Supporting Information

First Principles Study on Thickness Dependent Structural and Electronic Properties Unveiling Growth and Stability of 2D Layered II-VI Semiconducting Compounds.

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Table of Contents

Fig. S1- Cut-off energy optimization for WZ phase of MO and MX compounds.

Fig. S2 – CBM and VBM as a function of uniaxial strain of 2D-MO and 2D-MX surface slabs with thickness of 2L.

Fig. S3 - Ball and Stick model of various thicknesses of 2D-ZnS and 2D-CdS surface slabs.

Fig. S4 – Layer resolved DOS of 10L thick WZ-ZnTe slab.

Fig. S5 – Calculated E_{exf} values for various thick (2L to 10L) 2D-MO and 2D-MX surface slabs.

Fig. S6 – DOS and BS of 3L and 4L thick 2D-CdX surface slab.

Fig. S7 – DOS and BS of 10L thick WZ-CdX surface slab.

Fig. S8 – Partial change density of 2L thick 2D-ZnTe surface slab.

Table S1 – Zn-X bond distances of various thicknesses of 2D-ZnX surface slabs.

Table S2 – Cd-X bond distances of various thicknesses of 2D-CdX surface slabs.

Table S3 – Interlayer Zn-X distances of various thicknesses of 2D-ZnX surface slabs.

- Table S4 -- Interlayer Cd-X distances of various thicknessess of 2D-CdX surface slabs.
- Table S5 Interlayer M-X distances of various thicknessess of WZ-MX surface slabs.
- Table S6 Buckling distances of various thicknesses of 2D-ZnX surface slabs.
- Table S7 Buckling distances of various thicknesses of 2D-CdX surface slabs.
- Table S8 Mechanical properties of 2L 2D-MX surface slabs.

Table S9 – Band gap of various thicknesses of 2D-MX surface slabs.

Table S10 - Effective mass of various thicknesses of 2D-MX surface slabs.



Fig. S1 : Cut-off energy optimization for WZ phase of MO and MX compounds.



Fig. S2: CBM (red line) and VBM (blue line) as a function of uniaxial strain of MX 2L (high symmetry direction $\Gamma \rightarrow K$)



Fig. S3: Ball and stick model of optimized structures of various thick (1L to 10L) ZnS (lower diagonal) and CdS (upper diagonal) surface slabs. Grey, sandal and yellow coloured ball represent Zn, Cd and S atoms, respectively.



Fig. S4 : Layer resolved DOS of 10L thick WZ slab of ZnTe compound is given. For clarity, atomic structure is provided in right panel where layers are indexed. This figure clearly indicates the holes and electrons are spatially separated in the surface slab. This kind of feature can be seen in WZ slabs of these compounds.

nL	Zn-O	Zn-S	Zn-Se	Zn-Te
1	1.896	2.236	2.364	2.563
2	1.925	2.303	2.448	2.649
3	1.935	2.269 - 2.293	2.383 - 2.439	2.567 - 2.647
4	1.942	2.297 - 2.303	2.444 - 2.447	2.647 - 2.648
5	1.946	2.258 - 2.303	2.383 - 2.446	2.566 - 2.654
6	1.949	2.295 - 2.305	2.443 -2.449	2.648 - 2.650
7	1.952	2.304 - 2.277	2.375 - 3.449	2.599 - 2.671
8	1.954	2.294 - 2.304	2.385 - 2.469	2.648 - 2.650
9	1.955	2.295 - 2.305	2.383 - 2.449	2.564 - 2.652
10	1.956	2.295 - 2.306	2.390 - 2.455	2.646 - 2.648
Bulk	1.99	2.32	2.45	2.63

Table S1 : Typical Zn-X bond distances (in Å) along xy-axis of various thick (1L to 10L) of 2D-MX surface slabs. For comparison, bulk bond distances are given at last row.

Table S2 : Typical Cd-X bond distances (in Å) along xy-axis of various thick (1L to 10L) of 2D-MX surface slabs. For comparison, bulk bond distances are given at last row.

nL	Cd-O	Cd-S	Cd-Se	Cd-Te
1	2.115	2.446	2.572	2.760
2	2.153	2.517	2.649	2.840
3	2.170	2.497 - 2.510	2.594 - 2.646	2.758 - 2.840
4	2.179	2.513 - 2.525	2.642-6.50	2.840 - 2.842
5	2.185	2.508 - 2.528	2.589 - 2.658	2.756 - 2.844
6	2.190	2.512 - 2.531	2.639 - 2.652	2.838 - 2.842
7	2.193	2.516 - 2.537	2.587 - 2.666	2.756 - 2.844
8	2.196	2.518 - 2.538	2.640 - 2.655	2.801 - 2.868
9	2.198	2.519 - 2.540	2.597-2.662	2.743 - 2.848
10	2.199	2.521 - 2.540	2.643 - 2.656	2.800 - 2.873
Bulk	2.23	2.55	2.68	2.81

In these Tables (S1 & S2), M-X bond distances, along xy axis of layers, in odd nL are observed to varied significanly as compared to even nL, owing to instability of former case.

