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Deliverable 1.1

HARMLESS database with extensions to handle advanced materials

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Description of Task

Task 1.1 HARMLESS database development with extensions to handle advanced material types, (Lead: IDEA; all partners), duration month 1-19 The HARMLESS database will build on the open source data management solution eNanoMapper, which possess currently the largest searchable compilation of nanoEHS Environment, Health and Safety) (Nano data in Europe (https://search.data.enanomapper.net), from multiple completed (ENPRA, MARINA, NanoTest, NanoGenotox, NANOREG, caLIBRAte, Nanoreg2, PATROLS, GRACIOUS, BIORIMA) and many ongoing EU nanosafety projects (NanoinformaTIX, Gov4Nano, RISKGONE, Sbd4Nano, SABYDOMA and more). The HARMLESS-eNanoMapper database provides an infrastructure for data management of chemical substances and measurement, making use of generated unique material and study identifiers (Findable, F1), rich set of metadata parameters describing the experiment (Findable, F2, F3) and searchable data and metadata (Findable, F4). The Accessibility is ensured by the provided HTTP REST Application Programming Interface (API) with standard authentication and authorization (Oauth2 and Application Programming Interface (API) keys). The interoperability relies on a generic representation of the "measurement"10 and user friendly as well as automatic tools for annotation with controlled vocabularies and ontologies. The selection of the proper terminology as well as the Reusability criteria are typically domain specific and will be ensured by Task 1.2-T1.5. We will launch the HARMLESS database and populate initially with existing data. Support for advanced materials will be implemented, including representation of complex materials structure and appropriate ontology annotation. Text processing AI methods will be integrated to find gaps in existing ontologies, which will be annotated and updated to meet the requirements for advanced materials.



Introduction

WP1 launched HARMLESS eNanoMapper database, part of the NanoSafety Data Interface [1], at <u>https://search.data.enanomapper.net/projects/harmless</u>. The database was populated with data from multiple previous projects as well as data compiled in T1.2 (physicochemical characterization and test data available in scientific literature and NRCWE reports) and T1.3 (in vitro data sets from recently completed EU H2020 projects PATROLS and SMARTNanoTOX provided by partners SU and HMGU).

Data entry

Data entry for newly generated data is streamlined through the eNanoMapper Template Wizard. Unique material identifiers (ERM - European Registry of Materials [2]) have been assigned to 23 materials being tested by WP6 (Table 3) and integrated in the Template Wizard.

To facilitate the description of multicomponent materials, a new template for specifying complex compositions for multicomponent materials has been created, integrated within Template Wizard and tested with composition data for silica paper. As an agreed definition of advanced materials is still not publicly available, IDEA performed a feasibility study for automatic classification of materials into suggested categories using text processing AI methods. Also, IDEA is developing an open source software prototype for conversion of material description info into a SYBYL line notation together with a future conversion to NInChI notation, which will provide terse machine readable representation of multicomponent materials, compatible with other data resources supporting NInChI.

The programmatic access to data as well as user friendly tools are essential for supporting data analysis performed in HARMLESS. Guidance and assistance for programmatic access has been provided to partners for their use. The similarity method developed previously by IDEA has been reworked and transformed into an easily accessible web page, and is already being utilized by its partners.

Initial gap analysis

In the beginning of the HARMLESS project manual annotation of advanced materials in the database was attempted (PN), according to the then available classification [5], which is helping with data gap analysis (screenshots used in Penny's slides)





Figure 1. Example of visual gap analysis available in the Nanosafety Data Interface and HARMLESS database

