**Supporting information**

**Synthesizability of transition-metal dichalcogenides: a systematic first-principles evaluation**

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**Figure S1. Energy levels of transition-metal d orbitals under the T and H coordinations.**



**Figure S2. Energy levels of Pyrite-type and PdS2-type polytypes.**

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**Figure S3. Definition of the out-of-center distortion (**$∆\_{d}$**) in TX6 octahedron.** $θ\_{1}$, $θ\_{2}$ and $θ\_{3}$ represents the angles of $X\_{1}-T-X\_{4}$, $X\_{2}-T-X\_{5}$ and $X\_{3}-T-X\_{6}$, respectively.

**Table S1. Reference table of thermodynamic stability of TMDs.** Detailed information of phases is listed in Table 1. All the Ehull are present in meV. All the ids are extracted from ICSD (Ehull data can also be obtained from Atomly).

| **Formula** | **Phase** | **Ehull** | **ID** |  | **Phase** | **Ehull** | **ID** |  | **Phase** | **Ehull** | **ID** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| TiS2 | 1T | 0 | 41663 | TiSe2 | 1T | 0 | 43617 | TiTe2 | 1T | 0 | 80092 |
| Spinel | 16 | 72042 | Spinel | 24 | — | MnS2 | 40 | — |
| MnS2 | 22 | 41092 | MnS2 | 27 | — | Spinel | 44 | — |
| ZrS2 | 1T | 0 | 56012 | ZrSe2 | 1T | 0 | 182676 | ZrTe2 | 1T | 0 | 657478 |
| Spinel | 10 | — | Spinel | 12 | — | Spinel | 30 | — |
| MnS2 | 21 | — | MnS2 | 27 | — | MnS2 | 41 | — |
| HfS2 | 1T | 0 | 638851 | HfSe2 | 1T | 0 | 638902 | HfTe2 | 1T | 0 | 638959 |
| Spinel | 11 | — | Spinel | 14 | — | Spinel | 30 | — |
| MnS2 | 21 | — | MnS2 | 26 | — | MnS2 | 41 | — |
| VS2 | 2Ha | 0 | — | VSe2 | 3R | 0 | — | VTe2 | TaTe2 | 0 | 38369 |
| 3R | 0.25 | — | 2Hc | 1.35 | — | 1T’ | 7 | — |
| 2Hc | 0.26 | — | 2Ha | 1.55 | — | Td | 15 | — |
| 4Ha | 0.59 | — | 4Ha | 1.63 | — | Marcasite | 16 | — |
| 4Hb | 4 | — | 4Hb | 4 | — | 4Hb | 28 | — |
| 1T | 12 | 86519 | TaTe2 | 6 | — | 3R | 28 | — |
| MnS2 | 32 | — | 1T | 11 | 86520 | 4Ha | 29 | — |
|  |  |  | MnS2 | 35 | — | 2Ha | 29 | — |
|  |  |  | 1T’ | 47 | — | 1T | 30 | 603582 |
|  |  |  |  |  |  | 2Hc | 31 | — |
|  |  |  |  |  |  | Pyrite | 46 | — |
|  |  |  |  |  |  | RhSe2 | 48 | — |
| NbS2 | 2Ha | 10 | 43697 | NbSe2 | 2Ha | 0 | 16304 | NbTe2 | TaTe2 | 0 | 14389 |
| 4Ha | 12 | — | 4Ha | 3 | [] | 2Ha | 22 | — |
| 3R | 15 | 43696 | 3R | 5 | 18131 | 4Ha | 25 | — |
| 4Hb | 18 | — | 4Hb | 6 | 645379 | 4Hb | 26 | — |
| 2Hc | 18 | — | 2Hc | 10 | 82570 | 1T’ | 28 | — |
| 1T | 41 | 40706 | TaTe2 | 20 | — | Td | 29 | — |
| TaTe2 | 42 | — | 1T | 26 | 76576 | 3R | 30 | — |
|  |  |  |  |  |  | 2Hc | 38 | — |
|  |  |  |  |  |  | 1T | 44 | 645529 |
| TaS2 | 2Ha | 0 | 68488 | TaSe2 | 4Hb | 0 | 18133 | TaTe2 | TaTe2 | 0 | 86141 |
| 4Hb | 0.6 | — | 2Ha | 0 | 651950 | 1T’ | 15 | — |
| 4Ha | 0.7 | — | 3R | 0.5 | 24315 | Td | 16 | — |
| 3R | 1 | 43410 | 4Ha | 2 | 26249 | 4Hb | 39 | — |
| 2Hc | 3 | — | 2Hc | 3 | 651956 | 2Ha | 42 | — |
| TaTe2 | 16 | — | TaTe2 | 8 | — | 4Ha | 44 | — |
| 1T | 17 | 52115 | 1T | 15 | 24313 | 3R | 46 | — |
| MnS2 | 40 | 651086 | MnS2 | 44 | 651954 | 2Hc | 50 | — |
| Spinel | 45 | — |  |  |  | 1T | 50 | — |
| CrS2 | Marcasite | 0 | — | CrSe2 | Marcasite | 0 | — | CrTe2 | Marcasite | 0 | — |