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		6	_	7	_	5	_	3			a					6		Γ.		S.		3			Π		
YERS	1-2	2.63	2.65	2.63	2.65	2.62	2.69	3.43	2.81	2.66	2.62	9-10	ERS	YERS	1-2	3.00	4.57	3.01	4.57	2.98	4.55	3.00	4.55	2.84	2.84	9-10	RS
DD LA	2-3	3.42	3.46	3.49	3.43	3.43	3.11	2.64	2.72	3.44	3.45	8-9	LAYI	D LA	2-3	2.85	2.86	2.85	2.86	2.85	2.86	2.85	2.86	4.17	4.17	8-9	LAYE
OF O	3-4	2.67	2.64	2.66	2.70	2.95	3.39	2.66	2.63	2.65	2.64	7-8	EVEN	OF OI	3-4	4.14	4.17	4.15	4.18	4.13	4.16	2.84	2.84	2.84	2.84	7-8	EVEN
ANCE	4-5	3.44	3.45	3.41	2.99	2.72	2.65	3.43	3.45	3.42	3.42	6-7	CE OF	ANCE	4-5	2.83	2.84	2.83	2.84	2.83	2.84	4.17	4.16	4.16	4.16	6-7	E OF
RDIST	5-6	3.42	3.44	3.16	3.48	2.662	2.629	2.65	2.64	2.65	2.64	5-6	STAN	TSIU	5-6	4.16	4.17	4.18	4.18	2.84	2.84	2.84	2.84	2.84	2.84	5-6	STANC
LAYEI	6-7	2.64	2.65	2.68	2.63	3.433	3.454	3.40	3.40	3.42	3.42	4-5	VERDI	LAYEF	6-7	2.83	2.84	2.83	2.84	4.18	4.17	4.18	4.19	4.16	4.16	4-5	ERDI
INTER	7-8	3.44	3.47	2.66	2.63	2.65	2.65	2.64	2.65	2.64	2.65	3-4	ERLA	NTER	7-8	4.15	4.16	2.842	2.841	2.84	2.84	2.84	2.84	2.83	2.83	3-4	ERLAY
	8-9	2.65	2.63	3.46	3.47	3.45	3.43	3.46	3.44	3.45	3.43	2-3	INI	Ι	8-9	2.83	2.84	4.18	4.18	4.19	4.19	4.18	4.18	4.16	4.16	2-3	IIII
	ZUZ	2.64	2.64	2.63	2.66	2.63	2.66	2.63	2.66	2.62	2.66	1-2		E	Znle	2.83	2.83	2.84	2.84	2.84	2.83	2.83	2.84	2.83	2.84	1-2	
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S		5 9 A	0	7 7		8 5		1 3	+	0	nL S	0		SS		3 9 4	2	2 7		3 5	8	1 3	8		9 nL	9	
AYERS	1-2	2.36 9	2.39	2.37 7	2.40	2.38 5	2.41	2.41 3	2.44	2.39	2.36 nL	9-10	TERS	AYERS	1-2	2.93 9	4.02	2.92 7	4.01	2.93 5	4.03	2.91 3	4.03	2.71	2.69 nL	9-10	TERS
DDD LAYERS	2-3 1-2	2.39 2.36 9	2.38 2.39	2.39 2.37 7	2.39 2.40	2.41 2.38 5	2.40 2.41	2.44 2.41 3	2.44 2.44	2.38 2.39	2.38 2.36 nL	8-9 9-10	N LAYERS	DDD LAYERS	2-3 1-2	2.73 2.93 9	2.72 4.02	2.73 2.92 7	2.72 4.01	2.73 2.93 5	2.73 4.03	2.73 2.91 3	2.72 4.03	3.74 2.71	3.75 2.69 nL	8-9 9-10	N LAYERS
E OF ODD LAYERS	3-4 2-3 1-2	2.38 2.39 2.36 9	2.38 2.38 2.39	2.39 2.39 2.37 7	2.39 2.39 2.40	2.40 2.41 2.38 5	2.41 2.40 2.41	2.39 2.44 2.41 3	2.36 2.44 2.44	2.38 2.38 2.39	2.38 2.38 2.36 nL	7-8 8-9 9-10	F EVEN LAYERS	E OF ODD LAYERS	3-4 2-3 1-2	3.75 2.73 2.93 9	3.79 2.72 4.02	3.75 2.73 2.92 7	3.79 2.72 4.01	3.74 2.73 2.93 5	3.78 2.73 4.03	2.70 2.73 2.91 3	2.69 2.72 4.03	2.70 3.74 2.71	2.71 3.75 2.69 nL	7-8 8-9 9-10	F EVEN LAYERS
TANCE OF ODD LAYERS	4-5 3-4 2-3 1-2	2.38 2.38 2.39 2.36 9	2.38 2.38 2.38 2.39	2.39 2.39 2.39 2.37 7	2.39 2.39 2.39 2.40	2.41 2.40 2.41 2.38 5	2.38 2.41 2.40 2.41	2.39 2.39 2.44 2.41 3	2.39 2.36 2.44 2.44	2.37 2.38 2.38 2.39	2.38 2.38 2.38 2.36 nL	6-7 7-8 8-9 9-10	VCE OF EVEN LAYERS	TANCE OF ODD LAYERS	4-5 3-4 2-3 1-2	2.70 3.75 2.73 2.93 9	2.70 3.79 2.72 4.02	2.70 3.75 2.73 2.92 7	2.71 3.79 2.72 4.01	2.70 3.74 2.73 2.93 5	2.70 3.78 2.73 4.03	3.77 2.70 2.73 2.91 3	3.79 2.69 2.72 4.03	3.76 2.70 3.74 2.71	3.75 2.71 3.75 2.69 nL	6-7 7-8 8-9 9-10	ICE OF EVEN LAYERS
RDISTANCE OF ODD LAYERS	5-6 4-5 3-4 2-3 1-2	2.38 2.38 2.38 2.39 2.36 9	2.38 2.38 2.38 2.38 2.39	2.39 2.39 2.39 2.39 2.37 7	2.39 2.39 2.39 2.39 2.40	2.40 2.41 2.40 2.41 2.38 5	2.38 2.38 2.41 2.40 2.41	2.39 2.39 2.39 2.44 2.41 3	2.39 2.39 2.36 2.44 2.44	2.37 2.37 2.38 2.38 2.39	2.37 2.38 2.38 2.38 2.36 nL	5-6 6-7 7-8 8-9 9-10	USTANCE OF EVEN LAYERS	ERDISTANCE OF ODD LAYERS	5-6 4-5 3-4 2-3 1-2	3.79 2.70 3.75 2.73 2.93 9	3.80 2.70 3.79 2.72 4.02	3.77 2.70 3.75 2.73 2.92 7	3.79 2.71 3.79 2.72 4.01	2.70 2.70 3.74 2.73 2.93 5	2.69 2.70 3.78 2.73 4.03	2.71 3.77 2.70 2.73 2.91 3	2.71 3.79 2.69 2.72 4.03	2.70 3.76 2.70 3.74 2.71	2.70 3.75 2.71 3.75 2.69 nL	5-6 6-7 7-8 8-9 9-10	ISTANCE OF EVEN LAYERS
ULAYERDISTANCE OF ODD LAYERS	6-7 5-6 4-5 3-4 2-3 1-2	2.38 2.38 2.38 2.38 2.39 2.36 9	2.38 2.38 2.38 2.38 2.38 2.39	2.40 2.39 2.39 2.39 2.39 2.37 7	2.37 2.39 2.39 2.39 2.39 2.40	2.40 2.40 2.41 2.40 2.41 2.38 5	2.40 2.38 2.38 2.41 2.40 2.41	2.38 2.39 2.39 2.39 2.44 2.41 3	2.38 2.39 2.39 2.36 2.44 2.44	2.37 2.37 2.37 2.38 2.38 2.39	2.37 2.37 2.38 2.38 2.38 2.38 DL	4-5 5-6 6-7 7-8 8-9 9-10	YERDISTANCE OF EVEN LAYERS	ALAYERDISTANCE OF ODD LAYERS	6-7 5-6 4-5 3-4 2-3 1-2	2.70 3.79 2.70 3.75 2.73 2.93 9	2.71 3.80 2.70 3.79 2.72 4.02	2.70 3.77 2.70 3.75 2.73 2.92 7	2.70 3.79 2.71 3.79 2.72 4.01	3.80 2.70 2.70 3.74 2.73 2.93 5	3.80 2.69 2.70 3.78 2.73 4.03	3.78 2.71 3.77 2.70 2.73 2.91 3	3.78 2.71 3.79 2.69 2.72 4.03	3.76 2.70 3.76 2.70 3.74 2.71	3.76 2.70 3.75 2.71 3.75 2.69 nL	4-5 5-6 6-7 7-8 8-9 9-10	YERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.39 2.38 2.38 2.38 2.38 2.39 2.36 9	2.39 2.38 2.38 2.38 2.38 2.38 2.38 2.39	2.42 2.40 2.39 2.39 2.39 2.39 2.37 7	2.39 2.37 2.39 2.39 2.39 2.39 2.40	2.39 2.40 2.40 2.41 2.40 2.41 2.38 5	2.40 2.40 2.38 2.38 2.41 2.40 2.41	2.38 2.38 2.39 2.39 2.39 2.44 2.41 3	2.38 2.38 2.39 2.39 2.36 2.44 2.44	2.38 2.37 2.37 2.37 2.38 2.38 2.39	2.38 2.37 2.37 2.38 2.38 2.38 2.36 nL	3-4 4-5 5-6 6-7 7-8 8-9 9-10	TERLAYERDISTANCE OF EVEN LAYERS	INTERLAYERDISTANCE OF ODD LAYERS	7-8 6-7 5-6 4-5 3-4 2-3 1-2	3.79 2.70 3.79 2.70 3.75 2.73 2.93 9	3.81 2.71 3.80 2.70 3.79 2.72 4.02	2.71 2.70 3.77 2.70 3.75 2.73 2.92 7	2.70 2.70 3.79 2.71 3.79 2.72 4.01	2.71 3.80 2.70 2.70 3.74 2.73 2.93 5	2.70 3.80 2.69 2.70 3.78 2.73 4.03	2.71 3.78 2.71 3.77 2.70 2.73 2.91 3	2.71 3.78 2.71 3.79 2.69 2.72 4.03	2.71 3.76 2.70 3.76 2.70 3.74 2.71	2.71 3.76 2.70 3.75 2.71 3.75 2.69 nL	3-4 4-5 5-6 6-7 7-8 8-9 9-10	ERLAYERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.36 2.39 2.38 2.38 2.38 2.38 2.38 2.39 2.36 9	2.39 2.39 2.38 2.38 2.38 2.38 2.38 2.39	2.42 2.42 2.40 2.39 2.39 2.39 2.39 2.37 7	2.42 2.39 2.37 2.39 2.39 2.39 2.39 2.40	2.40 2.39 2.40 2.40 2.41 2.40 2.41 2.38 5	2.40 2.40 2.38 2.38 2.38 2.41 2.41	2.39 2.38 2.39 2.39 2.39 2.44 2.41 3	2.39 2.38 2.38 2.39 2.39 2.36 2.44 2.44	2.38 2.38 2.37 2.37 2.37 2.38 2.38 2.39	2.38 2.38 2.37 2.37 2.38 2.38 2.38 2.36 nL	2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS	INTERLAYERDISTANCE OF ODD LAYERS	8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.70 3.79 2.70 3.79 2.70 3.75 2.73 2.93 9	2.70 3.81 2.71 3.80 2.70 3.79 2.72 4.02	3.80 2.71 2.70 3.77 2.70 3.75 2.73 2.92 7	3.80 2.70 2.70 3.79 2.71 3.79 2.72 4.01	3.78 2.71 3.80 2.70 2.70 3.74 2.73 2.93 5	3.77 2.70 3.80 2.69 2.70 3.78 2.73 4.03	3.79 2.71 3.78 2.71 3.77 2.70 2.73 2.91 3	3.78 2.71 3.78 2.71 3.79 2.69 2.72 4.03	3.77 2.71 3.76 2.70 3.76 2.70 3.74 2.71	3.76 2.71 3.76 2.70 3.75 2.71 3.75 2.69 nL	2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	ZnO 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.44 2.36 2.39 2.38 2.38 2.38 2.38 2.38 2.39 2.36 9	2.44 2.39 2.38 2.38 2.38 2.38 2.38 2.39	2.39 2.42 2.42 2.40 2.39 2.39 2.39 2.39 2.37 7	2.43 2.42 2.39 2.37 2.39 2.39 2.39 2.39 2.40	2.37 2.40 2.39 2.40 2.40 2.41 2.41 2.41 2.38 5	2.40 2.40 2.40 2.40 2.38 2.38 2.41 2.40 2.41	2.36 2.39 2.38 2.39 2.39 2.39 2.44 2.41 3	2.39 2.39 2.38 2.38 2.39 2.39 2.36 2.44 2.44	2.36 2.38 2.38 2.37 2.37 2.37 2.38 2.39	2.39 2.38 2.38 2.37 2.37 2.38 2.38 2.38 2.38 D L	1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS	INTERLAYERDISTANCE OF ODD LAYERS	ZnSe 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.70 2.70 3.79 2.70 3.79 2.70 3.75 2.73 2.93 9	2.70 2.70 3.81 2.71 3.80 2.70 3.79 2.72 4.02	2.70 3.80 2.71 2.70 3.77 2.70 3.75 2.73 2.92 7	2.71 3.80 2.70 2.70 3.79 2.71 3.79 2.72 4.01	2.70 3.78 2.71 3.80 2.70 2.70 3.74 2.73 2.93 5	2.71 3.77 2.70 3.80 2.69 2.70 3.78 2.73 4.03	2.70 3.79 2.71 3.78 2.71 3.77 2.70 2.73 2.91 3	2.71 3.78 2.71 3.78 2.71 3.79 2.69 2.72 4.03	2.69 3.77 2.71 3.76 2.70 3.76 2.70 3.74 2.71	2.70 3.76 2.71 3.76 2.70 3.75 2.71 3.75 2.69 nL	1 -2 2 -3 3 -4 4 -5 5 -6 6 -7 7 -8 8 -9 9 -10	INTERLAYERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	nL ZnO 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2 2.44 2.36 2.39 2.38 2.38 2.38 2.38 2.38 2.39 2.36 9	2.44 2.39 2.39 2.38 2.38 2.38 2.38 2.38 2.39	4 2.39 2.42 2.40 2.39 2.39 2.39 2.37 7	2.43 2.42 2.39 2.37 2.39 2.39 2.39 2.39 2.40	6 2.37 2.40 2.39 2.40 2.40 2.41 2.41 2.40 2.41 2.38 5	2.40 2.40 2.40 2.40 2.38 2.38 2.41 2.40 2.41	8 2.36 2.39 2.38 2.38 2.39 2.39 2.39 2.44 2.41 3	2.39 2.38 2.38 2.38 2.39 2.39 2.34 2.44	10 2.36 2.38 2.37 2.37 2.37 2.38 2.39 2.39	2.39 2.38 2.38 2.37 2.37 2.38 2.38 2.38 2.36 nL	1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS	INTERLAYERDISTANCE OF ODD LAYERS	IL ZnSe 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2 2.70 2.70 3.79 2.70 3.79 2.70 3.75 2.73 2.93 9	2.70 2.70 3.81 2.71 3.80 2.70 3.79 2.72 4.02	4 2.70 3.80 2.71 2.70 3.77 2.70 3.75 2.73 2.92 7	2.71 3.80 2.70 2.70 3.79 2.71 3.79 2.72 4.01	6 2.70 3.78 2.71 3.80 2.70 2.70 3.74 2.73 2.93 5	2.71 3.77 2.70 3.80 2.69 2.70 3.78 2.73 4.03	8 2.70 3.79 2.71 3.78 2.71 3.77 2.70 2.73 2.91 3	2.71 3.78 2.71 3.78 2.71 3.79 2.69 2.72 4.03	10 2.69 3.77 2.71 3.76 2.70 3.76 2.70 3.74 2.71	2.70 3.76 2.71 3.76 2.70 3.75 2.71 3.75 2.69 nL	<u>1-2</u> 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS

Table S3 : Interlayer distances (in Å) of various thick (nL) of 2D-ZnX surface slabs are reported. Left and right diagonal panels correspond to even and odd number layered surface slabs, repectively.

Table S4 : Interlayer distances (in Å) of various thick (nL) of 2D-CdX surface slabs are reported. Left and right diagonal panels correspond to even and odd number layered surface slabs, repectively.

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		6		7		0		e			Ξ						9	_	7	_	S	_	3			п		
YERS	1-2	2.86	2.74	2.75	2.87	2.75	2.89	2.76	3.02	2.86	2.74	9-10	RS		VERS	1-2	3.21	4.82	3.20	4.80	3.22	4.82	3.20	4.80	3.08	3.07	9-10	ERS
DD LA	2-3	2.92	3.03	3.04	2.92	3.04	2.87	3.01	2.75	2.93	3.03	8-9	LAYF		DD LA	2-3	3.09	3.09	3.09	3.09	3.09	3.09	3.08	3.08	4.03	4.03	8-9	LAYE
OF 0]	3-4	2.87	2.82	2.83	2.91	2.86	3.03	2.86	2.75	2.86	2.82	7-8	EVEN		OF 0	3-4	4.00	4.02	3.99	4.01	3.99	4.01	3.08	3.07	3.08	3.08	7-8	EVEN
ANCE	4-5	2.86	2.90	2.91	2.83	2.90	2.75	2.97	3.06	2.89	2.91	6-7	CE OF		ANCE	4-5	3.07	3.08	3.07	3.08	3.07	3.07	4.03	4.04	4.02	4.02	6-7	CE OF
RDIST	5-6	2.90	2.86	2.92	3.05	2.86	2.76	2.85	2.82	2.85	2.85	5-6	STAN		RDIST	5-6	4.02	4.03	4.02	4.03	3.08	3.07	3.08	3.08	3.08	3.08	5-6	ISTAN
LAYE	6-7	2.82	2.87	2.87	2.75	3.07	3.13	2.95	2.95	2.91	2.89	4-5	YERDI		RLAYE	6-7	3.07	3.08	3.07	3.07	4.03	4.03	4.04	4.03	4.02	4.02	4-5	YERDI
INTER	7-8	3.03	2.92	2.85	2.78	2.83	2.83	2.82	2.85	2.82	2.86	3-4	ERLA		INTER	7-8	4.02	4.03	3.08	3.08	3.08	3.08	3.08	3.08	3.08	3.08	3-4	ERLA
	8-9	2.74	2.87	3.22	3.22	3.13	3.07	3.05	2.96	3.01	2.92	2-3	INI			8-9	3.07	3.07	4.05	4.05	4.04	4.03	4.04	4.03	4.03	4.03	2-3	INI
ç		2.83	2.84	2.78	2.86	2.76	2.86	2.75	2.86	2.74	2.86	1-2				CdTe	3.07	3.08	3.07	3.08	3.07	3.08	3.07	3.08	3.07	3.08	1-2	
,	1	2		4		9		×		10						L	17		4		6		8		10			
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VERS	1-2	2.49 9	2.50	2.50 7	2.50	2.51 5	2.51	2.54 3	2.54	2.50	2.49 nL	9-10	ERS		AYERS	1-2	2.89 9	2.92	2.89 7	2.92	2.86 5	2.96	2.94 3	3.69	2.93	2.90 nL	9-10	ERS
DD LAYERS	2-3 1-2	2.50 2.49 9	2.51 2.50	2.50 2.50 7	2.51 2.50	5.52 2.51 5	2.52 2.51	2.54 2.54 3	2.54 2.54	2.50 2.50	2.50 2.49 nL	8-9 9-10	V LAYERS		DD LAYERS	2-3 1-2	3.56 2.89 9	3.53 2.92	3.55 2.89 7	3.51 2.92	3.57 2.86 5	3.06 2.96	2.98 2.94 3	2.87 3.69	3.55 2.93	3.57 2.90 nL	8-9 9-10	N LAYERS
C OF ODD LAYERS	3-4 2-3 1-2	2.50 2.50 2.49 9	2.50 2.51 2.50	2.50 2.50 2.50 7	2.50 2.51 2.50	5.52 5.52 2.51 5	2.52 2.52 2.51	2.50 2.54 2.54 3	2.50 2.54 2.54	2.50 2.50 2.50	2.50 2.50 2.49 nL	7-8 8-9 9-10	FEVEN LAYERS		E OF ODD LAYERS	3-4 2-3 1-2	2.91 3.56 2.89 9	2.91 3.53 2.92	2.91 3.55 2.89 7	2.91 3.51 2.92	3.06 3.57 2.86 5	3.57 3.06 2.96	2.94 2.98 2.94 3	2.90 2.87 3.69	2.92 3.55 2.93	2.92 3.57 2.90 nL	7-8 8-9 9-10	F EVEN LAYERS
TANCE OF ODD LAYERS	4-5 3-4 2-3 1-2	2.50 2.50 2.50 2.49 9	2.50 2.50 2.51 2.50	2.50 2.50 2.50 2.50 7	2.50 2.50 2.51 2.50	2.51 5.52 5.52 2.51 5	2.51 2.52 2.52 2.51	2.51 2.50 2.54 2.54 3	2.50 2.50 2.54 2.54	2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.49 nL	6-7 7-8 8-9 9-10	CE OF EVEN LAYERS		FANCE OF ODD LAYERS	4-5 3-4 2-3 1-2	3.54 2.91 3.56 2.89 9	3.53 2.91 3.53 2.92	3.53 2.91 3.55 2.89 7	3.45 2.91 3.51 2.92	2.96 3.06 3.57 2.86 5	2.86 3.57 3.06 2.96	3.54 2.94 2.98 2.94 3	3.56 2.90 2.87 3.69	3.55 2.92 3.55 2.93	3.55 2.92 3.57 2.90 nL	6-7 7-8 8-9 9-10	ICE OF EVEN LAYERS
RDISTANCE OF ODD LAYERS	5-6 4-5 3-4 2-3 1-2	2.50 2.50 2.50 2.50 2.49 9	2.50 2.50 2.50 2.51 2.50	2.51 2.50 2.50 2.50 2.50 7	2.51 2.50 2.50 2.51 2.50	2.51 2.51 5.52 5.52 2.51 5	2.51 2.51 2.52 2.52 2.51	2.50 2.51 2.50 2.54 2.54 3	2.51 2.50 2.50 2.54 2.54	2.50 2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.50 2.49 nL	5-6 6-7 7-8 8-9 9-10	ISTANCE OF EVEN LAYERS		ERDISTANCE OF ODD LAYERS	5-6 4-5 3-4 2-3 1-2	2.91 3.54 2.91 3.56 2.89 9	2.91 3.53 2.91 3.53 2.92	2.89 3.53 2.91 3.55 2.89 7	2.97 3.45 2.91 3.51 2.92	2.94 2.96 3.06 3.57 2.86 5	2.90 2.86 3.57 3.06 2.96	2.92 3.54 2.94 2.98 2.94 3	2.92 3.56 2.90 2.87 3.69	2.92 3.55 2.92 3.55 2.93	2.92 3.55 2.92 3.57 2.90 nL	5-6 6-7 7-8 8-9 9-10	ISTANCE OF EVEN LAYERS
