Supporting Information

Computational discovery of new 2D materials using deep learning generative models

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Table S1: 92 Hypothetical 2D materials with DFT verified E_{form}[Layered] in eV/atom

| Formula	E_{form}	Formula	E_{form}	Formula	E_{form}	Formula	E_{form}
YF2	-3.5146	AlBr2	-0.7021	MnCl5	-0.4207	IrBr4	-0.1934
TaF4	-2.9431	SeF	-0.6987	BrSi	-0.4198	AlI2	-0.1824
TaWO5	-2.7473	V2S3	-0.6830	SbBr5	-0.4196	MoBr4	-0.1810
ZnTaF5	-2.7234	GaCl	-0.6627	SnAsClS2	-0.3600	O3C2	-0.1687
NbMoF6	-2.4596	S2O5	-0.6471	SF3C	-0.3421	CrSe3	-0.1620
TaF2	-2.3656	AlCl	-0.6413	NbBr2	-0.3383	NbI2	-0.1565
SiF3	-2.1204	TaBr3	-0.6374	AsCl2	-0.3117	PdSe3	-0.1537
WF3	-2.0915	CrCl4	-0.6322	CrS3	-0.2951	Se3Ge2	-0.1512
GeF3	-2.0228	ZrS4	-0.6257	AsFN2	-0.2878	WSe	-0.1461
OB	-2.0188	SF	-0.6211	WS3	-0.2765	CoBr4	-0.1444
YCl2	-1.9251	FNC	-0.6195	AgCl2	-0.2670	AlI	-0.1375
TiSeF	-1.9018	VS3	-0.5630	BrAs	-0.2613	Ga2S	-0.1003
ScYCl4	-1.8396	NbRuCl5S2	-0.5615	Cl2O5	-0.2590	AgBr2	-0.0796
AlClS	-1.2643	ScBiAs	-0.5156	SiN	-0.2562	Br2O5	-0.0753
YI2	-1.1979	V2Se5	-0.5154	CoCl3	-0.2434	GaS2	-0.0721
TiCl	-1.0923	MnCl4	-0.5095	SB	-0.2396	Cl4P	-0.0683
YS3	-1.0488	BiBr5	-0.5095	CrBr4	-0.2392	Sb2Se5	-0.0387
NbCl3	-1.0060	GeCl3	-0.5011	Mn2Se5	-0.2392	I2As	-0.0230
ScS3	-0.9223	FB	-0.4784	TaS4	-0.2248	MnI3	-0.0218
AuF2	-0.9102	PbBr4	-0.4629	Br3AsClS	-0.2068	Cl2P	-0.0199
GeCl2	-0.7719	AlBr	-0.4484	Br4P	-0.2054	Se5As2	-0.0197
YF3	-0.5113	AlSe	-0.4342	MnBr4	-0.2046	CoBr3	-0.0167
TaF5	-0.3895	TiS4	-0.4309	ClP	-0.2035	P2B	-0.0021
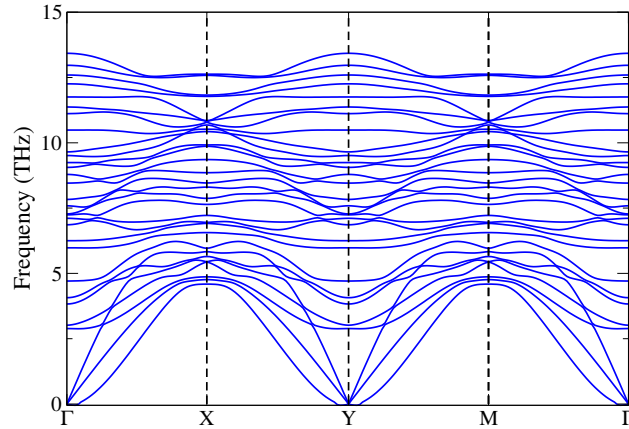
Figure S1: Phonon bands of V_2S_3 monolayer

Table S2: The 31 compositions with exfoliation energies found using DFT calculations. The formation energies of layered materials (E_{form}[Layered]), and monolayers (E_{form}[Monolayer]) are also stated.

Formula	E_{form}[Layered] (eV/atom)	E_{exf} (meV/atom)	E_{form}[Monolayer] (eV/atom)
S2O5	-0.6417	-87.8131	-1.4659
V2S3	-0.683	-11.7012	-0.8130
CoCl3	-0.2434	-2.4151	-1.8472
YI2	-1.1979	-1.1606	-1.2315
OB	-2.0188	-0.6184	-2.0268
TaF4	-2.9431	-0.1287	-2.8880
YCl2	-1.9251	0.5745	-3.3604
ScS3	-0.9223	1.6923	-0.8984
WS3	-0.2765	2.3043	-0.1630
SiF3	-2.1204	2.5126	-2.0726
GaCl	-0.6627	2.5508	-1.6550
PBr4	-0.2054	2.6124	-0.0463
SnAsS2Cl	-0.36	3.1929	-0.7259
GeCl3	-0.5011	3.6465	-2.0686
AlClS	-1.2643	3.8410	-1.9516
AlI	-0.1824	4.1322	-0.0680
GeCl2	-0.7719	4.1460	-2.1051
SF	-0.6211	4.4952	-0.5770
CrSe3	-0.2951	5.0601	-28.1131
TiSeF	-1.9018	5.6405	-14.2585
CNF	-0.6195	6.5108	-0.5164
VS3	-0.563	7.8693	-0.5678
Ga2S	-0.9223	8.9399	0.1495
WF3	-2.0915	9.0059	-2.1011
CrS3	-0.2951	10.0762	-0.2439
SiN	-0.2562	10.2146	-0.2511
GeF3	-2.0228	17.8999	-1.8943
YS3	-1.0488	18.6727	-1.1251
ClP	-0.2035	27.3343	-0.6743
FB	-0.4784	95.2095	-0.3436
WSe	-0.1461	156.6658	-16.4670