"Principle"	Ontology if available	HARMLESS case study	Database entries
(property/functionality-		material	(using principle key
based)			word(s))
High aspect ratio (HAR)	Aspect ratio	Metal-doped imogolite	Manual expert search, incl.
(aspect ratio > 3:1)*	[ENM_8000064]	nanotubes	Asbestos
	(Parent term "image		Crocidolite asbestos
	analysis descriptor")		Single-walled nanotubes
			Single-walled carbon
			nanotubes
			Multi-walled carbon
			nanotubes
			Carbon nanotubes
			Glass wool
			Nanofibrillar cellulose
Additive	Food additive	Silica additive in	2 entries, incl.
	[CHEBI_64047]	papermaking	Nanoemulsion
	Food additive carrier	Silica additive in paints	(poly(ethylene oxide)-
	[CHEBI_78059]		modified poly(epsilon-
	Fuel additive		caprolactone) (PEO-PCL)
	[CHEBI_62803]		nanoparticles)
	Freeze-thaw additive		
	[ENM_8000195]		
	Drying control chemical		
	additive [CHEBI_51268]		
Electrode	Ion-selective electrode	Transparent electrode on	16 entries, incl.
	[CHMO_0002393]	photovoltaics or displays	Silver NPs
			Quantum dots
Catalyst	Catalyst [CHEBI_35223]	Catalysts based on	3 entries, incl.
		perovskites	Iron oxide NPs
Light conversion	-	Light conversion based on	177 entries, incl.
		perovskites	Zinc NPs
			Silica NPs
			Barium sulfate NPs

Table 1.	"Complexity"	principles for	advanced	materials
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			Silver NPs
Insulation	-	Nano-enabled insulation	-
		materials	
Doped / Doping	Doped core	Metal-doped imogolite	9 ("doping") + 15 ("doped")
	[ENM_9000242]	nanotubes	entries, incl.
			CuO-doped silica NPs
			Boron-doped silica NPs

Many of the entries originate from caNanoLab DB with strong focus on nanomedicine. For regulatory purposes, fibres are defined on the basis of their size and shape (aspect ratio \geq 3:1, length \geq 5 µm, and width \leq 3 µm) and unlike other dusts are regulated by number per unit volume of air and not mass concentration per unit air [3].



Figure 2. With proper annotation we have the potential for viewing advanced materials and NAMs in the HARMLESS database





Figure 3. Example of the multicomponent materials in HARMLESS database (~2021)

By leveraging the HARMLESS database's annotation capabilities, advanced materials can be more easily identified, searched, and accessed. This makes it possible identify materials that are relevant to a particular research project or application.

Review material databases

Materials Genome Initiative (MGI) <u>https://www.mgi.gov/</u> is a US federal multi-agency initiative for discovering, manufacturing, and deploying advanced materials with the goal to support US institutions in the adoption of methods for accelerating materials development. Three databases that have received MGI support are the Materials Project (MP), AFLOWlib, and Open Quantum Materials Database (OQMD):

Materials Project (<u>https://materialsproject.org</u>) (Figure 4) is established in 2011 with an emphasis on battery research, but includes property calculations for many areas of clean energy systems such as photovoltaics, thermoelectric materials, and catalysts. Most of the known 35,000 molecules and over 130,000 inorganic compounds are included in the database. It provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools.



Figure 4. materialsproject.org. Example page showing perovskites

AFLOWlib <u>http://aflowlib.org/</u> is a software framework for high-throughput calculation of crystal structure properties of alloys, intermetallics and inorganic compounds. Includes 3,466,057 material compounds with over 679,347,172 calculated properties (and growing).

Open Quantum Materials Database (OQMD) <u>http://oqmd.org/</u> is a database of DFT calculated thermodynamic and structural properties of 815,654 materials.

NIST Materials Data Resources: see https://www.nist.gov/mgi/materials-data-resources

NIST Materials Data Repository <u>https://materialsdata.nist.gov/</u> is materials science data repository as part of an effort in coordination with the Materials Genome Initiative (MGI) to establish data exchange protocols and mechanisms.



NIST Materials Resource Registry <u>https://materials.registry.nist.gov/</u> MRR functions as a federated service, making the registered information from multiple institutions available for research to the materials community

The Materials Commons <u>https://materialscommons.org/</u> is an Information Repository and Collaboration Platform for the Materials Community.