LAYERDISTANCE OF ODD LAYERS	6-7 5-6 4-5 3-4 2-3 1-2	2.50 2.50 2.50 2.50 2.50 2.50 2.49 9	2.50 2.50 2.50 2.50 2.51 2.50	2.50 2.51 2.50 2.50 2.50 7	2.50 2.51 2.50 2.50 2.51 2.50	2.52 2.51 2.51 5.52 5.52 2.51 5	2.52 2.51 2.51 2.52 2.52 2.51	2.50 2.50 2.51 2.50 2.54 2.54 3	2.50 2.51 2.50 2.50 2.54 2.54	2.50 2.50 2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.50 2.50 2.49 nL	4-5 5-6 6-7 7-8 8-9 9-10	YERDISTANCE OF EVEN LAYERS		RLAYERDISTANCE OF ODD LAYERS	6-7 5-6 4-5 3-4 2-3 1-2	3.56 2.91 3.54 2.91 3.56 2.89 9	3.47 2.91 3.53 2.91 3.53 2.92	3.64 2.89 3.53 2.91 3.55 2.89 7	2.92 2.97 3.45 2.91 3.51 2.92	3.56 2.94 2.96 3.06 3.57 2.86 5	3.57 2.90 2.86 3.57 3.06 2.96	3.54 2.92 3.54 2.94 2.98 2.94 3	3.54 2.92 3.56 2.90 2.87 3.69	3.54 2.92 3.55 2.92 3.55 2.93	3.54 2.92 3.55 2.92 3.57 2.90 nL	4-5 5-6 6-7 7-8 8-9 9-10	YERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.49 9	2.50 2.50 2.50 2.50 2.50 2.51 2.50	2.53 2.50 2.51 2.50 2.50 2.50 2.50 7	2.52 2.50 2.51 2.50 2.50 2.51 2.50	2.51 2.52 2.51 2.51 5.52 5.52 2.51 5	2.57 2.52 2.51 2.51 2.52 2.52 2.51	2.51 2.50 2.50 2.51 2.50 2.54 2.54 3	2.51 2.50 2.51 2.50 2.50 2.54 2.54	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.50 2.50 2.50 2.49 nL	3-4 4-5 5-6 6-7 7-8 8-9 9-10	ERLAYERDISTANCE OF EVEN LAYERS		INTERLAYERDISTANCE OF ODD LAYERS	7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.89 3.56 2.91 3.54 2.91 3.56 2.89 9	2.98 3.47 2.91 3.53 2.91 3.53 2.92	2.94 3.64 2.89 3.53 2.91 3.55 2.89 7	2.91 2.92 2.97 3.45 2.91 3.51 2.92	2.92 3.56 2.94 2.96 3.06 3.57 2.86 5	2.92 3.57 2.90 2.86 3.57 3.06 2.96	2.91 3.54 2.92 3.54 2.94 2.98 2.94 3	2.92 3.54 2.92 3.56 2.90 2.87 3.69	2.92 3.54 2.92 3.55 2.92 3.55 2.93	2.92 3.54 2.92 3.55 2.92 3.57 2.90 nL	3-4 4-5 5-6 6-7 7-8 8-9 9-10	FERLAYERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.50	2.49 2.50 2.50 2.50 2.50 2.50 2.51 2.50	2.53 2.53 2.50 2.51 2.50 2.50 2.50 2.50 7	2.53 2.52 2.50 2.51 2.50 2.50 2.51 2.50	2.51 2.51 2.52 2.51 2.51 5.52 5.52 2.51 5	5.52 2.57 2.52 2.51 2.51 2.52 2.52 2.51	2.50 2.51 2.50 2.50 2.51 2.50 2.54 2.54 3	2.51 2.51 2.50 2.51 2.50 2.50 2.54 2.54	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.49 nL	2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS		INTERLAYERDISTANCE OF ODD LAYERS	8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	3.65 2.89 3.56 2.91 3.54 2.91 3.56 2.89 9	2.93 2.98 3.47 2.91 3.53 2.91 3.53 2.92	3.58 2.94 3.64 2.89 3.53 2.91 3.55 2.89 7	3.58 2.91 2.92 2.97 3.45 2.91 3.51 2.92	3.57 2.92 3.56 2.94 2.96 3.06 3.57 2.86 5	3.55 2.92 3.57 2.90 2.86 3.57 3.06 2.96	3.56 2.91 3.54 2.92 3.54 2.94 2.98 2.94 3	3.54 2.92 3.54 2.92 3.56 2.90 2.87 3.69	3.56 2.92 3.54 2.92 3.55 2.92 3.55 2.93	3.54 2.92 3.54 2.92 3.55 2.92 3.57 2.90 nL	2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS
INTERLAYERDISTANCE OF ODD LAYERS	CdO 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.55 2.50 2.50 2.50 2.50 2.50 2.50 2.50	2.55 2.49 2.50 2.50 2.50 2.50 2.50 2.51 2.50	2.52 2.53 2.53 2.50 2.51 2.50 2.50 2.50 2.50 7	2.52 2.53 2.52 2.50 2.51 2.50 2.50 2.51 2.50	2.51 2.51 2.51 2.52 2.51 2.51 5.52 5.52	2.51 5.52 2.57 2.52 2.51 2.51 2.52 2.51	2.50 2.50 2.51 2.50 2.50 2.51 2.51 2.54 2.54 3	2.50 2.51 2.50 2.51 2.50 2.51 2.54 2.54	2.49 2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.50	2.50 2.50 2.50 2.50 2.50 2.50 2.50 2.50	1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS		INTERLAYERDISTANCE OF ODD LAYERS	Cd3e 8-9 7-8 6-7 5-6 4-5 3-4 2-3 1-2	2.93 3.65 2.89 3.56 2.91 3.54 2.91 3.56 2.89 9	2.93 2.93 2.98 3.47 2.91 3.53 2.91 3.53 2.92	2.91 3.58 2.94 3.64 2.89 3.53 2.91 3.55 2.89 7	2.94 3.58 2.91 2.92 2.97 3.45 2.91 3.51 2.92	2.90 3.57 2.92 3.56 2.94 2.96 3.06 3.57 2.86 5	2.94 3.55 2.92 3.57 2.90 2.86 3.57 3.06 2.96	2.90 3.56 2.91 3.54 2.92 3.54 2.94 2.94 3	2.94 3.54 2.92 3.54 2.92 3.56 2.90 2.87 3.69	2.90 3.56 2.92 3.54 2.92 3.55 2.92 3.55 2.93	2.93 3.54 2.92 3.54 2.92 3.55 2.92 3.57 2.90 nL	1-2 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10	INTERLAYERDISTANCE OF EVEN LAYERS

