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Developing New 2D Materials and Heterostructures for Printed Digital Devices

2D-PRINTABLE - Deliverable report

D1.2 - Van der Waals DFT screening

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Project Scientific Abstract

The 2D-PRINTABLE project aims to integrate sustainable large-scale liquid exfoliation techniques with theoretical modelling to efficiently produce a wide range of new 2D materials (2DMs), including conducting, semiconducting, and insulating nanosheets. The focus includes developing the printing and liquid-phase deposition methods required to fabricate networks and multicomponent heterostructures, featuring layer-by-layer assembly of nanometer-thick 2DMs into ordered multilayers. The goal is to optimize these printed networks and heterostructures for digital systems, unlocking new properties and functionalities. The project also seeks to demonstrate various printed digital devices, including proof-of-principle, first-time demonstration of all-printed, all-nanosheet, heterostack light-emitting diodes (LEDs). In conclusion, 2D-PRINTABLE will prove 2D materials to be an indispensable material class in the field of printed electronics, capable of producing far-beyond-state-of-the-art devices that can act as a platform for the next generation of printed digital applications.

Public summary

We curated a database of novel 2D materials (2DMs) (https://www.materialscloud.org/discover/mc2d/) that can be exfoliated from known inorganic compounds and that now counts over 3,000 candidates.

The database has been created using high-throughput, van der Waals density functional theory (DFT) calculations to find layered three-dimensional (3D) materials that can be easily exfoliated into 2DMs.

The source databases are the Inorganic Crystal Structure Database (ICSD), the Crystallography Open Database (COD), and the Pauling File (MPDS). Overall, we considered 9,306 layered candidates, first performing a geometrical screening to allow a further selection of candidate materials, for which full first-principles calculations were performed.

This portfolio of novel monolayers will empower the search for novel materials for the 2D-Printable project, with outstanding electronic or optical properties.

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Abbreviations & Definitions

Abbreviation	Explanation
2DM	Two-dimensional materials
DFT	Density-functional theory
MC2D	Materials Cloud 2-dimensional Database
Van der Waals	vdW

[1] https://open-research-europe.ec.europa.eu/for-authors/data-guidelines#approvedrepositories

1 Introduction

2DM provide novel opportunities to venture into largely unexplored regions of the materials properties space. On one hand, their ultimate thinness makes them extremely promising for applications in electronics (from field-effect transistors, where a reduced device size is beneficial to improve performance and reduce short-channel effects between contacts, to optoelectronics). On the other hand, the physical properties of monolayers often change dramatically from those of parent 3D materials, providing a new degree of freedom in the applications (from light-emission to spin manipulation) while also unveiling novel physics. Moreover, vdW heterostructures have recently emerged as an additional avenue to engineer novel properties by stacking 2DM in a specifically designed fashion.

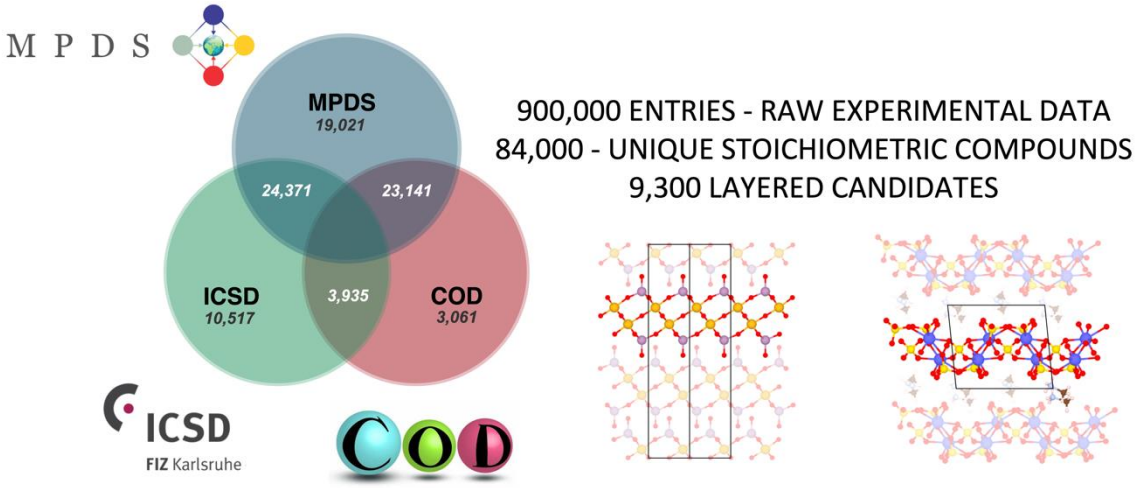

Fig. 1: out of ~900,000 experimentally known compounds, ~84,000 are stoichiometric and unique, and ~9,300 appear layered.