The Materials Data Facility (MDF) <u>https://materialsdatafacility.org/</u> offers Data Services to Advance Materials Science Research. It operates two cloud hosted services, data publication and data discovery, with features to promote open data sharing, self-service data publication and curation.

NREL MatDB <u>https://materials.nrel.gov/</u> is a computational materials database with the specific focus on materials for renewable energy applications including, but not limited to, photovoltaic materials, materials for photo-electrochemical water splitting, thermoelectrics, etc. The main goal of NRELMatDB is to enable and facilitate the access and exchange of computational data between different research groups following the guidelines outlined in the Materials Genome Initiative.

Matweb <u>http://www.matweb.com/</u> contains over 130,000 metals, plastics, ceramics, and composites.

The NIMS Materials Database (MatNavi) <u>https://mits.nims.go.jp/en/</u> aims to contribute to the development of new materials and the selection of materials. MatNavi includes:

-Polymer DB (chemical structures, polymerization, processing, physical properties, NMR spectra, etc.),

-Inorganic MaterialDB (crystal structures, phase diagrams, physical properties, etc.)

-Metallic Material DB (density, elastic constants, creep characteristics, etc.) and

-Computational Electronic Structure DB (band structures obtained by first-principles calculations, etc).

-also offers applications such as the Composite Design & Property Prediction System

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	About us Usage tips Data hierarchy System status Terms Privacy API license Editor-in-Chief: Pierre Villars. Section editors: Karin Cenzual, Ihor Savysyuk, Riccarda Caputo. Developed by <u>Tilde MI</u> .											



Figure 5. mdps.io

Other material databases are the Materials platform for data science (Figure 5), Materials cloud [4], MaterialsMine <u>https://materialsmine.org/</u> (an open source repository for nano composite data), and mechanical metamaterials data (Metamine).

The NOMAD Repository and Archive (NOvel MAterials Discovery) <u>https://nomad-lab.eu/</u> (Figure 6) contains results from more than 100 million open-access calculations (August 2021)

-NOMAD Repository is the largest repository for computational materials science worldwide, containing the input and output files from more than 100 million high-quality calculations.

-NOMAD Archive offers a homogeneous representation of the data from the repository as open-access, code-independent, machine-readable, and standardized data.

-NOMAD Encyclopedia – is a hugely powerful web tool for detailed searches of materials the NOMAD data store.

-NOMAD Artificial Intelligence Toolkit contains powerful tools for finding completely new patterns and information in materials science Big Data using the latest machine learning and artificial intelligence approaches.

Local nomad-lab can be installed for sharing simulation data privately.

The open source FAIR-mat is the next generation nomad-lab with strong focus on the newer interpretation of FAIR = Findable-AI-Ready[5]



Figure 6. nomad-lab.eu

Material databases interoperability is a good illustration of the distributed approach of designing independent but interoperable databases, where interoperability is based on implementation of a



common API [6] The common API allows more than 20 independently developed and hosted databases can be queried with the same query language by implementing a common specification (OPIMADE) (Figure 7).



Figure 7. OPTIMADE - common API for materials databases

There are number of ontologies addressing different subdomains of material design science and focused on specific types of materials or specific type of use. MatPortal (https://matportal.org/ontologies) comprises ontologies for materials science (in analogy of BioPortal for bioinformatics ontologies). Examples are Materials Design Ontology [7], European Materials Modelling Ontology (EMMO) developed by European Materials Modelling Council as well as attempts to define standard formats for material computational science [8].

