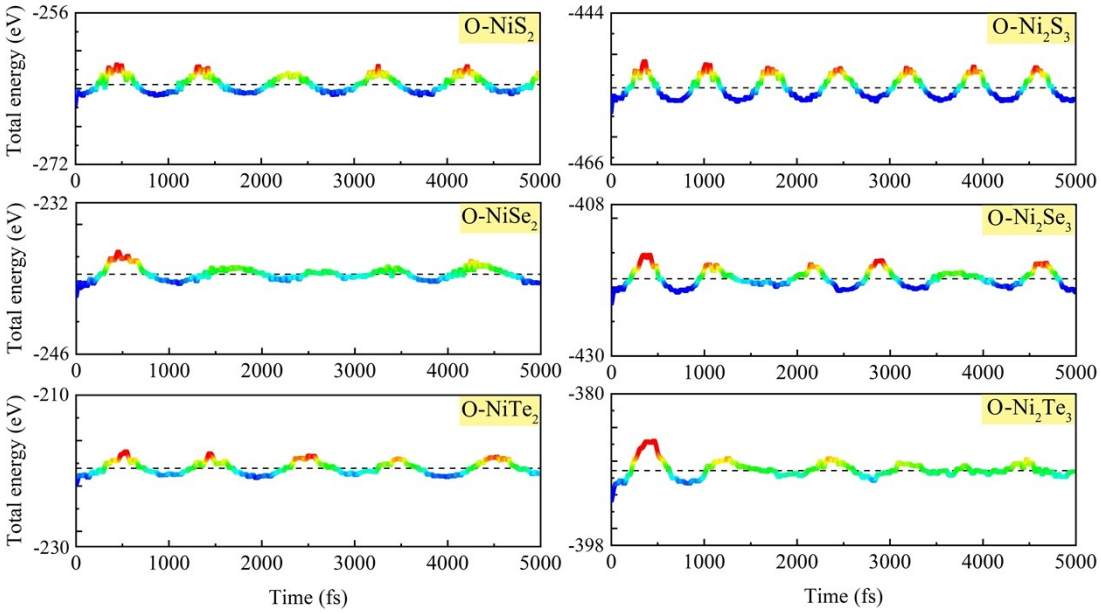

FIG. S1. The total energies of O-NiX_2 and O-Ni_2X_3 as a function of the time under the molecular dynamics simulations at 300K.

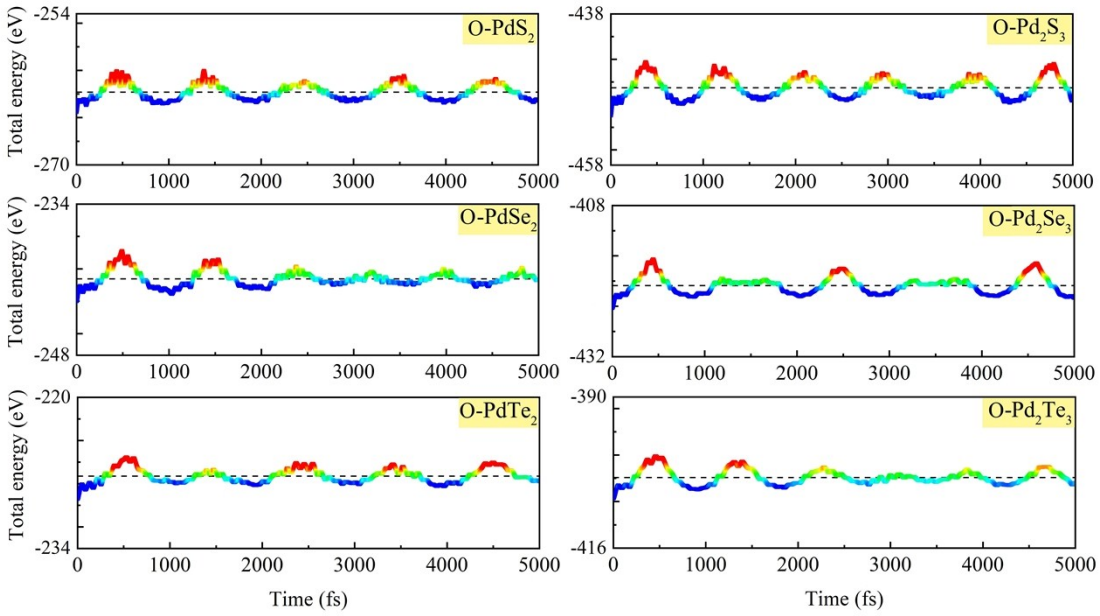

FIG. S2. The total energies of O-PdX_2 and O-Pd_2X_3 as a function of the time under the molecular dynamics simulations at 300K.