To date only a few dozens of 2DMs have been experimentally synthesised or exfoliated from 3D counterparts. Progress in this area will be strongly accelerated by the availability of a broader portfolio of potential realistic 2DM. To illustrate this point, we can compare the current situation for known 3D crystals, for which the knowledge accumulated in the past century (both the crystal structure and the measured physical properties) has been collected in databases such as the Pauling file, the Inorganic Crystal Structure Database or the Crystallographic Open Database (these, combined, contain to date close to a million entries) (Fig. 1). So, here we present a curated database of novel 2DMs that can be exfoliated from experimentally known inorganic compounds. In our search, we start from geometric and bonding criteria to identify layered materials among the 3D compounds contained in the experimental databases, independently of the layers' shape, crystallographic orientation or embedding. We then use first-principles vdW DFT simulations to validate these results. In particular, we compute the binding energy of all prospective layered structures and identify those that are held together by weak interactions and ready for mechanical or liquid-phase exfoliation, or, alternatively, directed growth.

2 Methods and core part of the report

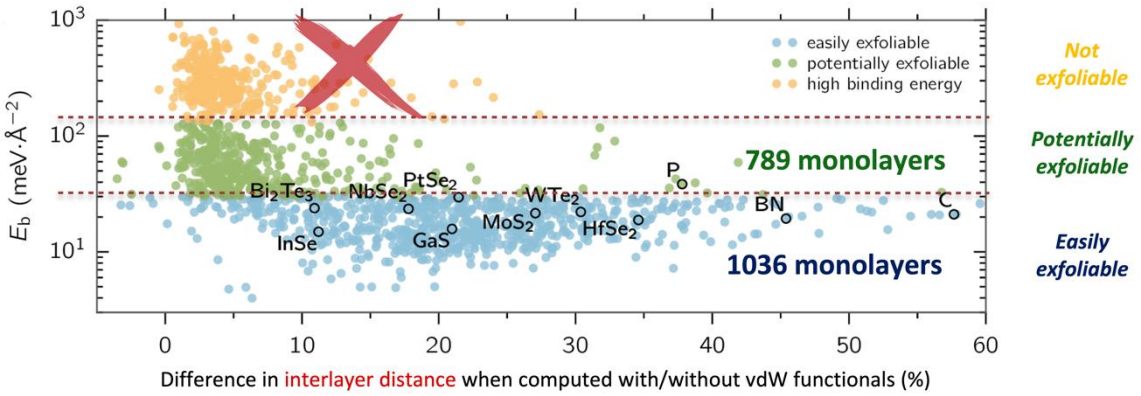

Fig. 2: the calculation of binding energies (vertical axis) and van der Waals character (horizontal axis) allow to cluster inorganic layered materials in three classes – not exfoliable, potentially exfoliable (maybe with electrochemical methods and ion insertion) and easily exfoliable – just like graphene or transition-metal dichalcogenides.

In our work, all the properties of the investigated materials are computed at the DFT-PBE level. The only exceptions are binding energies, which are calculated using the DF2-C09 and the rVV10 vdW functionals. Binding energies are always computed in a non-magnetic reference configuration, both for the 3D parent (Fig. 2) and for exfoliated monolayers. We checked that including magnetism for magnetic systems does not alter the binding energy by more than 10 meV/Å^2, and in most cases it does not alter the classification as easily exfoliable. The total and absolute magnetizations are defined, respectively, as $M_{tot}=\mu_B\int m(r)dr$ and $M_{abs}=\mu_B\int|m(r)|dr$, where $m(r)=n^{\uparrow}(r)-n^{\downarrow}(r)$ is the local magnetization and $n^{\uparrow}(r)/n^{\downarrow}(r)$ are the densities of spin-up/down electrons. A system is labelled non-magnetic (NM) if in the ground state $M_{tot}=M_{abs}=0$, while it is labelled anti-ferromagnetic (AF) if $M_{abs}\neq0$ and $M_{tot}<0.1$ μB. In all other cases the system is reported as ferromagnetic (FM). Magnetic band structures are plotted with two different colours for the two different spin states. Paths and special k-points follow the conventions for 2D systems from Ref. [1] as implemented in AiiDA [2]. All the structures, 3D and 2D, computed are treated as non-magnetic using spin-unpolarized DFT regardless of their true magnetic ground state, since the magnetic order has a negligible effect on the binding energies (caution is then needed when looking at the electronic properties of materials with element that might support a magnetic ground state – currently one PhD student in the project is working on identifying all the possible magnetic ground and excited states).