Results

Within T1.1 IDEA launched HARMLESS – eNanoMapper database [1] as part of the NanoSafety Data Interface [2], using the open source eNanoMapper data management solution [3]. The database is available online at <u>https://search.data.enanomapper.net/projects/harmless/</u> (Figure 8)





Figure 8. Main page of the HARMLESS eNanoMapper database. Each icon leads to a page with the corresponding functionality (search, Template Wizard, Dashboard, etc)

The data content includes physicochemical characterisation, data for toxicity and ecotoxicity endpoints from previous nanosafety projects (FP7 Nanoreg, FP7 SANOWORK, H2020 Nanoreg2, H2020 caLIBRAte). Compilation of NRCWE in-vivo data and data from H2020 PATROLS project was added through T1.2 and T1.3 respectively. Exposure data will be added through T1.5 efforts. The HARMLESS – eNanoMapper database is only accessible by project partners, at the moment 30 user accounts have been granted access. An overview of the content is shown in Table 2.

Table 2. Summary fo	or data from previous EU	projects available in HARMLESS	s eNanoMapper database
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eNanoMapper				Data
import	Project	Materials	Studies	points
HARMLESS T1.2	Danish Centre for Nanosafety 1	23	242	18514
HARMLESS T1.2	Danish Centre for Nanosafety 2	14	144	8917
HARMLESS T1.2	FP7 NanoMILE	11	103	4617
HARMLESS T1.2	FP7-NMP Gladiator	5	36	3532
HARMLESS T1.2	FP7-NMP NanoREG	20	118	10205
HARMLESS T1.2	FP7-NMP NanoSustain	16	149	9507
HARMLESS T1.2	H2020 Calibrate	10	88	5219
HARMLESS T1.2	Horizon 2020 NanoPack	4	27	1984
HARMLESS T1.2	Horizon2020 SmartNanoTox	6	51	6673
HARMLESS T1.2	Lund NanoWire	5	19	1426
HARMLESS T1.2	NPK	14	127	7708
HARMLESS T1.3	PATROLS	20	393	7838
	caLIBRAte	40	1141	28124



caNanoLab	1500	5963	21499
NANoREG	147	5178	39935
NanoReg2	41	793	3849
OMICS_DATA	209	397	850
SANOWORK	64	594	1060

All the data is also programmatically accessible through REST API (at <u>https://api.ideaconsult.net</u>), protected by standard authentication and authorization protocols as API keys and OAuth2 (Figure 9). IDEA has provided guidance and assistance for programmatic access to willing partners, with partner TNO already integrating eNanoMapper database access into the DSS (WP5). To support data analysis by project partners, both programmatic access and user-friendly tools are essential.

IDEAconsult API Portal × +				~	-		×
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Servers (https://api.ideaconsult.net/harmless) Authorize							1
Search Multi-DB aggregated free text and faceted search	~						
GET /select Apache Solr powered search solrquery_get	:						
POST /select Apache Solr powered search solrquery_point	:						
Structures Chemical structures	\sim						
GEI /enm/{db}/substance/{uuid}/composition SubstanceComposition getSubstanceComposition	•						
GEI /enm/{db}/substance/{uuid}/structures Centrolion as a getSubstanceStructure dataset							
GET /enm/{db}/query/compound/{term}/{representatio n} Exact chemical searchByIdentific search							
GET /enm/{db}/query/smarts Substructure search searchBySmart	•						
GET /enm/{db}/query/similarity Exact similarity search searchBySimilarit	/						
Substances Chemical substances and (nano)materials	>						
Studies Measurements or calculations attached to a substance	>						
Data analysis Machine learning algorithms and models, property prediction models	>						
Facets Summaries	>						

Figure 9. HARMLESS eNanoMapper database Application Programming Interface (API) interactive documentation

Tools for data analysis

The dose response and time series similarity method (without fitting curves) developed previously by IDEA [7] as a Jupyter notebook is now re-implemented as an easy to use web page and is already used by partners.