| 2Hc | 3 | — | 1T | 27 | 626718 | 1T | 6 | — |
| 3R | 4 | — | RhSe2 | 29 | — | RhSe2 | 19 | — |
|  | 4Ha | 6 | — |  | Pyrite | 47 | — |  | Pyrite | 37 | — |
| 2Ha | 8 | — | 2Hc | 48 | — | Spinel | 44 | — |
|  |  |  | 3R | 50 | — |  |  |  |
| MoS2 | 2Hc | 0 | 24000 | MoSe2 | 2Hc | 0 | 49800 | MoTe2 | 2Hc | 0 | 15431 |
| 3R | 0 | 43560 | 3R | 1 | 16948 | 3R | 4 | — |
| 4Ha | 2 | — | 4Ha | 4 | — | 4Ha | 9 | — |
| 2Ha | 5 | 644259 | 2Ha | 7 | 644346 | 2Ha | 14 | — |
|  |  |  |  |  |  | 1T’ | 18 | 14349 |
|  |  |  |  |  |  | Td | 18 | — |
| WS2 | 2Hc | 0 | 56014 | WSe2 | 2Hc | 0 | 40752 | WTe2 | 1T’ | 0 | — |
| 3R | 1 | 202367 | 3R | 2 | — | Td | 0 | 14348 |
| 4Ha | 3 | — | 4Ha | 5 | — | 2Hc | 20 | 653170 |
| 2Ha | 8 | — | 2Ha | 9 | — | 3R | 25 | — |
|  |  |  |  |  |  | 4Ha | 31 | — |
|  |  |  |  |  |  | 2Ha | 36 | — |
| MnS2 | Marcasite | 0 | 643441 | MnSe2 | 1T | 0 | — | MnTe2 | Spinel | 23 | — |
| 1T | 35 | — | Spinel | 2 | — | 4Hb | 42 | — |
| Spinel | 37 | — | MnS2 | 15 | — | Marcasite | 46 | — |
| ReS2 | 38 | — | Marcasite | 20 | — | RhSe2 | 47 | — |
| MnS2 | 48 | — | RhSe2 | 23 | — |  |  |  |
| 1T’ | 49 | — | 1T’ | 35 | — |  |  |  |
| Td | 49 | — | Td | 35 | — |  |  |  |
|  |  |  | ReS2 | 39 | — |  |  |  |
|  |  |  | 4Hb | 40 | — |  |  |  |
| TcS2 | ReS2 | 0 | 81816 | TcSe2 | ReS2 | 0 | — | TcTe2 | ReS2 | 0 | — |
| ReS2 | ReS2 | 0 | 75459 | ReSe2 | ReS2 | 0 | 26256 | ReTe2 | ReS2 | 0 | — |
| FeS2 | Marcasite | 0 | 26756 | FeSe2 | Marcasite | 0 | 25680 | FeTe2 | Marcasite | 0 | 25679 |
| Pyrite | 4 | 10422 | Pyrite | 17 | 633475 | Pyrite | 32 | 633869 |
| RuS2 | Pyrite | 8 | 24186 | RuSe2 | Pyrite | 0 | 24201 | RuTe2 | Pyrite | 4 | 24188 |
| Marcasite | 42 | — | Marcasite | 27 | — | Marcasite | 15 | 106001 |
| OsS2 | Pyrite | 1 | 300224 | OsSe2 | Pyrite | 2 | 24202 | OsTe2 | Pyrite | 4 | 24189 |
| Marcasite | 32 | — | Marcasite | 23 | — | Marcasite | 13 | — |
| CoS2 | Pyrite | 2 | 43715 | CoSe2 | RhSe2 | 0 | — | CoTe2 | RhSe2 | 2 | — |
| Marcasite | 12 | — | Marcasite | 7 | 42540 | Pyrite | 5 | 625403 |
| RhSe2 | 13 | — | Pyrite | 9 | 42539 | 1T | 8 | 625401 |
|  |  |  | 1T | 46 | — | Marcasite | 9 | 42728 |
| RhS2 | RhSe2 | 0 | — | RhSe2 | RhSe2 | 0 | 650286 | RhTe2 | Pyrite | 6 | 2179 |
| Pyrite | 40 | 105914 | Pyrite | 9 | 44868 | RhSe2 | 23 | — |
|  |  |  | Marcasite | 28 | — | Marcasite | 39 | — |
| IrS2 | RhSe2 | 0 | 80568 | IrSe2 | RhSe2 | 0 | 16728 | IrTe2 | RhSe2 | 0 | 93896 |
|  |  |  |  |  |  | 1T | 21 | 93891 |
|  |  |  |  |  |  | Pyrite | 37 | 641087 |
| NiS2 | Pyrite | 16 | 40328 | NiSe2 | 1T | 0 | — | NiTe2 | 1T | 0 | 42559 |
| Marcasite | 20 | 169570 | Pyrite | 11 | 40330 | Pyrite | 27 | 646897 |
|  |  |  | Marcasite | 18 | 5071 | Marcasite | 46 | — |
|  |  |  | RhSe2 | 27 | — | RhSe2 | 50 | — |
|  |  |  | MnS2 | 46 | — |  |  |  |
| PdS2 | PdS2- | 0 | 16694 | PdSe2 | 1T | 0 | — | PdTe2 | 1T | 0 | 42555 |
| Marcasite- | 44 | — | Pyrite- | 20 | — | Pyrite- | 38 | — |
|  |  |  | PdS2- | 23 | 16693 |  |  |  |
|  |  |  | Marcasite- | 38 | — |  |  |  |
| PtS2 | 1T | 0 | 41375 | PtSe2 | 1T | 0 | 41374 | PtTe2 | 1T | 0 | 105813 |
| Spinel | 45 | — |  |  |  |  |  |  |