2.1 Data Analysis

Fig. 3: landing page of the database of inorganic materials (https://mc2d.materialscloud.org/) that are layered and can be exfoliated, now containing more than 3000 inorganic compounds, of which 2000+ are easily exfoliable.

All the materials properties that have been calculated are openly accessible to the entire scientific community through the MC2D (Materials Cloud 2-dimensional Database), as shown in Fig. 3. Properties that have been calculated are the theoretical geometries of the 3D parent and of the 2D exfoliated monolayer, and the exfoliation energies.

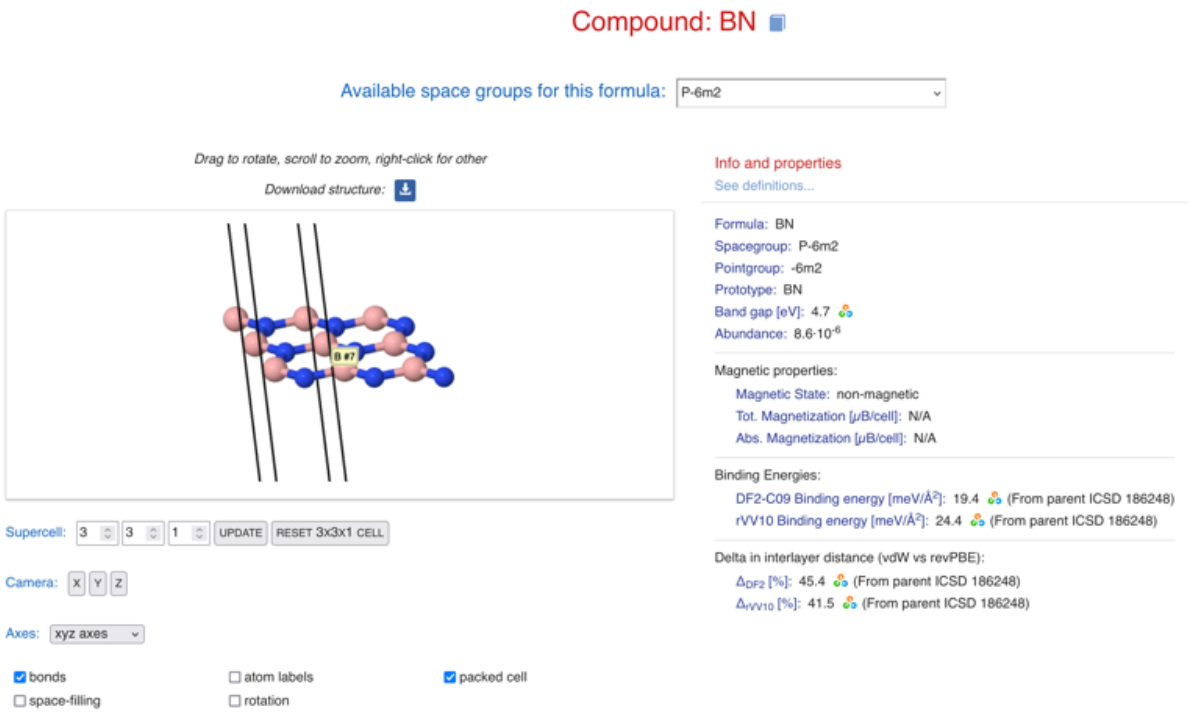

Fig. 4: the selection of a material (here, hexagonal boron nitride) provides core information: symmetry properties, magnetization, band gap, and especially binding energy.

Work is continuously in progress to add more properties – total and absolute magnetization, electronic band structure, and phonon dispersions, as shown in Figs. 4, 5 and 6.

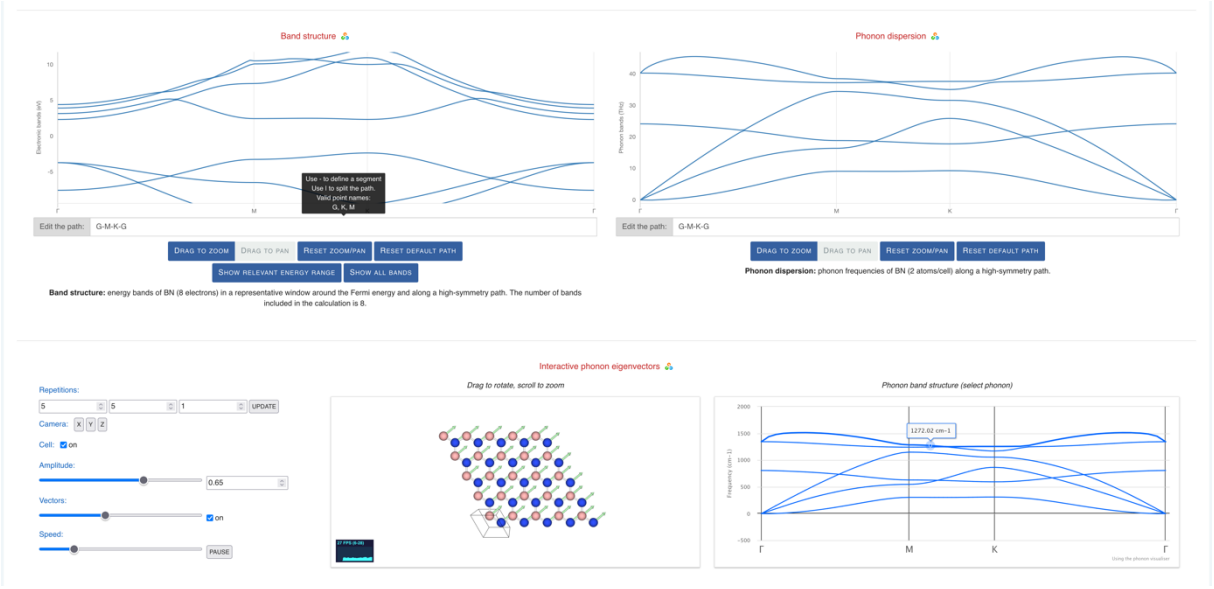

Fig. 5: whenever available, the electronic band structure and the phonon dispersions are also displayed. The user can probe and visualize interactively individual phonon modes.

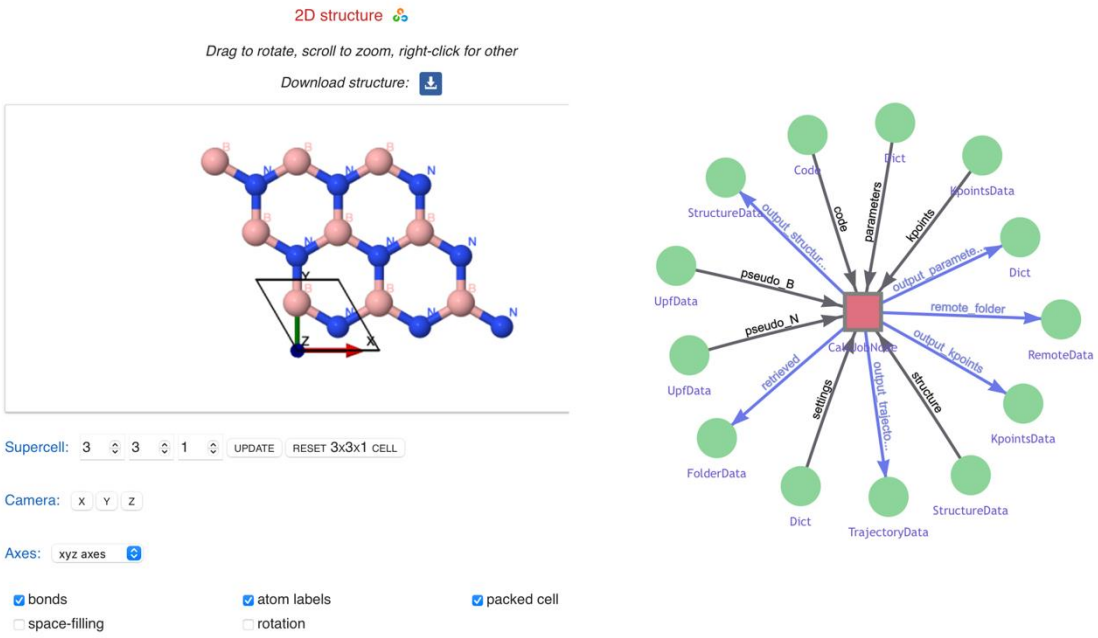

Fig. 6: the geometries of the 2DM (monolayer) are presented, together with the link to the data for the 3D parent (often contained in proprietary databases); the AiiDA directed acyclic graph recording the provenance of the entire simulation workflow can be browsed graphically (left panel) or downloaded in its

entirety from the Materials Cloud Archive (an open-access resource, recommended by the European Commission through Open Research Europe for the storage of materials data[2]).

Table 1: list of materials easily exfoliable into monolayers (containing 6 atoms or less in the unit cell) that are optimal lattice matched pairs with graphene.

Formula	N° atoms	strain	cell size 1	cell size 2	Formula	N° atoms	strain	cell size 1	cell size 2
Sn	3	0.3116	1	1	$Ga_2Ge_2Te_2$	104	0.0	25	9
In	3	0.3206	1	1	$Hf_2I_2N_2$	42	0.0001	9	4
BN	4	0.0084	1	1	CdClHO	34	0.0001	9	4
K	5	0.5682	2	1	Li_2P_2Pr	95	0.0001	25	9
FeO_2	5	0.4946	1	1	$CrTe_2$	275	0.0002	79	39
Br_2Cu	5	1.0098	1	1	Sb_2Te_3	178	0.0003	49	16
NiO_2	5	0.4981	1	1	KNO_3	173	0.0003	64	9
CrO_2	5	0.4648	1	1	Br_2V	173	0.0003	49	25
MnO_2	5	0.4705	1	1	FeO_2	275	0.0003	64	49
N_2Re	5	2.9608	1	1	CS_2Ta_2	77	0.0003	16	9
CoO_2	5	0.4966	1	1	Cl_2Sc_2	314	0.0003	79	39
InSe	6	6.2671	1	2	Cu_4Te_2	194	0.0003	49	16
AgTl	6	0.4545	2	1	Mg_6	198	0.0004	39	20
N_4	6	1.5954	1	1	Cl_2Ti	59	0.0004	16	9
Ba_2Hg	7	0.5241	2	1	$TaTe_2$	30	0.0004	9	4
$CrTe_2$	7	0.2259	2	1	$Ge_2I_2La_2$	312	0.0005	81	25
Br_2Ti	7	0.2251	2	1	CoO_2	275	0.0005	64	49
$AsSe_2$	7	0.2198	2	1	Br_2Cr	275	0.0005	79	39
Cl_2Cu	7	0.1774	2	1	$F_2Se_2Tm_2$	278	0.0005	64	25
BrNZr	7	0.2215	2	1	P_2	50	0.0005	16	9
$NbSe_2$	7	0.2185	2	1	$ReSe_2$	173	0.0005	49	25
Br_2Cr	7	0.2255	2	1	$Br_2H_2Zr_2$	392	0.0006	79	39
Se_2Ta	7	0.2186	2	1	HN_3OZn	86	0.0006	16	9
H_2MgO_2	7	13.6508	1	1	$LiMnSe_2$	228	0.0006	64	25
$NbSe_2$	7	0.2202	2	1	Sb_2	68	0.0007	25	9
Se_2Ta	7	0.2241	2	1	$Br_2S_2Y_2$	398	0.0007	115	28
$AgCuTe_2$	8	0.2761	2	1	Br_2Ti	275	0.0008	79	39
S_2Sn_2	8	0.4891	2	1	H_2MgO_2	407	0.0008	81	49
BrCdI	8	6.075	1	2	Au_2Br_2	240	0.0008	76	22
Br_2Hf_2	8	0.221	2	1	$H_2Li_2O_2$	584	0.0008	130	54
BaF_2	8	6.1633	1	2	CrO_2	401	0.0008	91	73
AsKSn	8	6.125	1	2	$SnTe_2$	77	0.0009	25	9
$PbTe_2$	8	6.0491	1	2	In	159	0.0009	61	37
STl_2	8	6.1889	1	2	Br_2La_2	86	0.0009	25	9
Ge_2Se_2	8	0.4559	2	1	NiO_2	275	0.001	64	49
PbS_2Sn	8	0.5545	2	1	$Se_2Si_2Zr_2$	518	0.001	115	48
Cl_2Sc_2	8	0.2258	2	1	$AsSn_2$	30	0.001	9	4
Se_2Sn_2	8	0.5589	2	1	$I_2S_2Tb_2$	408	0.001	120	28
F_4Sn	9	0.5218	2	1	CNb_2S_2	77	0.001	16	9
Sn	9	0.139	4	1	Cl_2Zr_2	198	0.001	49	25
Fe_2Te_2	10	0.1252	3	1	$H_2Na_2O_2$	416	0.0011	88	40
Ca_2Cl_2	10	0.1255	3	1	BH_4Li	104	0.0011	25	9
$Br_2H_2Zr_2$	10	0.2254	2	1	I_2Y_2	228	0.0012	64	25
HgO	10	0.1457	3	2	$Cl_2H_2Sc_2$	392	0.0013	79	39
$Cu_2Na_2Te_2$	10	0.579	2	1	$Br_2Ho_2O_2$	510	0.0014	123	44
$AsLi_3$	10	6.2753	1	2	Fe_2O_4	518	0.0014	103	52
Pb_2Se_2	10	8.8761	1	2	Bi_2SeTe_2	178	0.0014	49	16
$Cl_2N_2Zr_2$	10	0.3483	2	1	Br_2Zr_2	396	0.0014	100	49
Br_2Ca_3Si	10	0.5248	2	1	MnO_2	401	0.0014	91	73
AgTl	10	0.1091	4	1	H_2MgO_2	307	0.0014	61	37

[2] https://open-research-europe.ec.europa.eu/for-authors/data-guidelines#approvedrepositories

Table 2: list of materials easily exfoliable into monolayers (containing 6 atoms or less in the unit cell) that are optimal lattice matched pairs with hexagonal boron nitride.

Formula	N° atoms	strain	cell size 1	cell size 2
C_2	4	0.0081	1	1
Mg_2	4	0.3277	1	1
K	5	0.5436	2	1
FeO_2	5	0.4732	1	1
NiO_2	5	0.4765	1	1
MnO_2	5	0.45	1	1
Na	5	0.2222	2	1
N_2Re	5	2.8541	1	1
CoO_2	5	0.4751	1	1
InSe	6	6.0468	1	2
Bi_2	6	6.2011	1	2
C_2Li_2	6	2.4727	1	1
PbTe	6	6.0934	1	2
$MoTe_2$	7	0.2251	2	1
Te_2Zn	7	0.2249	2	1
PtS_2	7	0.2235	2	1
Se_2Ti	7	0.2201	2	1
Te_2W	7	0.2253	2	1
H_2MnO_2	7	2.9974	1	1
H_2Li_2Pd	7	0.3317	1	1
N_3W_2	7	2.9657	1	1
H_4Ti	7	0.3329	1	1
CdI_2	8	6.1393	1	2
Cu_4Te_2	8	1.18	1	1
Br_2Ca	8	6.1721	1	2
NS_2Zr	8	0.2227	2	1
$AgCuTe_2$	8	0.2624	2	1
BiClTe	8	6.1489	1	2
S_2Sn_2	8	0.4673	2	1
Br_2Zr_2	8	0.2196	2	1
N_4	8	0.2782	2	1
GeI_2	8	6.0997	1	2
Ge_2Se_2	8	0.4353	2	1
La_2S_2	8	0.5193	2	1
CdI_2	8	6.1277	1	2
$HfLiS_2$	8	0.2245	2	1
I_2Pr	8	6.1512	1	2
K	9	0.1163	4	1
Sn	9	0.1398	4	1
In	9	0.1393	4	1
CdH_2O_2	9	0.2259	2	1
F_2Zn	9	0.1256	3	1
Ga_2S_3	9	0.2226	2	1
$LiMnTe_2$	10	6.1079	1	2
Bi_2Mn_2	10	6.1222	1	2
HgO	10	0.1355	3	2
$Cu_2Na_2Te_2$	10	0.554	2	1
$AsLi_3$	10	6.0548	1	2
Cu_2S_2	10	0.1236	3	1
$C_2Br_2Gd_2$	10	0.2839	2	1