S HARMLESS

Home Proje

H2020 HARMLESS - eNanoMapper database : Similarity matrix



Figure 10. Screenshot of the online similarity assessment tool for dose response and/or time series

Data entry

Data entry for newly generated data is streamlined through the eNanoMapper Template Wizard, an online tool with harmonized data entry templates, shared across nanosafety projects. Existing templates for physicochemical will be reused and new ones are being integrated in collaboration with data providers i.e. FRAS and dynamic dissolution template provided by BASF ; updated exposure templates, NRCWE updated omics in-vivo templates (Figure 11)

🛞 H2020 HARMLESS	× +										~	-	>
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	Templates Wizar	d gallery							0				
	Show All Ph	ys-chem Ecotox	Dose response E	xposure & Release	Metadata	H2020 HAR	MLESS Ten	nplates					
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	Dynamic dissolution by HARMLESS	Define material composition by HARMLESS	Ferric Reduction Ability of Serum by HARMLESS	Omics metada	by ormaTIX,Gov4Na	Omics in-vivo metadata ano,HARMLESS pReg2,Nanoinfor	by rmaTIX,Gov4	Nano,HARMLI	ESS				

Figure 11. Overview of templates developed or updated by HARMLESS partners.



Unique material identifiers (ERM - European Registry of Materials [2]) have been assigned to 23 materials being tested by WP6 (Table 3) and integrated in the Template Wizard.

	. •	י ∂ •	÷								Te	stDataReco	ordingFo	rm_harm	less_FRAS	S (1).xlsx	- Excel						
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4			A			В		C		D	E	F	G	H	1 I	J	K	L	M	N	0	Р	Q
1	Harml	ess				IN-VITRO Test D	ata Reco	ording Form	TDRF)														
2	Please o	complete all a	pplicable field	ds below as fa	r as possible.	Aim to familiarise ye	ourself wit	h the Introduct	ory Guida	nce and E	xample Filled Te	mplates.											
3	While a	iming to star	dardise data	recording as	far as we car	n, flexibility may still	be needed	for some Test/A	ssay type	s and the	ir results:												
4	Thus it	t may be nece	ssary to add	additional ite	ms e.g. for fu	urther replicates, con	entration	s, timepoints, o	other va	riations o	n inputs, result	s outputs, etc.											
5	If so, p	please highlig	ht changes &	alterations e.	g. using colo	ur, and/or comments	in notes,	or adjacent to a	ata/tabk	es to flag	items, fluctuatio	ons from norm	, etc.										
6	TEST C	CONDITION	IS			Please ensure you	also com	plete a Test M	ethod De	escription	Form (TMDF)	for this test t	ype*.										
7																							
8				Project W	/ork Package:	WP6: Safe by Design	Case Stud	dies															
9			Pa	artner conductin	ng test/assay:	BASF																	
10			Lead	d Scientist & co	ntact for test:			E-mail addr	ess:														
11			As	say/Test work	conducted by:			E-mail addr	ess:														
12		Full name o	f test/assay (a	add OECD Test r	ef-ID if app.):	Ferric Reduction Abi	lity of Seru	ım															
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25				NM Co	re chemistry:	SiO2																	
26					CAS No:	7631-86-9																	
27				Mate	erial Supplier:	NOURYON																	
28				M	laterial State:																		
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38		Additiv	es used? If yes,	, specify which	& conc. used:																		
39																							
40				Aids use	d to disperse:			Sonication-B	ath:		Sonication-tip:		Vortexing:		Stirring:								
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	< ►	res	conalti	IONS Ra	w_data_F	KAS Kesult	_rKAS	Material	2	(+)								1 4					

Figure 12. The list of materials is integrated in the Template Wizard and materials are selected via drop down box within the data entry template.

ERM identifiers	Name	CAS	type	Supplier	Supplier code	Core
ERM00000487	Silica-SIL-S	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000488	Silica-SIL-M	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000489	Silica-SIL-L	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000490	Silica-NOSIL-S	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000491	Silica-NOSIL-M	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000492	Silica-NOSIL-L	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000493	Silica-REF-Std	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000494	Silica-ANIS-Std	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000495	Silica-ANIS-Al	7631- 86-9	NPO_1373	NOURYON		SiO2
ERM00000496	LaCoNi			BASF		LaCoNi



ERM00000497	LaCoNi_Pd	BASF	LaCoNi
ERM00000498	LaCoNi_Pt	BASF	LaCoNi
ERM00000499	LaCoNi(5)	BASF	LaCoNi
ERM00000500	LaCoNi(16)	BASF	LaCoNi
ERM00000501	LaNi(22)	BASF	LaNi
ERM00000502	Mat 1_OR	BASF	Aerogel
ERM00000503	Mat 2_ORIN	BASF	Aerogel
ERM00000504	Mat 3_CR	BASF	Aerogel
ERM00000505	Mat 4_PY	BASF	Aerogel
ERM00000506	Imo-OH	CEA	Aluminosilicate
ERM00000507	Imo-CH3	CEA	Aluminosilicate
ERM00000508	Imo-OH-Cu	CEA	Aluminosilicate
ERM00000509	Imo-CH3-Cu	CEA	Aluminosilicate

The procedure to register identifiers is explained in [2] and at <u>https://github.com/NanoCommons/identifiers/blob/master/index.md</u> (Figure 13).

⇒ C	github.com/NanoCommon	s/identifiers/blob/master/inde	ex.md				QE	¥		
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	How to register new n	naterials								
	The process to register new mater	als is described in this docur	ment <mark>and</mark> J. van Rijn et al							
	How to use the identif	ier								
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	Use in semantic web soluti	ons								
	For use in semantic web approach "https://nanocommons.github.io/i	es, an equivalent IRI version dentifiers/registry#".	is available with prefixes t	he short identifie	er with					
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials	es, an equivalent IRI version dentifiers/registry#".	is available with prefixes t	he short identifie	er with					
	For use in semantic web approach "https://nanocommons.github.io/ii Registered materials • the full list can be found at ht	es, an equivalent IRI version dentifiers/registry#". :ps://nanocommons.github.i	is available with prefixes the object of the	he short identifie le format)	er with					
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000057	es, an equivalent IRI version dentifiers/registry#". ps://nanocommons.github.ic ERM00000277-ERM000003	is available with prefixes the optimized optized optimized optimized optimized optimized optimiz	he short identifie le format) M00000461 for N	r with NanoSolve	т				
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM0000001-ERM00000057 • ERM00000058-ERM00000059	es, an equivalent IRI version dentifiers/registry#". ps://nanocommons.github.ic ERM00000277-ERM000003/ for NanoFASE	is available with prefixes the o/identifiers/registry (Turt) 00, and ERM00000326-ER	he short identifie le format) M00000461 for N	er with NanoSolve	т				
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000059 • ERM00000068-ERM00000067 RiskGONE	es, an equivalent IRI version dentifiers/registry#". eps://nanocommons.github.i ERM00000277-ERM0000003 for NanoFASE ERM00000083-ERM000000	is available with prefixes the oridentifiers/registry (Turt 00, and ERM00000326-ER 90, ERM00000099-ERM00	he short identifie le format) M00000461 for N 000276 and ERM	vanoSolve	T -ERM0000	00324 for	r		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000059 • ERM00000068-ERM00000067 RiskGONE • ERM00000068-ERM00000073	es, an equivalent IRI version dentifiers/registry#". tps://nanocommons.github.i ERM00000277-ERM0000003 for NanoFASE ERM00000083-ERM000000 for NanoTest	is available with prefixes the oridentifiers/registry (Turt 00, and ERM00000326-ER	he short identifie le format) M00000461 for N 000276 and ERM	vanoSolve	T -ERM0000	00324 foi	ŗ		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000059 • ERM00000068-ERM00000067 RiskGONE • ERM00000068-ERM00000073 • ERM00000074-ERM00000082	es, an equivalent IRI version