nL

nL

Table S5: Interlayer distances (in Å) of MX (expect CdO) various thick surface slabs (nL) are provided. Pink and yellow color marked boxes correspond to M-X bonding side and non-bonding side of surface slabs (refer Fig. 2), respectively.

			INTE	RLAYE	RDISTA	NCE O)F WUI	RZITE S	SLABS	
n	L	1-2	2-3	3-4	4-5	5-6	6-7	7-8	8-9	9-10
	7	2.16	2.13	2.12	2.13	2.14	2.22			
	<i>`</i>	2.88	3.00	3.02	3.02	3.01	2.94			
	8	2.14	2.09	2.08	2.08	2.09	2.10	2.18		
0	0	2.91	3.04	3.06	3.07	3.07	3.07	3.01		
Z	0	2.13	2.07	2.07	2.07	2.07	2.07	2.08	2.16	
	_	2.93	3.08	3.11	3.11	3.11	3.11	3.10	3.04	
	10	2.12	2.06	2.06	2.05	2.05	2.05	2.05	2.07	2.14
	10	2.94	3.10	3.14	3.14	3.14	3.14	3.13	3.13	3.07
	6	2.56	2.52	2.50	2.51	2.49				
	0	2.96	3.60	3.55	3.57	3.64				
	7	2.51	2.46	2.45	2.45	2.45	2.45			
	/	3.19	3.69	3.67	3.67	3.67	3.74			
S	0	2.43	2.40	2.39	2.39	2.39	2.39	2.40		
Z	0	3.71	3.80	3.79	3.79	3.79	3.79	3.87		
	0	2.42	2.38	2.38	2.38	2.38	2.38	2.38	2.39	
	9	3.75	3.82	3.82	3.82	3.82	3.81	3.81	3.89	
	10	2.41	2.37	2.37	2.37	2.37	2.37	2.37	2.38	2.39
	10	3.77	3.84	3.83	3.82	3.82	3.83	3.83	3.83	3.90
	_	2.62	2.64	2.68	2.67					
	5	3.89	3.77	3.92	2.82	1				
1		2.59	2.60	2.60	2.63	2.66				
	6	3.96	3.85	3.83	3.93	2.84				
	-	2.56	2.56	2.56	2.57	2.59	2.65	1		
Se	7	4.00	3.91	3.92	3.90	3.96	2.88	1		
Zn	•	2.53	2.53	2.53	2.54	2.54	2.57	2.66		
	8	4.02	3.94	3.96	3.96	3.93	3.97	2.91		
		2.52	2.52	2.51	2.52	2.52	2.53	2.56	2.67	
	9	4.04	3.97	3.98	3.98	3.98	3.95	3.98	2.91	
	10	2.52	2.51	2.51	2.51	2.51	2.51	2.52	2.56	2.67
	10	4.05	3.99	4.00	4.00	4.00	4.00	3.97	3.99	2.92
		2.86	2.92	2.82			-			
	4	4.24	4.44	2.88						
	_	2.77	2.78	2.81	2.80					
	5	4.39	4.24	4.40	2.88					
		2.73	2.74	2.74	2.76	2.79				
	6	4.44	4.31	4.28	4.37	2.90				
le	_	2.70	2.71	2.71	2.71	2.73	2.79	1		
Zn]	7	4.48	4.33	4.33	4.29	4.37	2.90	1		
		2.69	2.70	2.70	2.70	2.70	2.72	2.78		
	8	4.51	4.35	4.35	45	4.30	4.36	2.91		
		2.68	2.69	2.71	2.69	2.69	2.69	2.71	2.78	
	9	4.52	4.37	4.38	4.37	4.37	4.33	4.38	2.91	
		2.68	2.68	2.68	2.68	2.68	2.68	2.68	2.70	2.78
	10	4.53	4.38	4.37	4.37	4.37	4.36	4.31	4.35	2.91

			INTER	RLAYE	RDISTA	ANCE O	OF WUI	RZITE S	SLABS	
n	L	1-2	2-3	3-4	4-5	5-6	6-7	7-8	8-9	9-10
	8	2.66	2.71	2.69	2.70	2.70	2.73	2.75		
		3.46	3.42	3.47	3.47	3.41	3.54	3.02		
dS	9	2.63	3.64	2.64	2.64	2.64	2.64	2.67	2.77	
Ũ	-	3.76	3.70	3.72	3.72	3.72	3.69	3.72	3.10	
	10	2.62	2.62	2.61	2.61	2.61	2.62	2.62	2.65	2.76
	10	3.85	3.81	3.83	3.83	3.83	3.84	3.80	3.81	3.15
	-	2.75	2.76	2.76	2.76	2.80	2.86			
		4.06	3.94	3.96	3.90	4.06	3.08			
		2.73	2.73	2.73	2.73	2.74	2.78	2.88		
Se	0	4.15	4.06	4.08	4.07	4.03	4.43	3.10		
Cq	0	2.72	2.71	2.71	2.71	2.72	2.72	2.77	2.88	
	,	4.20	4.13	4.14	4.14	4.13	4.08	4.16	3.11	(
	10	2.72	2.71	2.70	2.70	2.71	2.71	2.73	2.76	2.89
	10	4.22	4.16	4.17	4.17	4.17	4.15	4.11	4.16	3.11
	6	2.94	2.95	2.95	2.98	3.00				
	0	4.63	4.47	4.43	4.61	3.13		_		
	7	2.91	2.92	2.92	2.93	2.96	3.01			
		4.69	4.53	4.53	4.48	4.64	3.15			
Te	0	2.89	2.90	2.90	2.90	2.91	2.95	3.01		
Cd	°	4.73	4.56	4.57	4.57	4.53	4.68	3.16		
	0	2.89	2.88	2.89	2.89	2.89	2.90	2.95	3.01	
	9	4.76	4.59	4.59	4.59	4.60	4.54	4.69	3.17	
	10	2.88	2.88	2.88	2.88	2.88	2.88	2.89	2.94	3.01
	10	4.78	4.61	4.61	4.61	4.60	4.60	4.54	4.68	3.17

Note that in last two layers (particularly for MSe, MTe cases), the M-X interlayer distances in both bonding and non-bonding sides are almost equal due to formation of bilayer in the WZ slabs.

Layer	1L	2L	3L	4L	5L	6L	7L	8L	9L	10L
1L	0.02									
2L	0.473	-0.475	I — — — —						Z	nS
3L	0.254	0.006	0.26							
4L	0.402	-0.33	0.331	-0.4						
5L	0.318	-0.171	0.005	0.162	-0.309					
6L	0.371	-0.275	0.213	-0.212	0.279	-0.372				
7L	0.007	-0.005	0.002	0	0.002	0.005	-0.007			
8L	0.335	-0.222	0.134	-0.108	0.109	-0.135	0.228	-0.336		
9L	0.324	-0.203	0.096	-0.045	0.002	-0.035	0.089	-0.194	0.318	
10L	0.318	-0.197	0.099	-0.06	0.044	-0.046	0.064	-0.103	0.202	-0.321
1L	0.409									C
2L	0.724	-0.723							Zr	iSe
3L	0.271	0.477	-0.584							
4L	0.688	-0.656	0.653	-0.658						
5L	0.022	-0.018	0	0.018	-0.022					
6L	0.684	-0.65	0.632	-0.632	0.649	-0.682	I 			
7L	0.658	-0.629	0.595	-0.595	0.51	-0.426	-0.297			
8L	0.679	-0.642	0.626	-0.622	0.622	-0.623	0.642	-0.677		
9L	0.658	-0.63	0.603	-0.609	0.597	-0.599	0.511	-0.426	-0.296	
10L	0.673	-0.637	0.619	-0.619	0.618	-0.619	0.621	-0.623	0.641	-0.675
1L	0.565								а	T
2L	0.985	-0.984	I	_					Zn	ı'l'e
3L	0.66	0.942	-0.948		-					
4L	0.98	-0.974	0.974	-0.98	L					
5L	0.662	0.94	-0.938	0.966	-0.965	I				
6L	0.981	-0.974	0.971	-0.972	0.973	-0.981				
7L	0.663	0.939	-0.936	0.962	-0.954	0.969	-0.97			
8L	0.98	-0.973	0.969	-0.97	0.97	-0.969	0.973	-0.98		
9L	0.668	0.942	-0.939	0.962	-0.955	0.964	-0.957	0.969	-0.968	
10L	0.978	-0.97	0.97	-0.969	0.969	-0.968	0.969	-0.969	0.969	-0.978

Table S6- Buckling distances (Δz in Å) of various thick 2D – ZnX (X=S, Se, Te) surface slabs.

This buckling distances is higher value of MTe case, owing to having high covalency.

Layer	1L	2L	3L	4L	5L	6L	7L	8L	9L	10L
1L	0.04									
2L	0.5	-0.5							C	dS
3L	0.429	0.348	-0.272							
4L	0.477	-0.444	0.446	-0.476						
5L	0.458	-0.392	0.074	0.364	-0.441					
6L	0.472	-0.44	0.421	-0.42	0.441	-0.473				
7L	0.461	-0.436	0.382	-0.343	0.082	0.401	-0.458			
8L	0.476	-0.443	0.427	-0.419	0.418	-0.423	0.439	-0.469		
9L	0.448	-0.392	0.029	0.359	-0.391	0.42	-0.42	0.444	-0.469	
10L	0.469	-0.438	0.422	-0.416	0.416	-0.417	0.416	-0.421	0.438	-0.469
1L	0.293									C.
2L	0.728	-0.727							Ca	Se
3L	-0.445	0.669	-0.682							
4L	0.711	-0.701	0.695	-0.712						
5L	-0.44	0.663	-0.663	0.705	-0.707	I 				
6L	0.712	-0.702	0.695	-0.699	0.707	-0.717		_		
7L	0.438	0.655	-0.658	0.695	-0.685	0.703	-0.703		_	
8L	0.711	-0.702	0.695	-0.693	0.696	-0.694	0.706	-0.713		
9L	-0.437	0.657	-0.66	0.695	-0.688	0.698	-0.696	0.705	0.704	
10L	0.719	-0.706	0.693	-0.694	0.698	-0.699	0.696	-0.692	0.7	-0.713
1L	0.46								-	
2L	0.95	-0.95	I	_					Cd	Те
3L	0.642	0.905	-0.898	I	_				<u> </u>	
4L	0.945	-0.943	0.943	-0.944	I	_				
5L	0.689	0.887	-0.878	0.908	-0.903	I	-			
6L	0.945	-0.945	0.945	-0.944	0.94	-0.941				
7L	0.649	0.918	-0.911	0.941	-0.935	0.941	-0.942			
8L	0.947	-0.944	0.942	-0.943	0.945	-0.944	0.941	-0.943		
9L	0.65	0.922	-0.913	0.936	-0.943	0.943	-0.935	0.943	-0.939	
10L	0.946	-0.944	0.945	-0.945	0.947	-0.945	0.945	-0.946	0.947	0.948

Table S7- Buckling distances (in Å) of various thick 2D– CdX (X=S, Se, Te) surface slabs.