Formula	N° atoms	strain	cell size 1	cell size 2
$HfSe_2$	30	0.0	9	4
Te_2Ti	30	0.0	9	4
$PdTe_2$	203	0.0	64	25
H_2MnO_2	278	0.0001	49	36
BiITe	146	0.0001	49	16
BrCdI	77	0.0001	25	9
Bi_2Te_3	178	0.0001	49	16
SSb_2Te_2	95	0.0002	25	9
$CrSe_2$	233	0.0002	61	37
$Cl_2H_2Zr_2$	86	0.0002	16	9
CdH_2O_2	353	0.0002	79	39
DyI_2	237	0.0002	81	25
NiO_2	354	0.0002	81	64
$I_2S_2Tb_2$	312	0.0002	81	25
Br_2Zn	30	0.0003	9	4
CoO_2	354	0.0003	81	64
CCl_2Gd_2	38	0.0004	9	4
NbS_2	59	0.0004	16	9
$MnNaTe_2$	86	0.0005	25	9
H_2Li_2Pt	172	0.0006	36	20
Te_2W	275	0.0006	79	39
Te_2V	347	0.0006	100	49
Br_2Tb_2	228	0.0006	64	25
CdClO	275	0.0006	79	39
$CrTe_2$	173	0.0007	49	25
$LiOS_2Ti$	77	0.0007	16	9
Cl_2Sc_2	198	0.0007	49	25
$MoTe_2$	275	0.0008	79	39
LiO	260	0.0008	81	49
OTl_2	275	0.0008	79	39
$Cl_2Hf_2N_2$	392	0.0008	79	39
Br_2Pr_2	34	0.0009	9	4
Br_2Cd	203	0.0009	64	25
Bi_2S_3	253	0.0009	64	25
$Dy_2I_2S_2$	312	0.0009	81	25
Br_2Mn	347	0.0009	100	49
NS_2Ta	172	0.0009	36	25
Br_2Cr	173	0.001	49	25
Te_2Zn	275	0.001	79	39
CBr_2Y_2	38	0.001	9	4
$Br_2H_2Zr_2$	248	0.0011	49	25
Br_2PY_2	253	0.0011	64	25
FeO_2	354	0.0011	81	64
$PbTe_2$	77	0.0011	25	9
Cl_2V	233	0.0011	61	37
GeI_3Rb	37	0.0011	16	1
Br_2Cu	281	0.0011	88	35
Br_2Ho_2	228	0.0011	64	25
Te_2V	275	0.0011	79	39
N_2Re	275	0.0012	64	49

3 Results & Discussion

3.1 Results

We have curated the data of a portfolio of 3000+ monolayers [4], that provides the starting point to calculated more complex materials properties, such as mobilities or optical absorption or emission, that are currently in progress.

3.2 Contribution to project (linked) Objectives

This deliverable contributed directly to the objective of combining “theoretical modelling, crystal growth and large-scale liquid-exfoliation, to scalably produce >20 new 2DM, including conducting, semiconducting and insulating nanosheets, with targeted properties”.

3.3 Contribution to major project exploitable result

This deliverable underpins the experimental efforts that are ongoing in 2D-Printable to identify novel 2DM that can be incorporated in next-generation printed electronic devices.

4 Conclusion and Recommendation

A very extensive portfolio of 2DMs has been identified theoretically; for these, the most pressing needs are the calculation of optoelectronic properties (starting from the direct band gaps), currently in progress, and of mechanical properties and bending rigidities.

Calculation of direct/indirect band gaps requires in principle very extensive (and expensive) sampling of the Brillouin zone, for which we have recently developed very accurate Wannier interpolation techniques. Work is very advanced, and in the next 2-3 months we'll be able to release all the band structures and direct/indirect band gap of ~2000+ easily exfoliable materials.

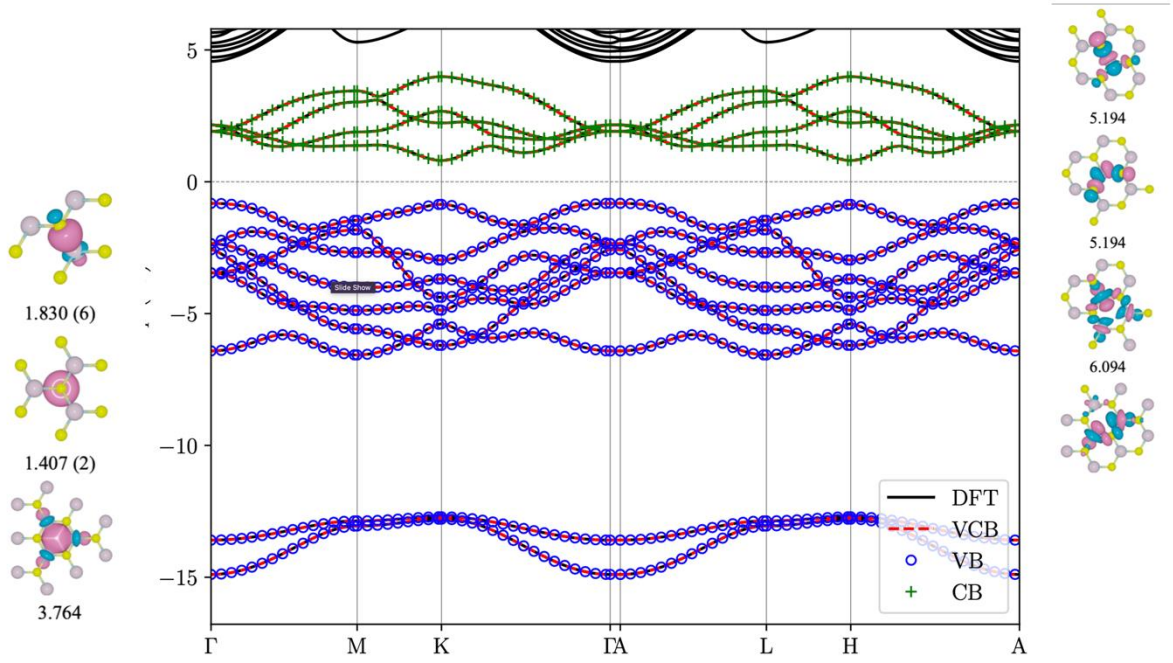

Fig. 7: maximally localized Wannier function for monolayer MoS_2, perfectly interpolating the DFT data and allowing to identify with great precision maxima and minima in the band edges.

5 Risks and interconnections

5.1 Risks/problems encountered

The risks are related to the accuracy (or lack thereof) of DFT simulations – binding energies have very moderate errors, of 10-20%, but band gaps are always underestimated (by a factor of 2), whereas much more expensive many-body perturbation theory/GW calculations should be performed for few, selected most promising candidates.

5.2 Interconnections with other deliverables

D1.2 underpins the calculations of D1.4 and D1.6, bur especially the experimental efforts in D4.1 and D4.2

6 Deviations from Annex 1

No deviations.

7 References

[1] R. Ramírez, and M. C. Böhm, *Simple geometric generation of special points in Brillouin-zone integrations: Two-dimensional bravais lattices*, Int. J. Quantum Chem. 30, 391-411 (1986).

[2] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, *AiiDA: automated interactive infrastructure and database for computational science*, Computational Materials Science 111, 218-230 (2016).

[3] The curation of the data is made openly accessible at *https://mc2d.materialscloud.org/*; the original research work includes Ref. [4] and Ref. [5].

[4] N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi & N. Marzari, *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, Nature Nanotechnology 13, 246-252 (2018), with the accompanying data: N. Mounet et al., Materials Cloud Archive 2020.158, doi: 10.24435/materialscloud:az-b2 (2020).

[5] D. Campi, N. Mounet, M. Gibertini, G. Pizzi & N. Marzari, *Expansion of the Materials Cloud 2D Database* ACS Nano 17, 12, 11268-11278 (2023), with the accompanying data: D. Campi et al., Materials Cloud Archive 2022.84, doi: 10.24435/materialscloud:36-nd (2022).

8 Acknowledgement

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Project partners:

#	Partner short name	Partner Full Name
1	TCD	TCD THE PROVOST, FELLOWS, FOUNDATION SCHOLARS & THE OTHER MEMBERS OF BOARD, OF THE COLLEGE OF THE HOLY & UNDIVIDED TRINITY OF QUEEN ELIZABETH NEAR DUBLIN
2	UNISTRA	UNIVERSITE DE STRASBOURG
3	UKa	UNIVERSITAET KASSEL
4	BED	BEDIMENSIONAL SPA
5	TUD	TECHNISCHE UNIVERSITAET DRESDEN
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8	UniBw M	UNIVERSITAET DER BUNDESWEHR MUENCHEN
9	EPFL	ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE

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9 Appendix A - Quality Assurance Review Form

The following questions should be answered by all reviewers (WP Leader, reviewer, Project Coordinator) as part of the Quality Assurance procedure. Questions answered with NO should be motivated. The deliverable author will update the draft based on the comments. When all reviewers have answered all questions with YES, only then can the Deliverable be submitted to the EC.

NOTE: This Quality Assurance form will be removed from Deliverables with dissemination level "Public" before publication.

Question	**WP Leader**	**Reviewer**	**Project Coordinator**
	NAME (Organisation)	NAME (Organisation)	Jonathan Coleman (TCD))
1. *Do you accept this Deliverable as it is?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
2. *Is the Deliverable complete?* - *All required chapters?* - *Use of relevant templates?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
3. *Does the Deliverable correspond to the DoA?* - *All relevant actions preformed and reported?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
4. *Is the Deliverable in line with the 2D-PRINTABLE objectives?* - *WP objectives* - *Task Objectives*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
5. *Is the technical quality sufficient?* - *Inputs and assumptions correct/clear?* - *Data, calculations, and motivations correct/clear?* - *Outputs and conclusions correct/clear?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
6. *Is created and potential IP identified and are protection measures in place?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
7. *Is the Risk Procedure followed and reported?*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)
8. *Is the reporting quality sufficient?* - *Clear language* - *Clear argumentation* - *Consistency* - *Structure*	Yes / No (elaborate)	Yes / No (elaborate)	Yes / No (elaborate)

10 Appendix B - <<Appendix Title>>