HORIZON EUROPE PROGRAMME
HORIZON-CL4-2023-DIGITAL-EMERGING-01-33

GA No. 101135196

Developing New 2D Materials and Heterostructures for Printed Digital Devices

2D-PRINTABLE - Deliverable data (+ report)

D1.1 – Database on available materials

Funded by
the European Union

Deliverable No.	D1.1	
Related WP	WP 1	
Deliverable Title	Database on available materials	
Deliverable Date	2024-03-31	
Deliverable Type	DATA (+ REP)	
Dissemination level	Public (PU)	
Author(s)	Joka Buha (BeD) Sebastiano Bellani (BeD)	2024-03-04
Reviewed by	Francesco Bonaccorso (BeD) Jonathan Coleman (TCD)	2024-03-18 2024-03-27
Approved by	Jonathan Coleman (TCD) - Project Coordinator	2024-03-28
Status	Final	2024-03-28

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

This deliverable is a database of exfoliable three-dimensional (3D) layered materials available for 2D-PRINTABLE, and the corresponding two-dimensional (2D) materials produced by project partners by means of various exfoliation methods in liquid media, including liquid-phase exfoliation method (LPE), electrochemical exfoliation (EE) and chemical exfoliation (CE). Exfoliable 3D layered materials are those synthesized and currently available at VSCHT facilities, while LPE-produced 2D materials are those produced by BeD, UKa, TCD TUD and VSCHT. The database includes the main specifications for exfoliable 3D layered materials, including their (physical) form (*e.g.*, powder/crystal and corresponding dimension), stoichiometry and doping, as well as the material amount that can be supplied within the consortium. For 2D materials, the database reports the references to public documents (e.g., paper in international peer-reviewed journal or public repositories) showing material characterizations. The following report is annexed to D1.1 database (available https://zenodo.org/communities/2d-printable/), listing and explaining the information given in the database, as well as giving the instruction to correctly report such information and to name the .ppt files with unpublished characterization of the materials.

Contents

1 Introduction 6
2 Methods and core part of the report 7
2.1 D1.1 Database description 7
2.2 Instruction for hyperlink creation 7
3 Results & Discussion 8
3.1 Results 8
3.2 Contribution to project (linked) Objectives 8
3.3 Contribution to major project exploitable result 8
4 Conclusion and Recommendation 9
5 Risks and interconnections 10
5.1 Risks/problems encountered 10
5.2 Interconnections with other deliverables 10
6 Deviations from Annex 1 11
7 References 13
8 Acknowledgement 12
9 Appendix A - Quality Assurance Review Form 15

Abbreviations & Definitions

Abbreviation	Explanation
2D	Two-dimensional
3D	Three-dimensional
AFM	Atomic force microscopy
CE	Chemical exfoliation
DFT	Density Functional Theory
EE	Electrochemical exfoliation
KER	Key Exploitable Result
LPE	Liquid-phase exfoliation
SEM	Scanning electron microscopy
TEM	Transmission electron microscopy
TMD	Transition metal dichalcogenides
XRD	X-ray diffraction

Introduction

This deliverable is a database of exfoliable three-dimensional (3D) layered materials available for 2D-PRINTABLE, and the corresponding two-dimensional (2D) materials produced in WP1, as well as in activities before this project, by means of various exfoliation methods in liquid media, including liquid-phase exfoliation method (LPE), electrochemical exfoliation (EE) and chemical exfoliation (CE). Exfoliable 3D layered materials are those synthesized and currently available at VSCHT facilities (Task 1.2), while LPE-produced 2D materials are those produced by BeD, UKa, TCD TUD and VSCHT (Task 1.3 and Task 1.4). The database includes the main specifications for exfoliable 3D layered materials, including their (physical) form (*e.g.*, powder/crystal and corresponding dimension), stoichiometry and doping, as well as the material amount that can be supplied within the consortium. For 2D materials, the database reports the references to public documents (*e.g.*, paper in international peer-reviewed journal or public repositories) showing material characterizations, as well as the hyperlinks to .ppt file containing unpublished characterizations (accessible from partners only, thus, kept as confidential until their publication). This database will be updated during the projects, reporting new exfoliable 3D layered materials and 2D materials produced considering the outcomes from Task 1.1 (*Theory-driven identification of novel 2D materials from exfoliable 3D layered materials*) and the specifications needed for the printed digital devices targeted in WP6 (Proof-of-concept digital devices based on printed networks and heterostructures). Also, this database will be used in Task 1.1, where available 3D materials will permit to extend current ICSD, the COD and the MPDS databases, enabling the identification of a core portfolio of novel exfoliable materials through high-throughput calculations using van der Waals Density Functional Theory (DFT).

The objectives of D1.1 have been reached without any deviation from DoA.

1 Methods and core part of the report

1.1 D1.1 Database description

D1.1 Database is realized in form of Excel spreadsheet, in which rows of information are called records and columns of information are called fields. The following column headings have been used to identify fields for exfoliable 3D layered materials and corresponding 2D materials.

- *3D (bulk) layered material:* chemical name of available 3D layered materials, as synthesized by VSCHT;
- *Formula:* chemical formula of 3D layered materials;
- *CAS Registry Number:* unique and unambiguous identifier for a specific substance that allows clear communication and links together all available data and research about that substance. Governmental agencies rely on CAS Registry Numbers for substance identification in regulatory applications because they are unique, easy validated, and internationally recognized (see https://www.cas.org/cas-data/cas-registry);
- *Physical form(s):* physical form of the 3D layered materials (*e.g.*, crystal or powder), including main dimension characteristics (e.g., crystal size, powder mesh, *etc*.);
- *Amount that can be supplied:* amount of 3D layered materials that can be supplied by VSCHT to project partners;
- *Exfoliation method(s) (LPE, EE, CE, other); *external:* list of the methods that have been used to produce 2D materials from available 3D layered materials. LPE: liquid-phase exfoliation; EE: electrochemical exfoliation; CE: chemical exfoliation; other: methods different from LPE, EE and CE, including methods not performed in liquid media. * is used to indicate methods reported in previous literature from research groups not belonging to 2D-PRINTABLE consortium;
- *Partners:* list of the 2D-PRINTABLE partners that can produce and supply 2D materials to project consortium;
- *Ease of supply:* indication (yes/not) on ease of supply of 2D materials, qualitatively informing the request applicant about the efforts needed to produce 2D materials;
- *Characterization data and notes:* general notes (e.g., available phases) are also reported in this heading.
- *References; * external:* link to reference(s) reporting the characterization of 2D materials. * is used to indicate literature published from research group not belonging to 2D-PRINTABLE CONSORTIUM. The link to references is given in form of a Digital Object Identifier (DOI) link, adding the DOI of the article (located alongside the citation information) to the following url: https://doi.org/.

2 Results & Discussion

2.1 Results

By reporting the database of exfoliable three-dimensional (3D) layered materials available for 2D-PRINTABLE, and the corresponding two-dimensional (2D) materials produced by project partners, D1.1 deliverable represent the playground for the activities of subsequent WPs, from WP2 to WP7.

2.2 Contribution to project (linked) Objectives

D1.1 database allows the access to an exhaustive list of available exfoliable 3D layered materials, which can be used to achieve one of the main target of 2D-PRINTABLE, namely the production of novel 2D nanosheets (D1.5, M24), paving the way towards the initiation of the activities of subsequent WP2, including chemical modification of nanosheets (WP2), printing and deposition of networks and heterostructures with controlled interfaces (WP3), Characterization of nanosheets, networks and heterostructures (WP4), electrical Characterization of nanosheets, heterostructures and networks (WP5), ending with the realization of proof-of-concept digital devices based on printed networks and heterostructures (WP6).

2.3 Contribution to major project exploitable result

This deliverable contributes reaching several Key Exploitable Results (KERs), including:

1. Overarching KERs (Target Groups: Research Community -academic & industry-, Industry, European Associations, Coordinators of EU projects related to 2D materials
    a. High-performance materials for printed electronics applications
2. Materials KERs (Target Groups: Nanomaterial manufacturers):
    a. ≥20 novel 2D materials for different printed electronic applications as printable inks, powders and films (WP1–2);
    b. Novel nanosheets/networks with tunable properties
3. Printed electronics & devices KERs (Target Groups: Consumer electronic companies, Mobile healthcare and diagnostics industry & wearable monitoring devices)
    a. Light-emitting 2D materials

Conclusion and Recommendation

The database of exfoliable three-dimensional (3D) layered materials available for 2D-PRINTABLE, and the corresponding two-dimensional (2D) materials produced by project partners by means of various exfoliation methods in liquid media, including liquid-phase exfoliation method (LPE), electrochemical exfoliation (EE) and chemical exfoliation (CE), has been created. This report is annexed to the D1.1 database, listening the information given by the database and the instructions to fill it.
The database will be updated during the continuation of the project.

3 Risks and interconnections

3.1 Risks/problems encountered

The risks are those identified in the 2D-PRINTABLE proposal, as listed here below:

Risk No.	What is the risk	Probability of risk occurrence[1]	Effect of risk[1]	Solutions to overcome the risk
1	Insufficient exfoliation yield for novel 3D materials, leading to insufficient amount of 2D materials for practical applications.	3	1	Theoretical and experimental screening of a large portfolio of solvents and their mixtures; screening various of exfoliation techniques and their combinations
2	Insufficient control of defect formation in 2D materials during exfoliation	2	2	Use defective bulk materials (*e.g.*, nonstoichiometric composition); apply post-exfoliation defect engineering
3	New materials are prone to degradation/oxidation in ambience.	1	2	Develop inert processing and device encapsulation; use chemical defect passivation during exfoliation
4	Green solvents are not suitable for exfoliation	2	3	Implement solvent recycling and reuse

[1)] Probability risk will occur: 1 = high, 2 = medium, 3 = Low

3.2 Interconnections with other deliverables

D1.1 is clearly interconnected with the WP1 deliverables (D1.2-1-6), as well as with D2.1 (Tuneable functionalization of TMDs), D2.2 (Functionalization of 2D materials beyond TMDs), D3.1 (Ink production/printing), D4.1 (Characterization of nanosheets, networks and heterostacks built from initially available 2D materials), D4.2 (Characterization of new materials identified through theory)

4 Deviations from Annex 1

No deviations from the original plan have to be made.

Acknowledgement

The author(s) would like to thank the partners in the project for their valuable comments on previous drafts and for performing the review.

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
6	VSCHT	VYSOKA SKOLA CHEMICKO-TECHNOLOGICKA V PRAZE
7	UNR	UNIRESEARCH BV
8	UniBw M	UNIVERSITAET DER BUNDESWEHR MUENCHEN
9	EPFL	ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE

Disclaimer/ Acknowledgment

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101135196. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.