This buckling distances is higher value of MTe case, owing to having high covalency,

We calculated the exfoliation energy (E_{exf}) to form *n* number of monolayers from respective surface slabs, with their thicknesses varying from 2L to 10L, from following equation.

$$E_{exf} = \frac{n * E_{1L} - E_{nL}}{n}$$

where E_{nL} is total energy of surface slab with thickness of nL, E_{1L} is the energy of the monolayer and *n* is the number of layer. Deduced E_{exf} values for 2D-MO and 2D-MX surface slabs are given in Fig. S5. It shows that thinner slabs are easier to exfoliate, as compared to thicker slabs.



Fig. S5: Calculated E_{exf} values for various thick (2L to 10L) 2D-MO and 2D-MX surface slabs are shown.



Fig. S6: DOS (a) and BS (b) of 3L (red line) and 4L (blue line) layered 2D- CdX surface slabs.



Fig. S7: DOS (a) and BS (b) of 10L thick WZ surface slab of MX compounds.

MX	Elas	stic Cons (N/m)	tants	Layer modulus	Young modulus	Poisson's ratio
	C ₁₁	C ₁₂	C ₆₆	(γ)	(N/m)	(v)
ZnO	124.4	79.09	22.66	90.43	74.139	0.636
ZnS	72.98	28.36	22.31	39.51	61.967	0.389
ZnSe	61.45	21.61	19.92	31.57	53.85	0.352
ZnTe	54.08	16.74	18.67	26.07	48.895	0.31
CdO	95.40	76.74	9.33	81.40	33.673	0.804
CdS	53.30	27.98	12.66	34.31	38.608	0.525
CdSe	42.93	19.38	11.77	25.27	34.178	0.452
CdTe	39.41	15.85	11.78	21.74	33.027	0.402

Table S7 : Elastic constants (C₁₁, C₁₂, C₂₂, C₆₆ in unit of N/m), layer modulus (γ , N/m), Young's modules (Y, N/m), Poisson's ratio (υ) of 2L 2D-MX compounds are given.

These following formulae are used to calculate mechanical properties mentioned in table as follows:

$$\gamma = \frac{1}{4} (c_{11} + c_{12} + 2c_{12})$$

$$Y = \frac{(C_{11}C_{22} - C_{12}C_{21})}{C_{22}}$$

$$v = \frac{c_{21}}{C_{22}}$$



Fig. S8: Occupied DOS of 2L ZnTe is shown, where different discrete peaks (a to e) are marked. The partial change density isosurface plots are plotted for those peaks and their side and top views are presented.

Despite of vdW driven interlayer interaction in 2D-MX surface slabs, the bonding nature within layer is explored by performing partial charge density diagrams for 2L ZnTe cases and they are shown in Fig. S5. Structurally, sp³ hybridized cations (M) are located in the centre of tetrahedra that is formed by X atoms. Each X atom interacts with three M atoms and holding one lone pair, forming trigonal pyramid shape with bond angle of 107° . It is also seen in the charge density diagrams, donut like shapes (mixing of p_x and p_y orbitals) that are presented in the both sides of bonding states (sp³ orbitals).

nL	ZnO	ZnS	ZnSe	ZnTe	CdO	CdS	CdSe	CdTe
1	1.66	2.61	1.91	1.694	0.83	1.68	1.33	1.31
2	1.41	2.66	1.85	1.01	0.55	1.87	1.61	1.11
3	1.28	1.54	0.62	0.06	0.39	1.60	0.66	0.00
4	1.20	2.34*	1.67	0.91	0.30	1.61*	1.28*	0.99
5	1.15	1.98	0.55	0.047	0.24	1.44*	0.85*	0.00
6	1.11	2.12*	1.55*	0.885	0.20	1.52*	1.09*	0.96
7	1.08	1.86	0.52	0.073	0.17	1.47	0.51	0.00
8	1.07	2.00*	1.46*	0.883	0.14	1.47*	0.98*	0.90
9	1.05	1.91	0.54	0.07	0.12	1.43*	0.47*	0.00
10	1.04	1.96*	1.40*	0.87	0.10	1.42*	0.90	0.88
∞L	0.94	1.81	1.29	0.93	0.00	1.25	0.74	1.06
WZ Bulk	0.76	2.28	1.40	1.36	0.00	1.23	0.67	0.78

Table S9: Band gap (in eV) of various thicknesses (nL) of 2D-MX surface slabs are shown, along with WZ bulk.

The band gap is calculated by deducing BS calculations. We observed direct band gap in all the cases. It is also noticed that indirect band gap value, in a few cases (* marked), is also lied closer to direct band gap.

nL		electron	(e_{e}^{*})			hole (e *)	
IIL	ZnO	ZnS	ZnSe	ZnTe	ZnO	ZnS	ZnSe	ZnTe
1	0.28	0.19	0.14	0.12	1.07	0.72	0.71	0.97
2	0.24	0.21	0.15	0.12	1.19	1.35	1.03	1.38
3	0.22	0.2	0.15	0.11	1.26	0.68	0.74	1
4	0.21	0.2	0.15	0.12	1.3	1.03	1.12	1.12
5	0.2	0.19	0.15	0.12	1.33	0.8	0.82	0.66
6	0.2	0.19	0.15	0.13	1.36	1.26	0.4	1.01
7	0.2	0.19	0.15	0.12	1.37	0.82	0.82	0.99
8	0.19	0.19	0.15	0.13	1.39	1.72	3.31	1.1
9	0.19	0.19	0.15	0.12	1.43	2.92	0.82	0.98
10	0.19	0.19	0.15	0.13	1.44	2.56	3.07	1.1

Table S10 (a): Effective mass (e^*) of various thicknesses of 2D-ZnX various surface slabs

Table S10 (b): Effective mass (e^*) of various thicknesses of 2D-CdX various surface slabs.

nĬ		electro	e_{e}^{*}			hole	(e_h^*)	
	CdO	CdS	CdSe	CdTe	CdO	CdS	CdSe	CdTe
1	0.2	0.16	0.14	0.13	0.53	0.65	0.69	0.67
2	0.17	0.12	0.19	0.13	0.76	1.13	0.89	0.93
3	0.16	0.16	0.14	0.13	1.31	0.86	0.89	0.99
4	0.16	0.18	0.16	0.14	1.41	0.89	2.66	1.22
5	0.16	0.16	0.13	0.14	1.87	0.91	0.75	1
6	0.17	0.17	0.15	0.16	1.4	1.49	0.28	1.26
7	0.18	0.17	0.15	0.13	1.4	1.06	0.89	1.01
8	0.19	0.2	0.14	0.13	1.92	1.21	0.8	1.69
9	0.21	0.18	0.14	0.13	1.72	1.28	0.9	1
10	0.22	0.19	0.13	0.13	1.64	1.41	1.58	1.54