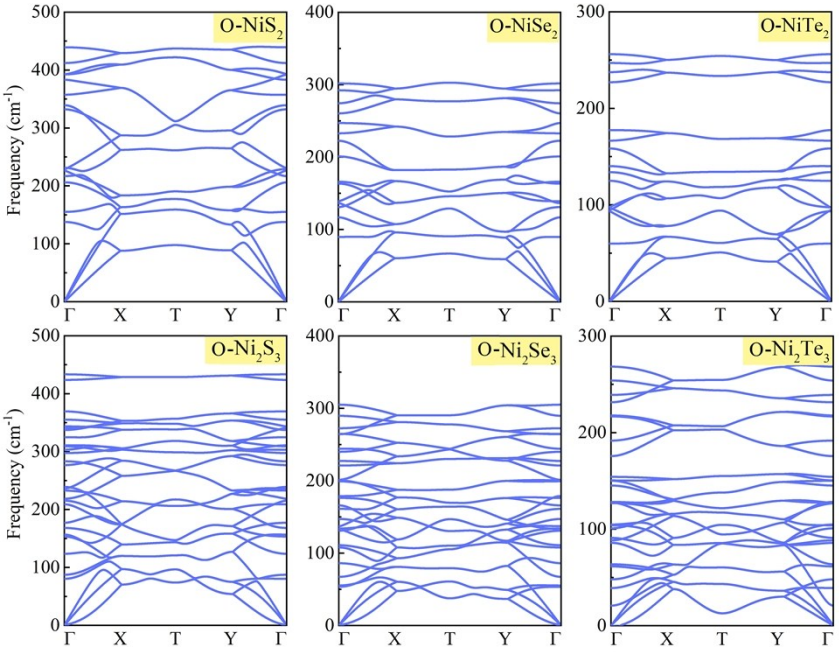

FIG. S3. The phonon dispersions of monolayer O-NiX_2 and O-Ni_2X_3.

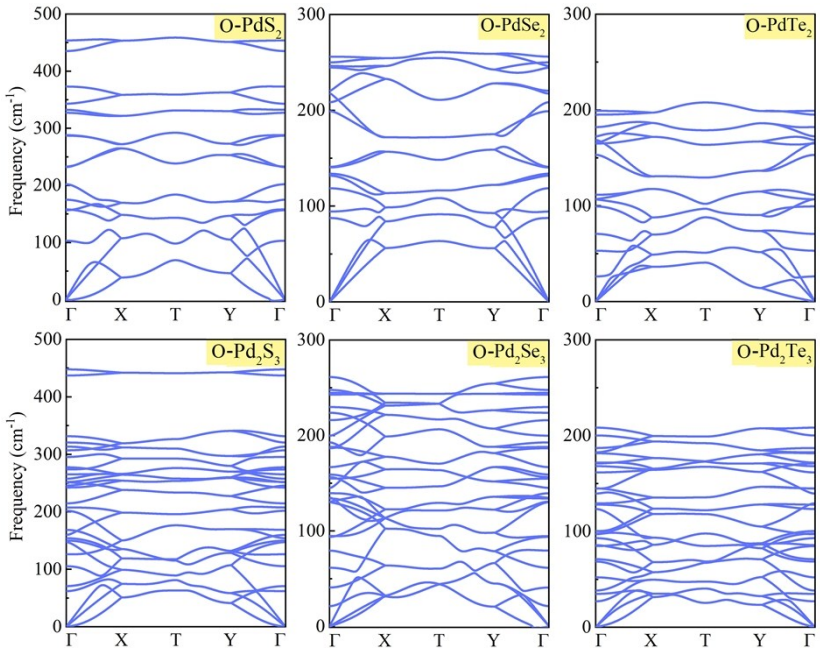

FIG. S4. The phonon dispersions of monolayer O-PdX_2 and O-Pd_2X_3.

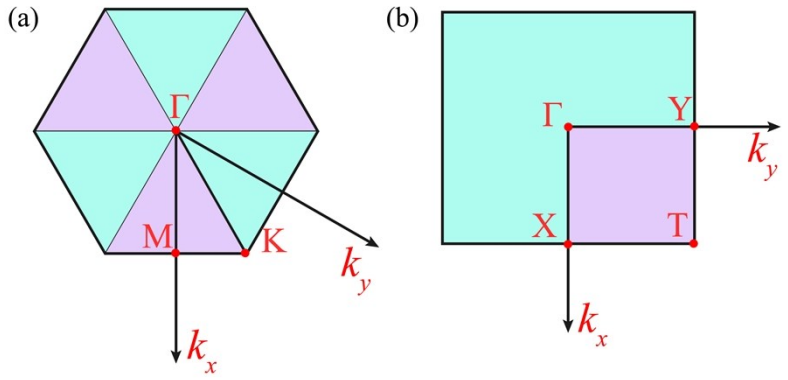

FIG. S5. The diagrams of first Brillouin zone for (a) hexagonal and (b) orthorhombic phases, respectively.

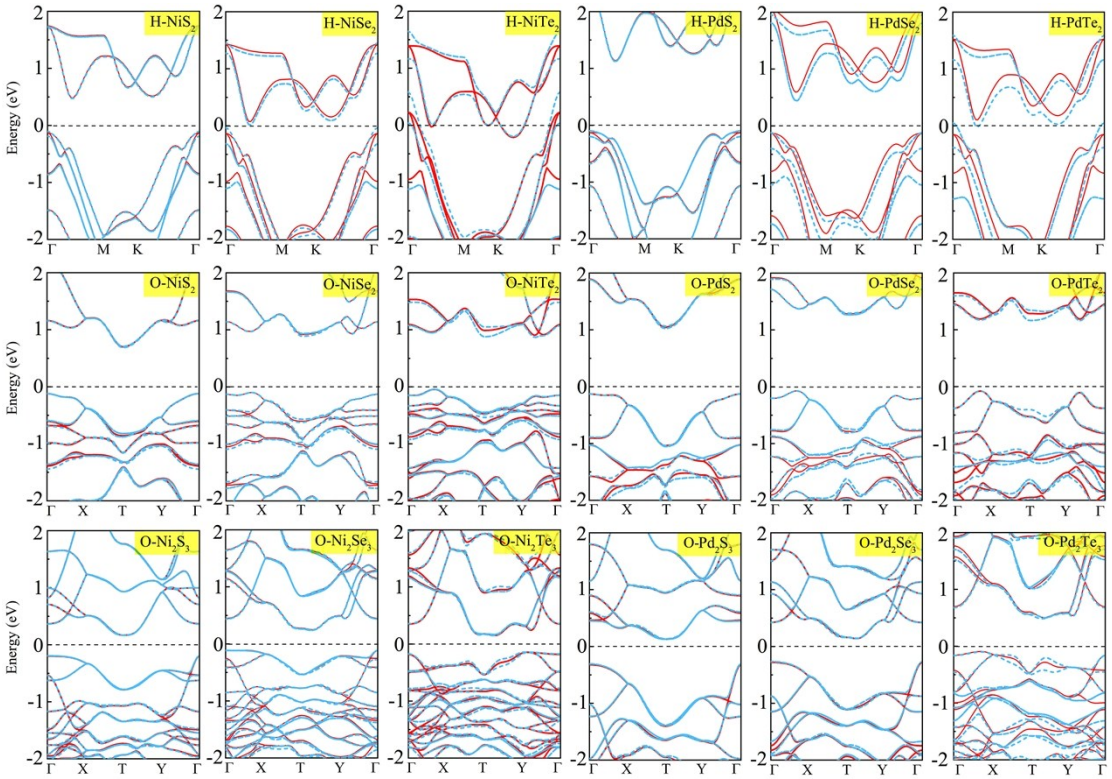

FIG. S6. The PBE and PBE+SOC band structures of monolayer TMCs.

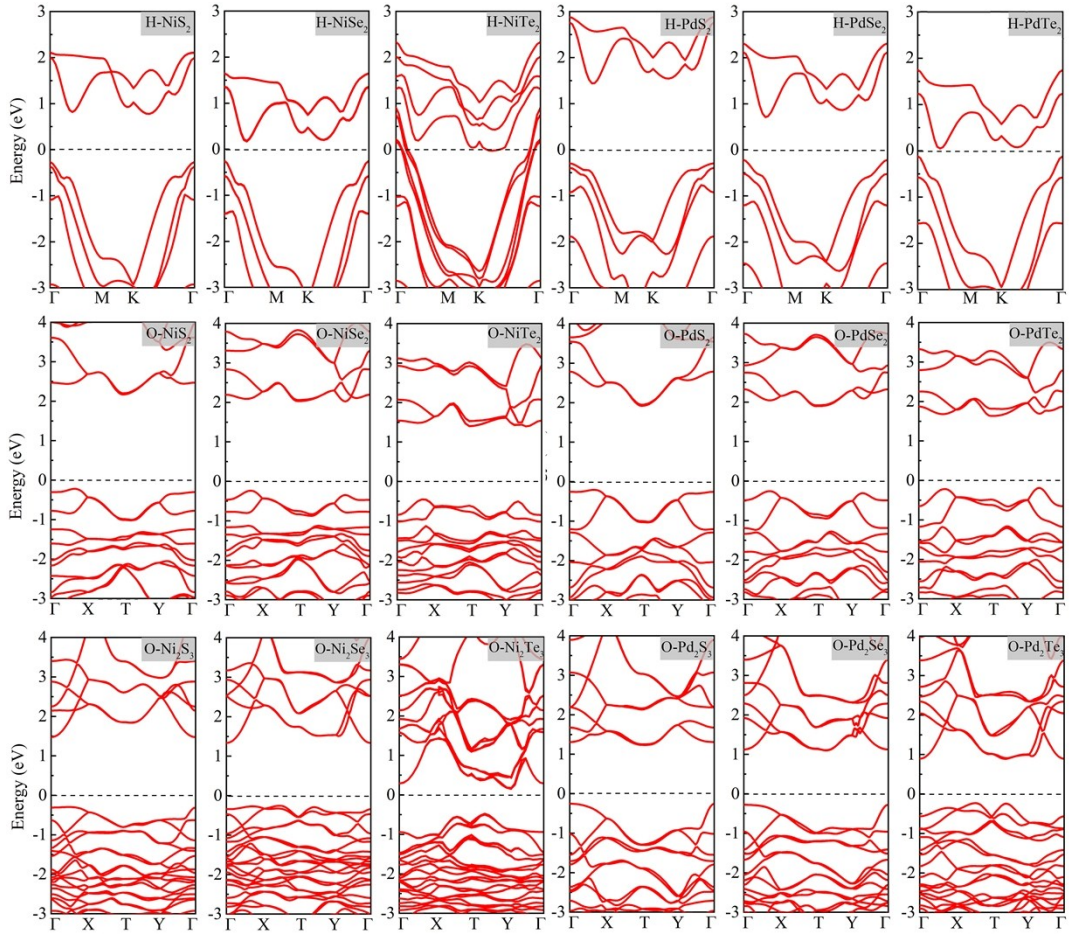

FIG. S7. The HSE06+SOC band structures of monolayer TMCs.

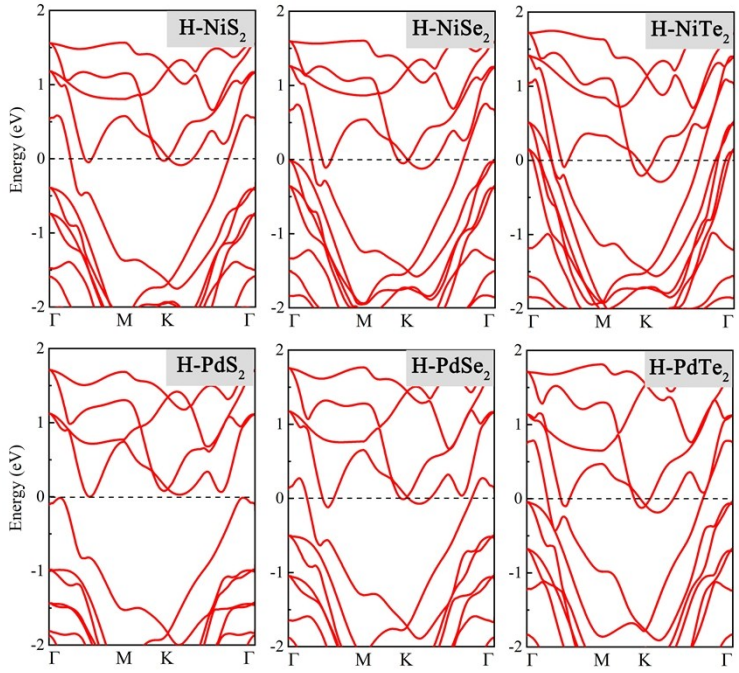

FIG. S8. The HSE06 band structures of bilayer H-MX_2, indicating their metallic characters.

TABLE S1. Calculated elastic stiffness (C_{ij}), Young's modulus (Y), Poisson's ratio (v) of monolayer TMCs along the x and y directions.

	C_{11} (N/m)	C_{22} (N/m)	C_{12} (N/m)	C_{66} (N/m)	Y_x (N/m)	Y_y (N/m)	v_x	v_y
H-NiS_2	81.166	81.259	22.462	29.293	74.957	75.043	0.276	0.277
H-$NiSe_2$	55.072	55.447	16.348	19.01	50.252	50.595	0.295	0.297
H-$NiTe_2$	35.27	35.793	7.031	14.543	33.889	34.392	0.196	0.199
H-PdS_2	67.127	67.072	18.771	24.188	61.874	61.823	0.28	0.28
H-$PdSe_2$	54.969	54.952	15.873	19.511	50.384	50.368	0.289	0.289
H-$PdTe_2$	41.059	41.281	12.829	13.788	37.072	37.272	0.311	0.312
O-NiS_2	59.253	93.034	5.778	32.385	58.894	92.47	0.062	0.098
O-$NiSe_2$	37.442	72.81	-1.335	26.51	37.417	72.762	-0.018	-0.036
O-$NiTe_2$	22.679	60.781	-2.259	23.821	22.595	60.556	-0.037	-0.1
O-PdS_2	56.622	78.41	2.993	23.709	56.508	78.251	0.038	0.053
O-$PdSe_2$	37.729	61.576	1.509	19.602	37.692	61.516	0.025	0.04
O-$PdTe_2$	23.214	51.031	-0.049	17.885	23.214	51.031	-0.001	-0.002
O-Ni_2S_3	63.029	54.077	33.148	28.372	42.709	36.643	0.613	0.526
O-Ni_2Se_3	45.364	40.261	29.865	24.51	23.211	20.6	0.742	0.658
O-Ni_2Te_3	35.324	31.641	28.531	21.108	9.597	8.596	0.902	0.808
O-Pd_2S_3	58.448	51.785	27.806	23.446	43.517	38.556	0.537	0.476
O-Pd_2Se_3	41.081	38.156	22.495	21.519	27.819	25.838	0.59	0.548
O-Pd_2Te_3	28.077	28.188	18.393	20.923	16.075	16.139	0.653	0.655

TABLE S2. The work function (*W*), conduction band edge (E_CBM), valence band edge (E_VBM), potential difference ΔE_C (ΔE_V) between CBM (VBM) and reduction potential (oxidation potential) for monolayer TMCs.

				pH=0		pH=7	
	W (eV)	*E_CBM* (eV)	*E_VBM* (eV)	ΔE_C (eV)	ΔE_V (eV)	ΔE_C (eV)	ΔE_V (eV)
H-NiS_2	6.03	-5.17	-6.27	-	0.60	-	1.01
H-$NiSe_2$	5.24	-4.95	-5.54	-	-	-	0.28
H-$NiTe_2$	4.44	-	-	-	-	-	-
H-PdS_2	6.55	-5.04	-6.84	-	1.17	-	1.58
H-$PdSe_2$	5.71	-4.81	-5.94	-	0.27	-	0.68
H-$PdTe_2$	4.66	-4.42	-4.94	0.02	-	-	-
O-NiS_2	6.06	-3.88	-6.28	0.56	0.61	0.15	1.02
O-$NiSe_2$	5.89	-3.89	-6.16	0.55	0.49	0.14	0.9
O-$NiTe_2$	5.47	-3.90	-5.79	0.54	0.12	0.13	0.53
O-PdS_2	5.99	-4.10	-6.24	0.34	0.57	-	0.98
O-$PdSe_2$	5.85	-3.91	-6.07	0.53	0.40	0.12	0.81
O-$PdTe_2$	5.48	-3.82	-5.72	0.62	0.05	0.21	0.46
O-Ni_2S_3	6.02	-4.52	-6.30	-	0.63	-	1.04
O-Ni_2Se_3	5.74	-4.42	-6.03	0.02	0.36	-	0.77
O-Ni_2Te_3	5.03	-4.34	-5.39	0.10	-	-	0.13
O-Ni_2S_3	5.64	-4.36	-5.86	0.08	0.19	-	0.60
O-Ni_2Se_3	5.38	-4.23	-5.62	0.21	-	-	0.36
O-Ni_2Te_3	5.11	-4.19	-5.42	0.25	-	-	0.16