**Table S2. Reference table of relative energy of single-layer TMDs.** Detailed information of phases is listed in Table 2. All the ΔE are present in meV (energy data can also be obtained from Atomly).

| **Formula** | **Phase** | **ΔE (meV/atom)** | **Formula** | **Phase** | **ΔE (meV/atom)** | **Formula** | **Phase** | **ΔE (meV/atom)** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| TiS2 | ML-T | 0 | CrS2 | ML-H | 0 | RuTe2 | ML-T’ | 0 |
| TiSe2 | ML-T | 0 | CrSe2 | ML-H | 0 | ML-ReS2 | 3 |
| TiTe2 | ML-T | 0 | ML-TaTe2 | 43 | OsS2 | ML-T’ | 0 |
| ZrS2 | ML-T | 0 | CrTe2 | ML-TaTe2 | 0 | ML-ReS2 | 25 |
| ZrSe2 | ML-T | 0 | ML-T’ | 18 | OsSe2 | ML-T’ | 0 |
| ZrTe2 | ML-T | 0 | ML-T | 23 | ML-ReS2 | 18 |
| HfS2 | ML-T | 0 | MoS2 | ML-H | 0 | OsTe2 | ML-T’ | 0 |
| HfSe2 | ML-T | 0 | MoSe2 | ML-H | 0 | ML-ReS2 | 9 |
| HfTe2 | ML-T | 0 | MoTe2 | ML-H | 0 | CoS2 | ML-TaTe2 | 0 |
| VS2 | ML-H | 0 | ML-T’ | 14 | ML-T | 3 |
| ML-T | 14 | WS2 | ML-H | 0 | CoSe2 | ML-T | 0 |
| VSe2 | ML-H | 0 | WSe2 | ML-H | 0 | CoTe2 | ML-T | 0 |
| ML-T | 15 | WTe2 | ML-T’ | 0 | RhS2 | ML-T’ | 0 |
| VTe2 | ML-T’ | 0 | ML-H | 30 | ML-TaTe2 | 33 |
| ML-TaTe2 | 4 | MnS2 | ML-ReS2 | 0 | ML-T | 42 |
| ML-T | 6 | ML-T | 3 | RhSe2 | ML-T’ | 0 |
| ML-H | 6 | ML-T’ | 25 | ML-TaTe2 | 23 |
| NbS2 | ML-H | 0 | MnSe2 | ML-T | 0 | ML-T | 28 |
| ML-TaTe2 | 36 | ML-T’ | 42 | RhTe2 | ML-T | 0 |
| ML-T | 37 | MnTe2 | ML-T | 0 | IrS2 | ML-T’ | 0 |
| NbSe2 | ML-H | 0 | TcS2 | ML-ReS2 | 0 | ML-T | 31 |
| ML-TaTe2 | 26 | TcSe2 | ML-ReS2 | 0 | IrSe2 | ML-T’ | 0 |
| ML-T | 27 | TcTe2 | ML-ReS2 | 0 | ML-TaTe2 | 31 |
| NbTe2 | ML-TaTe2 | 0 | ReS2 | ML-ReS2 | 0 | ML-T | 36 |
| ML-H | 16 | ReSe2 | ML-ReS2 | 0 | IrTe2 | ML-T | 0 |
| ML-T | 21 | ReTe2 | ML-ReS2 | 0 | NiS2 | ML-PdS2 | 0 |
| ML-T’ | 28 | FeS2 | ML-T’ | 0 | ML-T | 7 |
| TaS2 | ML-H | 0 | FeSe2 | ML-T’ | 0 | NiSe2 | ML-T | 0 |
| ML-TaTe2 | 20 | FeTe2 | ML-ReS2 | 0 | NiTe2 | ML-T | 0 |
| ML-T | 23 | ML-T’ | 12 | PdS2 | ML-PdS2 | 0 |
| TaSe2 | ML-H | 0 | ML-TaTe2 | 40 | PdSe2 | ML-T | 0 |
| ML-TaTe2 | 15 | ML-T | 46 | ML-PdS2 | 23 |