dentifiers/registry#". ps://nanocommons.github.i ERM00000277-ERM0000003 for NanoFASE ERM00000083-ERM000000 for NanoTest for caLIBRAte	is available with prefixes the oridentifiers/registry (Turt 00, and ERM00000326-ER	he short identifie le format) M00000461 for N 000276 and ERM	vr with NanoSolve	T -ERM0000	00324 for	r		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000057 • ERM00000063-ERM00000067 RiskGONE • ERM00000068-ERM00000073 • ERM00000064-ERM00000082 • ERM00000091-ERM00000088	es, an equivalent IRI version dentifiers/registry#". eps://nanocommons.github.i ERM00000277-ERM0000003 for NanoFASE ERM00000083-ERM0000000 for NanoTest for caLIBRAte and ERM00000301-ERM000	is available with prefixes the oridentifiers/registry (Turt 00, and ERM00000326-ER 090, ERM00000099-ERM00	he short identifie le format) M00000461 for N 000276 and ERM	vr with NanoSolve 100000307	T -ERM0000	00324 for	r		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000057 • ERM00000063-ERM00000067 RiskGONE • ERM0000068-ERM00000082 • ERM00000064-ERM00000088 • ERM0000001-ERM00000088 • ERM000000462-ERM00000088	es, an equivalent IRI version dentifiers/registry#". eps://nanocommons.github.i ERM00000277-ERM000003 for NanoFASE ERM00000083-ERM0000000 for NanoTest for caLIBRAte and ERM00000301-ERM000 for POLYRISK	is available with prefixes the oridentifiers/registry (Turt 00, and ERM00000326-ER 090, ERM00000099-ERM00	he short identifie le format) M00000461 for N 000276 and ERM	vr with NanoSolve	T -ERM0000	00324 for	r		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000057 • ERM00000068-ERM00000067 RiskGONE • ERM0000068-ERM00000082 • ERM00000074-ERM00000082 • ERM00000048-ERM0000088 • ERM0000048-ERM0000088 • ERM00000487-ERM00000509	es, an equivalent IRI version dentifiers/registry#". eps://nanocommons.github.i ERM00000277-ERM000003 for NanoFASE ERM00000083-ERM0000000 for NanoTest for caLIBRAte and ERM00000301-ERM000 for POLYRISK for HARMLESS	is available with prefixes the optimized state of the optized state of the optimized state of the optimized state	he short identifie le format) M00000461 for N 000276 and ERM	vr with NanoSolve	T -ERM0000	00324 for	r		
	For use in semantic web approach "https://nanocommons.github.io/i Registered materials • the full list can be found at ht • ERM00000001-ERM00000057 • ERM00000008-ERM00000067 RiskGONE • ERM0000068-ERM00000073 • ERM0000068-ERM00000088 • ERM00000462-ERM00000488 • ERM00000462-ERM00000489 • ERM00000462-ERM00000509 • ERM00000487-ERM00000509	es, an equivalent IRI version dentifiers/registry#". eps://nanocommons.github.i ERM00000277-ERM000003 for NanoFASE ERM00000083-ERM0000000 for NanoTest for caLIBRAte and ERM00000301-ERM000 for POLYRISK for HARMLESS for SABYDOMA	is available with prefixes the optimized of the optized of the optimized of the optimized of the optimized o	he short identifie le format) M00000461 for N 000276 and ERM	vr with	T -ERM0000	00324 for	r		

Figure 13. Github repository for ERM identifiers, indicating the ERM range assigned to HARMLESS test cases materials.



To facilitate the description of multicomponent materials, a new template for specifying complex compositions for multicomponent materials has been created, integrated within Template Wizard (<u>https://search.data.enanomapper.net/projects/harmless/datatemplates/pchem/index.html?templ ate=COMPOSITION</u>). Figure 14 illustrates an example with composition data for silica paper, provided by partner.

	А	В	С	D	E	F	G	н	1	J	к	L	м	N
1			Material							Component				
2	Id	entifiers			Comp	Component	FUNCTION			Component identif	iers		Pro	portion
3	Short name	Long name	Substance type	Supplier	onent	type		EINECS	CAS	Name	Tradename	SMILES	lower %	upper %
4	EXAMPLE1	example1	NPO_1373	NOURYON	1	HAS_ADDITIVE	SOLVENT		7732-18-5	water	water	0		
5	EXAMPLE1	example1	NPO_1373	NOURYON	2	HAS_ADDITIVE	DISPERSANT			sodium salt of a maleic and	Orotan 731			
6	EXAMPLE1	example1	NPO_1373	NOURYON	3	HAS_ADDITIVE	DEFOAMER			polyether siloxane	Tego Foamex 810			
7	EXAMPLE1	example1	NPO_1373	NOURYON	4	HAS_ADDITIVE	RHEOLOGY_MO	DIFIER		hydrophobically modified p	Aquaflow NLS-205			
8	EXAMPLE1	example1	NPO_1373	NOURYON	5	HAS_ADDITIVE	PIGMENT			TiO2 - rutile surface treate	Kronos 2190			
9	EXAMPLE1	example1	NPO_1373	NOURYON	6	HAS_ADDITIVE	FILLER		471-34-1	Calcium carbonate	Hydrocarb OG	C(=O)([O-])[O-]	.[Ca+2]	
10	EXAMPLE1	example1	NPO_1373	NOURYON	7	HAS_COMPONEN	COMPONENT		1318-74-7	Siliceous Earth - Silica and	Sillitin Z 89			
11	EXAMPLE1	example1	NPO_1373	NOURYON	8	HAS_ADDITIVE	DEAERATOR			polyether siloxane	Tego Airex 902 W			
12	EXAMPLE2	example2	NPO_1373	NOURYON	1	HAS_ADDITIVE	SOLVENT		7732-18-5	Water	Water	0		
13	EXAMPLE2	example2	NPO_1373	NOURYON	2	HAS_ADDITIVE	COUPLING_AID	252-104-2	34590-94-8	Dipropylene glycol mono p	Dowanol DPnP	CCC(0)0CCCOC		
14	EXAMPLE2	example2	NPO_1373	NOURYON	3	HAS_ADDITIVE	BINDER			acrylic copolymer dispersion	Alberdingk AC 2019	VP		
15	EXAMPLE2	example2	NPO_1373	NOURYON	4	HAS_ADDITIVE	RHEOLOGY_MO	DIFIER		hydrophobically modified p	Aquaflow NLS-205			
16														

Figure 14. Data entry template for multicomponent materials.

Once imported into the eNanoMapper database, the composition of the material can be explored as displayed at Figure 15 or programmatically via the REST API.

^	Substance Name	\$	Substance UUID	\$	Subst	ance Type 🕴	Public name	÷	Reference substance UU	ID \$		Dwner 🕴	I	nfo \$
0 - 1 - @	EXAMPLE1		HRMZ-ce6fafaf ©		NPO_1373		EXAMPLE1	XLSX-0a05	5544c		HARML	<u>ESS</u>	Supplier - NOUR	YON
	Put	Compo Compo rity of IU	sition name: Siliceous E sition UUID: HRMZ-1a0 C Substance:	arth - Si 807f2-7d	ica And Kaolinite,S 0d-3e69-9197-61a	illitin Z 89 (0 % (w/w)) 1941d8230d								
	Туре 🔺		Name	Þ	EC No. 0	CAS No.	typical concentra	tion 0	Concentrat	ion ranges	4)		Structure \$
	Additive (SOLVENT)	& Water				7732-18-5	0 % (w/w)		>=0 %	<=0 %		Also	contained in	H ₂ O
	Additive (DISPERSANT)		731,Sodium Salt Of A Maleic Copolymer				0 m (ww)		>=0 %	<=0 %		Also	contained in	~
	Additive (DEFOAMER)	🕈 Tego Fr	samex 810,Polyether Siloxane				0 % (%)w)		>=0 %	<=0 %		Also (contained in	~
	Additive (RHEOLOGY_MODIFIER)	Aquafic Modified Pr	w Nis-205, Hydrophobically olyacetal Polyether				0 % (n/w)		>=0 %	<=0 %		Also I	contained in	~
	Additive (PIGMENT)		2190, Tio2 - