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

Supplementary Materials
High-throughput Analysis of Tetragonal Transition-Metal Xenes

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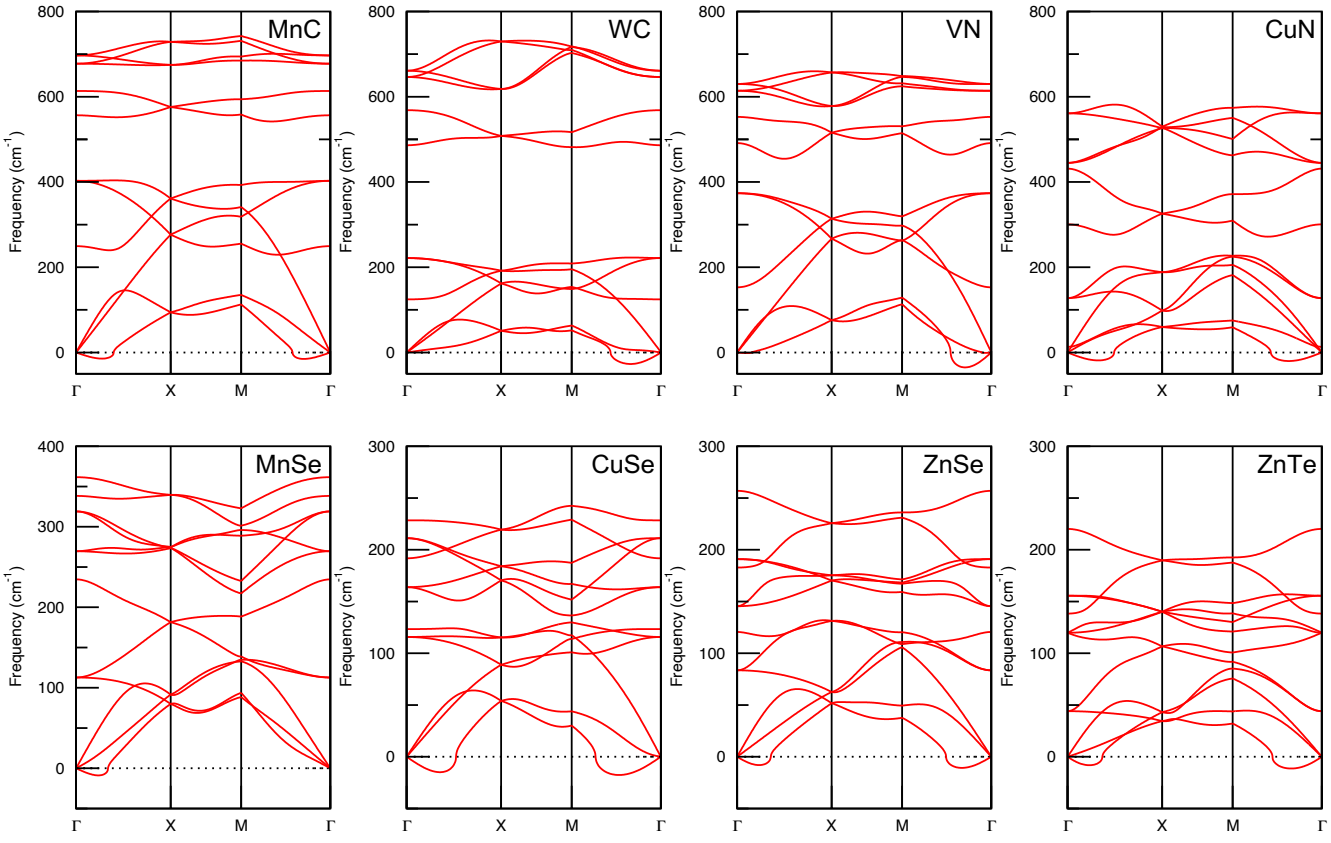

FIG. 1. Phonon band dispersions of single layer MnC, WC, VN, CuN, MnSe, CuSe, ZnSe, and ZnTe.

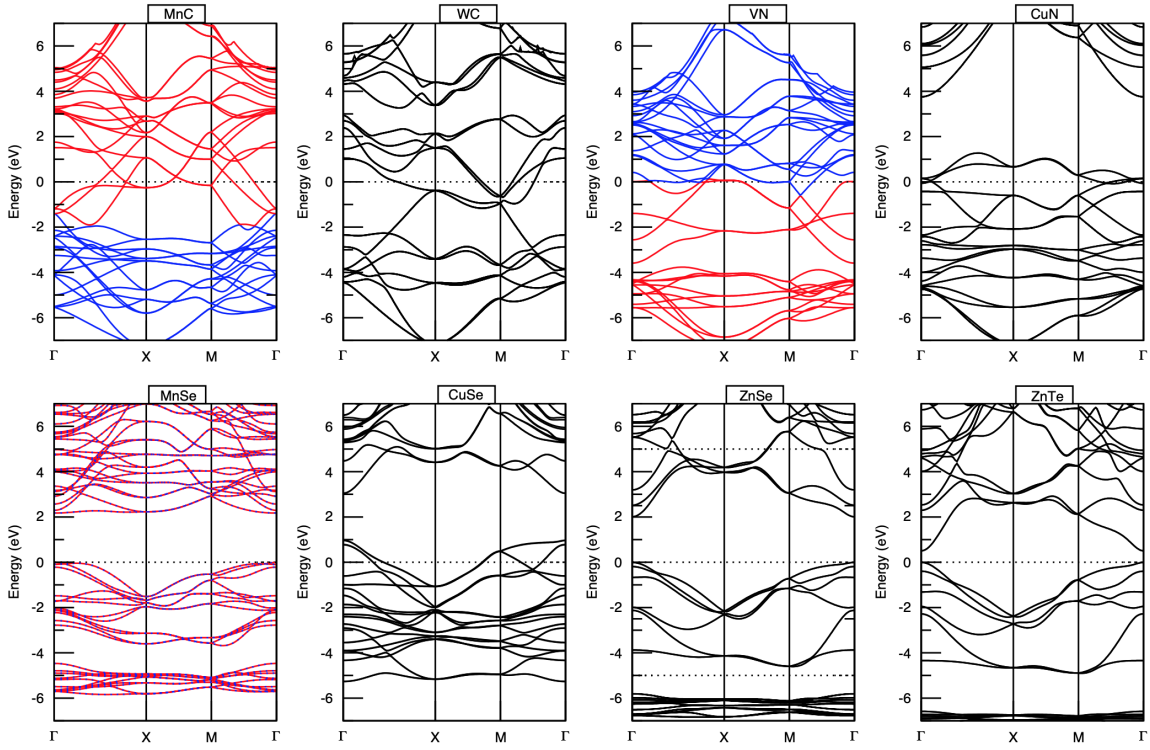

FIG. 2. Electronic structures of single layer MnC, WC, VN, CuN, MnSe, CuSe, ZnSe, and ZnTe. In all figures, blue, red and black lines correspond to spin-up, spin-down and non-magnetic case, respectively.

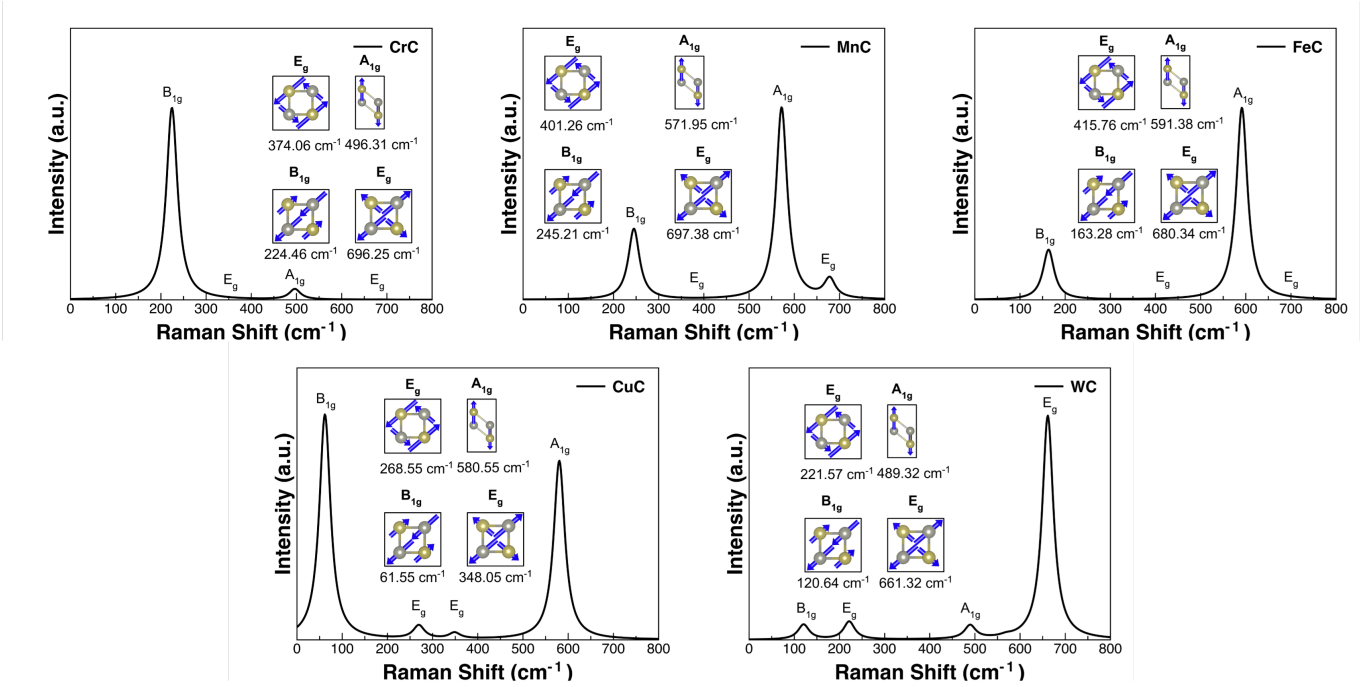

FIG. 3. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer CrC, MnC, FeC, CuC, and WC.

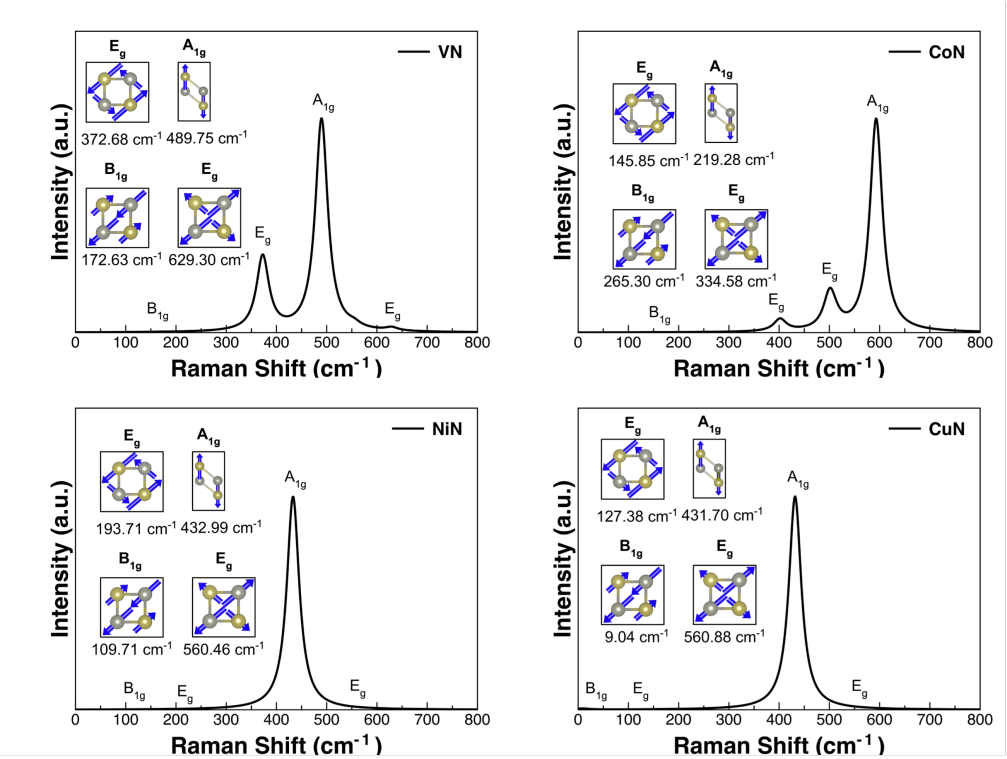

FIG. 4. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer VN, CoN, NiN, and CuN.

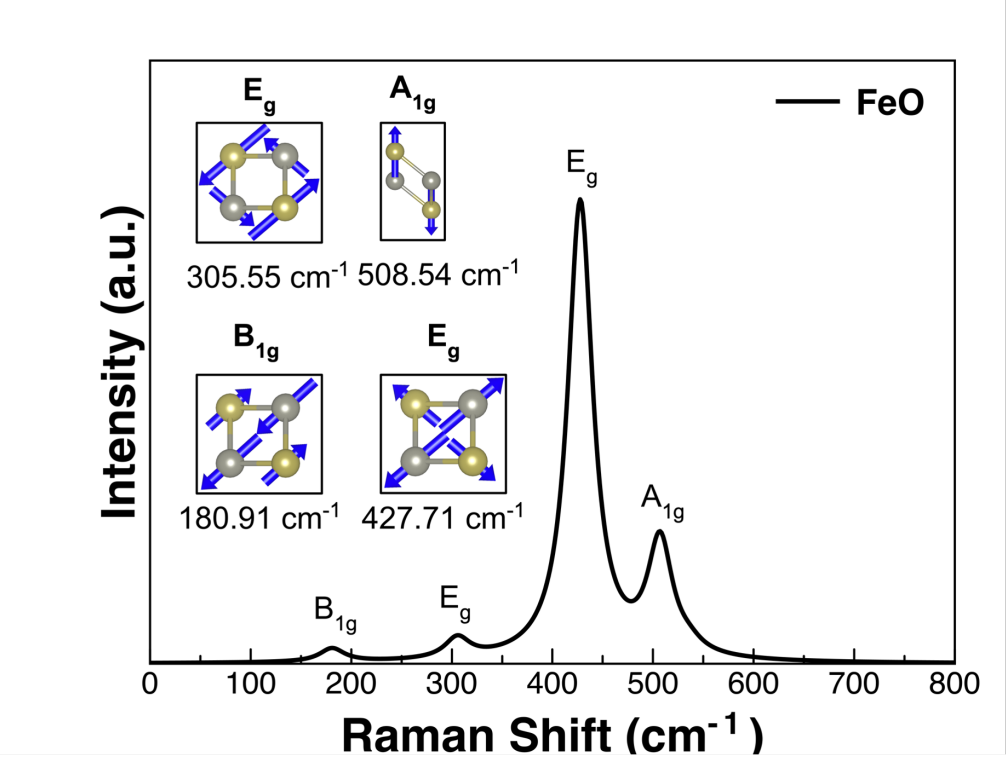

FIG. 5. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer FeO.

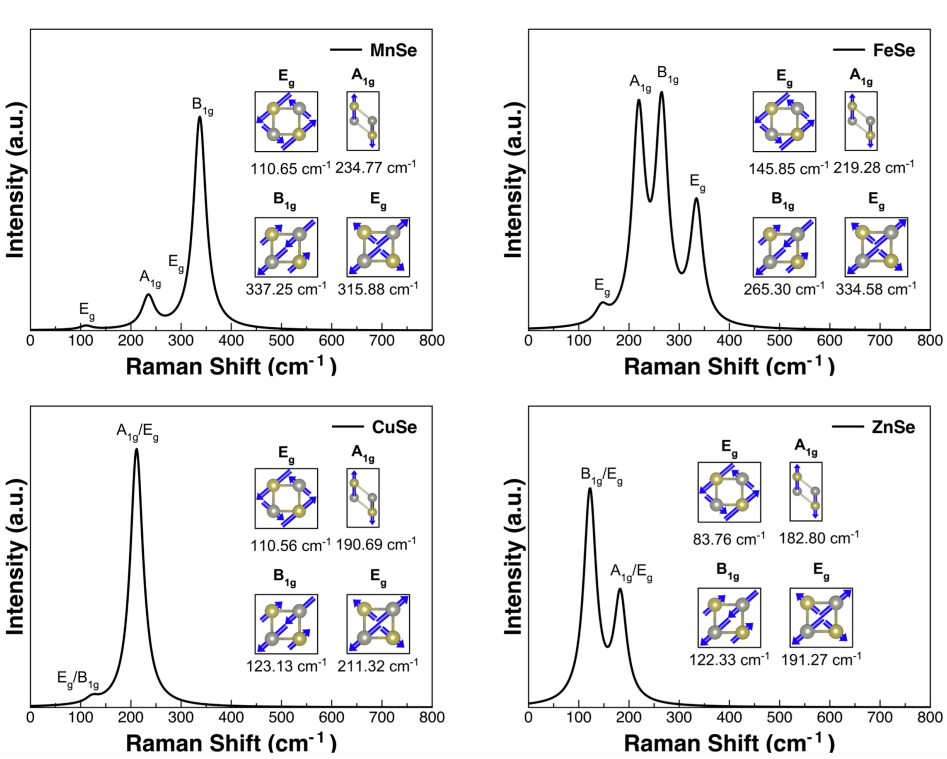

FIG. 6. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer MnSe, FeSe, CuSe and ZnSe.

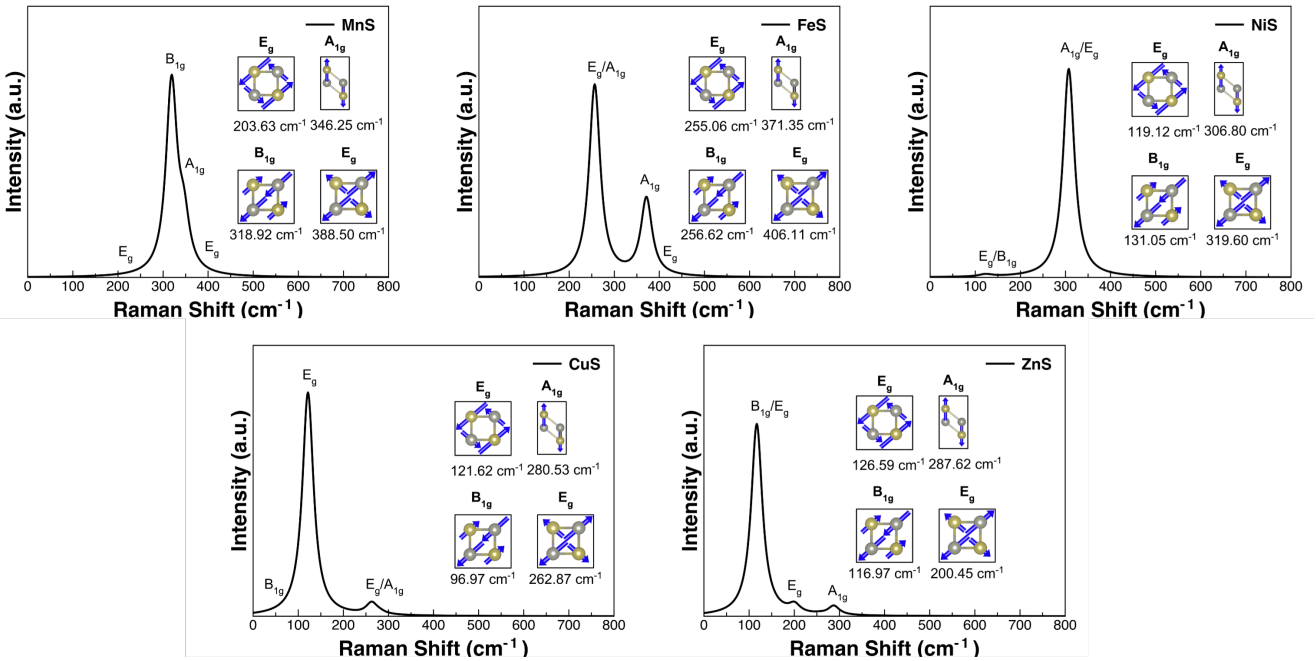

FIG. 7. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer MnS, FeS, NiS, CuS and ZnS.

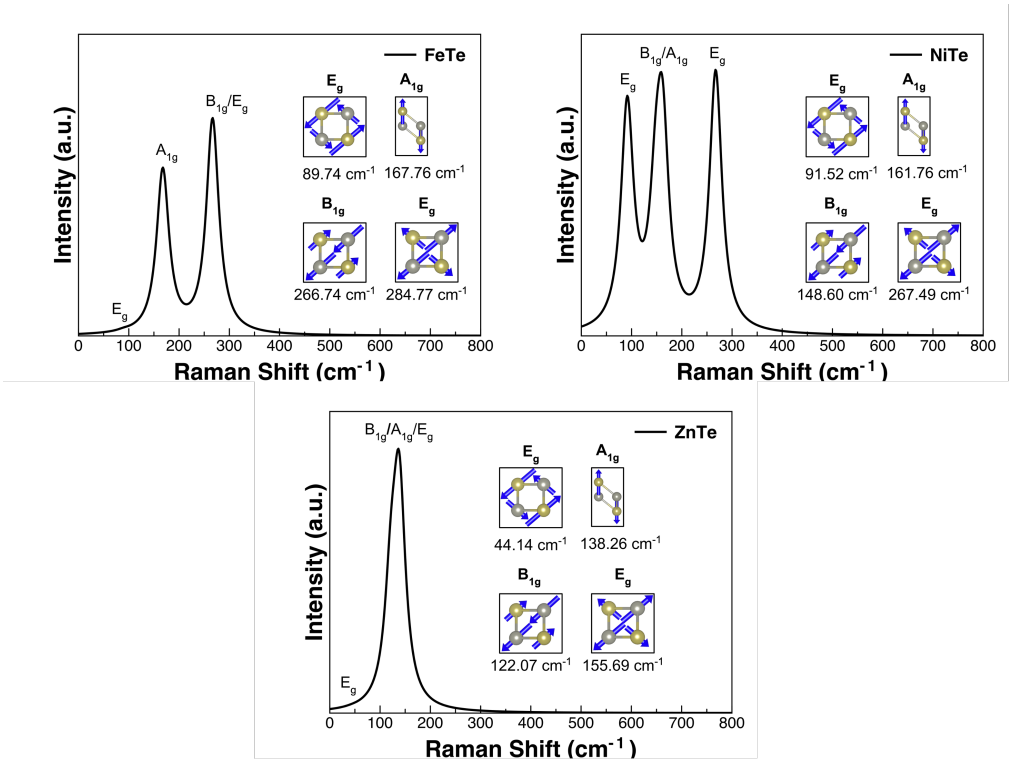

FIG. 8. Raman spectra and the vibrational characteristics of the Raman-active phonon modes for the single-layer FeTe, NiTe, and ZnTe.

TABLE I. Mechanical and dynamical stability of monolayer t-TMX are shown. The mechanical stability (Mech. Stability), the dynamical stablity (Dyn. Stability), stable (S) and unstable (UNS) are indicated for each material.

Structure	Mech. Stability	Dyn. Stability	Structure	Mech. Stability	Dyn. Stability	Structure	Mech. Stability	Dyn. Stability
ScC	S	UNS	ScO	UNS	-	ScS	UNS	-
TiC	S	UNS	TiO	UNS	-	TiS	UNS	-
VC	UNS	-	VO	UNS	-	VS	S	UNS
CrC	S	S	CrO	UNS	-	CrS	UNS	-
MnC	S	S	MnO	UNS	-	MnS	S	S
FeC	S	S	FeO	S	S	FeS	S	S
CoC	UNS	-	CoO	S	UNS	CoS	S	UNS
NiC	S	UNS	NiO	S	UNS	NiS	S	S
CuC	S	S	CuO	S	UNS	CuS	S	S
ZnC	S	UNS	ZnO	UNS	-	ZnS	S	S
ZrC	S	UNS	ZrO	UNS	-	ZrS	UNS	-
NbC	UNS	-	NbO	S	UNS	NbS	UNS	-
MoC	UNS	-	MoO	UNS	-	MoS	UNS	-
HfC	UNS	-	HfO	S	UNS	HfS	UNS	-
TaC	UNS	-	TaO	UNS	-	TaS	S	UNS
WC	S	S	WO	UNS	-	WS	UNS	-
ScN	UNS	-	ScSe	UNS	-	ScTe	UNS	-
TiN	UNS	-	TiSe	UNS	-	TiTe	UNS	-
VN	S	S	VSe	S	UNS	VTe	UNS	-
CrN	S	UNS	CrSe	UNS	-	CrTe	UNS	-
MnN	S	UNS	MnSe	S	S	MnTe	S	UNS
FeN	S	UNS	FeSe	S	S	FeTe	S	S
CoN	S	S	CoSe	S	UNS	CoTe	UNS	-
NiN	S	S	NiSe	S	UNS	NiTe	S	S
CuN	S	S	CuSe	S	S	CuTe	UNS	-
ZnN	S	UNS	ZnSe	S	S	ZnTe	S	S
ZrN	UNS	-	ZrSe	UNS	-	ZrTe	UNS	-
NbN	UNS	-	NbSe	UNS	-	NbTe	UNS	-
MoN	S	UNS	MoSe	UNS	-	MoTe	UNS	-
HfN	UNS	-	HfSe	UNS	-	HfTe	UNS	-
TaN	UNS	-	TaSe	UNS	-	TaTe	S	UNS
WN	UNS	-	WSe	UNS	-	WTe	UNS	-

TABLE II. Linear-elastic parameters for the monolayers of t-TMX structures.

Structure	C11	C12	C22	Structure	C11	C12	C22	Structure	C11	C12	C22
ScC	118.6	51.4	118.6	ScO	16.9	128.9	16.9	ScS	20.3	32.4	20.3
TiC	41.5	26.5	41.5	TiO	10.1	107.3	10.1	TiS	21.8	50.6	21.8
VC	62.4	99.2	62.4	VO	-54.4	189.1	-54.4	VS	56.6	15.7	56.6
CrC	88.9	75.5	88.9	CrO	46.4	167.2	46.4	CrS	60.3	88.6	60.3
MnC	134.8	72.6	134.8	MnO	16.1	114.0	16.1	MnS	50.7	30.0	50.7
FeC	136.3	92.3	136.3	FeO	78.2	73.6	78.2	FeS	75.5	46.7	75.5
CoC	82.8	138.3	82.8	CoO	94.8	47.7	94.8	CoS	61.1	14.3	61.1
NiC	73.0	21.6	73.0	NiO	137.0	74.5	137.0	NiS	47.8	12.5	47.8
CuC	103.8	-5.7	103.8	CuO	125.9	63.6	125.9	CuS	23.9	10.7	23.9
ZnC	59.9	-9.8	59.9	ZnO	-2.0	68.2	-2.0	ZnS	44.7	7.2	44.7
ZrC	115.9	28.7	115.9	ZrO	-169.8	320.8	-169.8	ZrS	21.1	59.2	21.1
NbC	61.5	112.7	61.5	NbO	81.7	78.3	81.7	NbS	6.8	107.0	6.8
MoC	84.3	114.6	84.3	MoO	72.8	189.4	72.8	MoS	71.5	113.4	71.5
HfC	-52.7	218.1	-52.7	HfO	113.5	19.7	113.5	HfS	28.4	66.5	28.4
TaC	81.4	112.9	81.4	TaO	57.3	91.1	57.3	TaS	38.9	36.1	38.9
WC	129.4	94.8	129.4	WO	80.0	225.6	80.0	WS	83.2	149.3	83.2
ScN	-22.4	167.4	-22.4	ScSe	19.2	24.1	19.2	ScTe	14.0	17.4	14.0
TiN	78.8	81.5	78.8	TiSe	14.8	40.0	14.8	TiTe	8.0	33.7	8.0
VN	90.7	83.2	90.7	VSe	64.9	35.8	64.9	VTe	14.4	65.9	14.4
CrN	103.9	70.7	103.9	CrSe	64.5	73.3	64.5	CrTe	56.1	57.9	56.1
MnN	136.9	47.3	136.9	MnSe	76.1	39.0	76.1	MnTe	65.2	28.4	65.2
FeN	120.4	105.9	120.4	FeSe	58.0	22.1	58.0	FeTe	52.3	15.5	52.3
CoN	107.5	86.4	107.4	CoSe	44.1	0.6	44.1	CoTe	16.3	-22.4	16.3
NiN	98.9	54.6	98.9	NiSe	25.4	17.4	25.4	NiTe	43.3	33.6	43.3
CuN	122.6	46.2	122.6	CuSe	31.2	21.7	31.2	CuTe	21.2	31.7	21.2
ZnN	84.1	38.7	84.1	ZnSe	45.5	4.3	45.5	ZnTe	43.7	0.8	43.7
ZrN	22.7	138.4	22.7	ZrSe	14.0	48.4	14.0	ZrTe	-0.1	44.2	-0.1
NbN	27.5	105.6	27.5	NbSe	61.2	81.8	61.2	NbTe	64.3	65.2	64.2
MoN	129.3	99.1	129.3	MoSe	66.2	101.5	66.2	MoTe	61.4	80.3	61.4
HfN	52.3	130.7	52.3	HfSe	15.8	57.4	15.8	HfTe	-2813.4	2850.2	-2813.4
TaN	98.5	106.0	98.5	TaSe	77.2	75.0	77.2	TaTe	80.7	70.8	80.7
WN	79.8	135.4	79.8	WSe	82.1	130.2	82.1	WTe	73.3	106.6	73.3