| ML-T | 22 | ML-H | 49 | PdTe2 | ML-T | 0 |
| TaTe2 | ML-TaTe2 | 0 | RuS2 | ML-T’ | 0 | PtS2 | ML-T | 0 |
| ML-H | 34 | ML-ReS2 | 18 | PtSe2 | ML-T | 0 |
| ML-T | 34 | RuSe2 | ML-T’ | 0 | PtTe2 | ML-T | 0 |
| ML-T’ | 41 | ML-ReS2 | 11 |  |  |

**Table S3. The compound list of the 2D TMDs that have been experimentally discovered.** The ΔE and the phonon stability (from C2DB [47, 48]) are provided for comparison.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Formula** | **Phase** | **ΔE (meV/atom)** | **Phonon stability** | **Synthesized** |
| TiS2 | ML-T | 0 | N | [1] |
| TiSe2 | ML-T | 0 | N | [2] |
| TiTe2 | ML-T | 0 | Y | [3] |
| ZrS2 | ML-T | 0 | Y | [4] |
| ZrSe2 | ML-T | 0 | Y | [5] |
| ZrTe2 | ML-T | 0 | Y | [6] |
| HfS2 | ML-T | 0 | Y | [7] |
| HfSe2 | ML-T | 0 | Y | [8] |
| HfTe2 | ML-T | 0 | Y | [9] |
| VS2 | ML-T | 14 | Y | [10] |
| VSe2 | ML-T | 15 | Y | [11] |
| VTe2 | ML-T | 6 | N | [12] |
| ML-H | 6 | Y | [13] |
| NbS2 | ML-H | 0 | N | [14] |
| ML-T | 37 | Y | [15] |
| NbSe2 | ML-H | 0 | Y | [16] |
| ML-T | 27 | Y | [17] |
| NbTe2 | ML-T | 21 | Y | [18] |
| TaS2 | ML-H | 0 | Y | [19] |
| ML-T | 23 | Y | [20] |
| TaSe2 | ML-H | 0 | N | [21] |
| ML-T | 22 | Y | [21] |
| TaTe2 | ML-TaTe2 | 0 | Y | [22] |
| ML-H | 34 | N | [23] |
| ML-T | 34 | Y | [24] |
| CrTe2 | ML-T | 23 | N | [25] |
| MoS2 | ML-H | 0 | Y | [26] |
| MoSe2 | ML-H | 0 | Y | [27] |
| MoTe2 | ML-H | 0 | Y | [28] |
| ML-T’ | 14 | Y | [29] |
| WS2 | ML-H | 0 | Y | [30] |
| WSe2 | ML-H | 0 | Y | [27] |
| WTe2 | ML-T’ | 0 | Y | [31] |
| ML-H | 30 | Y | [32] |
| MnSe2 | ML-T | 0 | Y | [33] |
| MnTe2 | ML-T | 0 | Y | [34] |
| ReS2 | ML-ReS2 | 0 | Y | [35] |
| ReSe2 | ML-ReS2 | 0 | Y | [36] |
| FeTe2 | ML-T | 46 | N | [37] |
| ML-H | 49 | Y | [37] |
| CoS2 | ML-T | 3 | N | [38] |
| CoSe2 | ML-T | 0 | N | [39] |
| CoTe2 | ML-T | 0 | N | [39] |
| NiS2 | ML-T | 7 | Y | [40] |
| NiSe2 | ML-T | 0 | Y | [41] |
| NiTe2 | ML-T | 0 | Y | [42] |
| PdSe2 | ML-PdS2 | 23 | Y | [43] |
| PdTe2 | ML-T | 0 | Y | [44] |
| PtS2 | ML-T | 0 | Y | [45] |
| PtSe2 | ML-T | 0 | Y | [46] |
| PtTe2 | ML-T | 0 | Y | [44] |

**Table S4. Reference table of exfoliability of TMDs.** Detailed information of phases is listed in Table 1. All the Eexf and Ehull are present in meV (Ehull data can also be obtained from Atomly).

|  |
| --- |
| **Easily Exfoliable** |
| **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** |
| TiS2 | 1T | 85 | 0 | VSe2 | 3R | 90 | 0 | MoSe2 | 2Hc | 96 | 0 |
| MnS2 | 63 | 22 | 2Hc | 89 | 1.3 | 3R | 95 | 1 |
| TiSe2 | 1T | 99 | 0 | 2Ha | 89 | 1.5 | 4Ha | 92 | 4 |
| MnS2 | 71 | 27 | 4Ha | 89 | 1.6 | 2Ha | 89 | 7 |
| TiTe2 | MnS2 | 77 | 40 | 4Hb | 93 | 5 | MoTe2 | 2Ha | 98 | 14 |
| ZrS2 | 1T | 81 | 0 | TaTe2 | 98 | 7 | WS2 | 2Hc | 86 | 0 |
| MnS2 | 60 | 21 | 1T | 93 | 12 | 3R | 85 | 1 |
| ZrSe2 | 1T | 94 | 0 | MnS2 | 70 | 35 | 4Ha | 83 | 3 |
| MnS2 | 67 | 27 | 1T’ | 57 | 47 | 2Ha | 81 | 6 |
| ZrTe2 | MnS2 | 76 | 41 | TaS2 | 2Ha | 94 | 0 | WSe2 | 4Ha | 99 | 5 |
| HfS2 | 1T | 81 | 0 | 4Ha | 93 | 0.7 |  | 2Ha | 95 | 8 |
| MnS2 | 60 | 21 | 3R | 93 | 1 | MnS2 | 1T | 60 | 35 |
| HfSe2 | 1T | 93 | 0 | 2Hc | 91 | 3 | ReS2 | 54 | 38 |
| MnS2 | 66 | 27 | TaTe2 | 98 | 16 | MnS2 | 47 | 48 |
| HfTe2 | MnS2 | 77 | 41 | MnS2 | 77 | 40 | 1T’ | 68 | 49 |
| VS2 | 2Ha | 82 | 0 | TaSe2 | MnS2 | 83 | 44 | Td | 68 | 49 |
| 3R | 82 | 0.2 | CrS2 | 2Hc | 71 | 3 | MnSe2 | 1T | 71 | 0 |
| 2Hc | 82 | 0.2 | 3R | 70 | 4 | MnS2 | 56 | 15 |
| 4Ha | 81 | 0.6 | 4Ha | 68 | 5 | 1T’ | 79 | 35 |
| 4Hb | 85 | 4 | 2Ha | 66 | 7 | Td | 78 | 35 |
| 1T | 84 | 12 | CrSe2 | 2Hc | 83 | 49 | ReS2 | 32 | 39 |
| MnS2 | 64 | 32 | 3R | 82 | 50 | 4Hb | 94 | 40 |
| NbS2 | 2Ha | 99 | 11 | MoS2 | 2Hc | 84 | 0 | TcS2 | ReS2 | 76 | 0 |
| 4Ha | 97 | 13 | 3R | 84 | 0 | TcSe2 | ReS2 | 89 | 0 |
| 3R | 95 | 15 | 4Ha | 81 | 2 | ReS2 | ReS2 | 78 | 0 |
| 2Hc | 91 | 18 | 2Ha | 79 | 5 | ReSe2 | ReS2 | 95 | 0 |
| **Feasibly Exfoliable** |
| **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** |
| TiTe2 | 1T | 117 | 0 | NbTe2 | 1T | 125 | 44 | MoTe2 | 4Ha | 103 | 9 |
| 4Hb | 124 | 46 | 2Hc | 127 | 38 | Td | 107 | 19 |
| ZrTe2 | 1T | 117 | 0 | 3R | 135 | 30 | 1T’ | 107 | 18 |
| 4Hb | 120 | 48 | 4Ha | 139 | 25 | 3R | 107 | 4 |
| HfTe2 | 1T | 118 | 0 | 4Hb | 140 | 26 | 2Hc | 112 | 0 |
| VTe2 | 2Hc | 112 | 31 | 2Ha | 143 | 22 | WSe2 | 3R | 102 | 2 |
| 1T | 112 | 31 | Td | 147 | 29 | 2Hc | 104 | 0 |
| 2Ha | 113 | 30 | 1T’ | 147 | 29 | TaTe2 | 3R | 134 | 46 |
| 4Ha | 113 | 30 | TaTe2 | 148 | 0 | 4Ha | 136 | 44 |
| 3R | 115 | 28 | TaS2 | 1T | 100 | 17 | 2Ha | 138 | 42 |
| 4Hb | 115 | 28 | 4Hb | 105 | 0.6 | 4Hb | 141 | 39 |
|  | Td | 121 | 16 |  | 2Hc | 102 | 3 |  | TaTe2 | 147 | 0 |
| 1T’ | 130 | 7 | 4Ha | 103 | 2 | 4Ha | 103 | 9 |
| TaTe2 | 141 | 0 | TaSe2 | 3R | 105 | 0.4 | MoTe2 | Td | 107 | 19 |
| NbS2 | TaTe2 | 104 | 42 | 2Ha | 105 | 0 | 1T’ | 107 | 18 |
| 1T | 106 | 41 | 1T | 112 | 15 | 3R | 107 | 4 |
| 4Hb | 110 | 18 | TaTe2 | 113 | 8 | 2Hc | 112 | 0 |
| NbSe2 | 2Hc | 106 | 10 | 4Hb | 117 | 0 | WSe2 | 3R | 102 | 2 |
| 3R | 111 | 5 | TaTe2 | 3R | 134 | 46 | 2Hc | 104 | 0 |
| 4Ha | 113 | 3 | 4Ha | 136 | 44 | TaTe2 | 3R | 134 | 46 |
| 2Ha | 116 | 0 | 2Ha | 138 | 42 | 4Ha | 136 | 44 |
| 1T | 118 | 26 | 4Hb | 141 | 39 | MoTe2 | 4Ha | 103 | 9 |
| TaTe2 | 122 | 20 | TaTe2 | 147 | 0 | Td | 107 | 19 |
| 4Hb | 123 | 6 |  |  |  | WSe2 | 3R | 102 | 2 |
|  |  |  |  |  |  | 2Hc | 104 | 0 |
| **Possibly Exfoliable** |
| **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** | **Formula** | **Phase** | **Eexf (meV)** | **Ehull (meV)** |
| TiS2 | 4Hb | 84 | 72 | TaTe2 | 2Hc | 130 | 50 | MnS2 | 4Hb | 43 | 95 |
| TiSe2 | 4Hb | 99 | 58 | 1T | 130 | 51 | MnTe2 | MnS2 | 78 | 56 |
| TiTe2 | 2Ha | 125 | 96 | MnS2 | 90 | 90 | 2Ha | 132 | 83 |
| 4Ha | 122 | 100 | CrS2 | 4Hb | 95 | 96 | 3R | 128 | 87 |
| ZrS2 | 4Hb | 75 | 98 | CrSe2 | 4Ha | 79 | 52 | 2Hc | 127 | 88 |
| ZrSe2 | 4Hb | 90 | 76 | 2Ha | 77 | 54 | TcS2 | 1T’ | 78 | 86 |
| ZrTe2 | 2Ha | 120 | 99 | CrTe2 | MnS2 | 95 | 63 | Td | 77 | 88 |
| HfSe2 | 4Hb | 89 | 91 | 4Hb | 142 | 75 | TcSe2 | 1T’ | 90 | 92 |
| HfTe2 | 4Hb | 121 | 62 | TaTe2 | 54 | 81 | Td | 89 | 93 |
| VTe2 | MnS2 | 80 | 63 | MoTe2 | 4Hb | 98 | 95 | TcTe2 | 1T’ | 111 | 84 |
| NbS2 | MnS2 | 78 | 69 | TaTe2 | 103 | 96 | Td | 111 | 84 |
| NbSe2 | MnS2 | 84 | 59 | WSe2 | Td | 99 | 100 | ReS2 | 1T’ | 78 | 95 |
| NbTe2 | MnS2 | 83 | 86 | 1T’ | 99 | 100 | Td | 78 | 95 |

Structural distortions in TMDs

Structural distortions may have a great impact on both the electronic states and the stable configurations of materials. Therefore, we made statistics on the structural distortions in TMDs, as shown in Table S4. Here, we chose two quantities to describe the distortions, namely the out-of-center distortion (labeled by $Δ\_{d}$) and the ratio of the shortest and longest T-X bond lengths (labeled by $R\_{l}$) [49, 50]. $Δ\_{d}$ and $R\_{l}$ are calculated as follows:

$∆\_{d}=\frac{|L\_{T-X\_{1}}-L\_{T-X\_{4}}|}{|\cos(θ\_{1})|}+\frac{|L\_{T-X\_{2}}-L\_{T-X\_{5}}|}{|\cos(θ\_{2})|}+\frac{|L\_{T-X\_{3}}-L\_{T-X\_{6}}|}{|\cos(θ\_{3})|}$ (1)

$R\_{l}=\frac{L\_{min}}{L\_{max}}$ (2)

$Δ\_{d}$ quantifies the magnitude of the out-of-center distortion (the specific meaning of the symbols in Equation (1) is shown in Fig. S3), and a nonzero value can be obtained if the transition metal deviates from its octahedral site. $R\_{l}$ refers to the ratio of the shortest and longest bond lengths among the six T-X bonds in one octahedron. It can represent not only the uneven degree of bond lengths, but also the strength of the metal-metal bonding [49].

**Table S5. Reference table of structural distortions of TMDs.** Detailed information of phases is listed in Table 1. There are two types: NL and L represent non-layered and layered, respectively (structural data can also be obtained from Atomly).

| **Formula** | **Phase** | $$Δ\_{d}$$ | $$R\_{l}$$ | **Type** | **Formula** | **Phase** | $$Δ\_{d}$$ | $$R\_{l}$$ | **Type** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| TiS2 | RhSe2 | 0.247 | 0.931 | NL | MoTe2 | 1T’ | 0.324 | 0.962 | L |
| Marcasite | 0 | 0.951 | NL | Td | 0.335 | 0.961 | L |
| TiSe2 | RhSe2 | 0.248 | 0.938 | NL | TaTe2 | 0.471 | 0.923 | L |
| TiTe2 | RhSe2 | 0.159 | 0.955 | NL | WSe2 | Td | 0.295 | 0.956 | L |
| Marcasite | 0 | 0.973 | NL | 1T’ | 0.295 | 0.957 | L |
| ZrS2 | RhSe2 | 0.141 | 0.961 | NL | WTe2 | 1T’ | 0.332 | 0.961 | L |
| Marcasite | 0 | 0.967 | NL | Td | 0.337 | 0.961 | L |
| ZrSe2 | RhSe2 | 0.187 | 0.955 | NL | MnS2 | Marcasite | 0 | 0.987 | NL |
| ZrTe2 | RhSe2 | 0.172 | 0.962 | NL | ReS2 | 0.397 | 0.916 | L |
| HfS2 | RhSe2 | 0.121 | 0.965 | NL | 1T’ | 0.256 | 0.927 | L |
| Marcasite | 0 | 0.969 | NL | Td | 0.266 | 0.925 | L |
| HfSe2 | RhSe2 | 0.175 | 0.956 | NL | RhSe2 | 0.093 | 0.980 | NL |
| HfTe2 | RhSe2 | 0.175 | 0.962 | NL | MnSe2 | Marcasite | 0 | 0.975 | NL |
| VS2 | Marcasite | 0 | 0.983 | NL | RhSe2 | 0.08 | 0.959 | NL |
| RhSe2 | 0.178 | 0.936 | NL | 1T’ | 0.29 | 0.928 | L |
| VSe2 | TaTe2 | 0.424 | 0.912 | L | Td | 0.296 | 0.926 | L |
| 1T’ | 0.279 | 0.943 | L | ReS2 | 0.424 | 0.919 | L |
| Marcasite | 0 | 0.986 | NL | MnTe2 | Marcasite | 0 | 0.985 | NL |
| RhSe2 | 0.152 | 0.948 | NL | RhSe2 | 0.096 | 0.976 | NL |
| VTe2 | TaTe2 | 0.451 | 0.919 | L | TcS2 | ReS2 | 0.395 | 0.916 | L |
| 1T’ | 0.295 | 0.945 | L | Marcasite | 0 | 0.986 | NL |
| Td | 0.189 | 0.958 | L | 1T’ | 0.235 | 0.935 | L |
| RhSe2 | 0.098 | 0.972 | NL | Td | 0.225 | 0.935 | L |
| NbS2 | TaTe2 | 0.163 | 0.954 | L | TcSe2 | ReS2 | 0.406 | 0.921 | L |
| NbSe2 | TaTe2 | 0.321 | 0.922 | L | 1T’ | 0.29 | 0.94 | L |
| NbTe2 | TaTe2 | 0.448 | 0.924 | L | Td | 0.262 | 0.94 | L |
| 1T’ | 0.251 | 0.955 | L | TcTe2 | ReS2 | 0.41 | 0.929 | L |
| Td | 0.265 | 0.951 | L | 1T’ | 0.275 | 0.943 | L |
| RhSe2 | 0.329 | 0.942 | NL | Td | 0.268 | 0.941 | L |
| TaS2 | TaTe2 | 0.168 | 0.952 | L | Marcasite | 0 | 0.984 | NL |
| RhSe2 | 0.226 | 0.926 | NL | ReS2 | ReS2 | 0.345 | 0.924 | L |
| TaSe2 | TaTe2 | 0.294 | 0.926 | L | 1T’ | 0.202 | 0.941 | L |
| TaTe2 | TaTe2 | 0.439 | 0.921 | L | Td | 0.203 | 0.942 | L |
| 1T’ | 0.145 | 0.954 | L | ReSe2 | ReS2 | 0.369 | 0.926 | L |
| Td | 0.147 | 0.953 | L | ReTe2 | ReS2 | 0.397 | 0.93 | L |
| CrS2 | RhSe2 | 0.094 | 0.973 | NL | FeS2 | RhSe2 | 0.088 | 0.982 | NL |
| CrSe2 | RhSe2 | 0.082 | 0.979 | NL | FeSe2 | RhSe2 | 0.072 | 0.979 | NL |
| CrTe2 | RhSe2 | 0.088 | 0.982 | NL | FeTe2 | RhSe2 | 0.152 | 0.972 | NL |
| TaTe2 | 0.097 | 0.981 | L | NiS2 | Marcasite | 0 | 0.982 | NL |
| OsSe2 | 1T’ | 0.195 | 0.932 | L | RhSe2 | 0.1 | 0.962 | NL |
| Td | 0.189 | 0.932 | L | NiSe2 | Marcasite | 0 | 0.985 | NL |
| CoS2 | Marcasite | 0 | 0.985 | NL | RhSe2 | 0.119 | 0.949 | NL |
|  | RhSe2 | 0.112 | 0.959 | NL | NiTe2 | Marcasite | 0 | 0.988 | NL |
| CoSe2 | RhSe2 | 0.146 | 0.971 | NL | RhSe2 | 0.161 | 0.963 | NL |
| CoTe2 | RhSe2 | 0.199 | 0.962 | NL | PdS2 | PdS2 | 0 | 0.728 | L |
| RhS2 | RhSe2 | 0.144 | 0.951 | NL | Marcasite | 0 | 0.954 | NL |
| RhSe2 | RhSe2 | 0.152 | 0.970 | NL | PdSe2 | PdS2 | 0 | 0.83 | L |
| RhTe2 | RhSe2 | 0.201 | 0.965 | NL | RhSe2 | 0.052 | 0.873 | NL |
| IrS2 | RhSe2 | 0.224 | 0.958 | NL | PdTe2 | RhSe2 | 0.138 | 0.967 | NL |
| IrSe2 | RhSe2 | 0.214 | 0.963 | NL | PtS2 | PdS2 | 0 | 0.676 | L |
| IrTe2 | RhSe2 | 0.208 | 0.964 | NL |  |  |  |  |

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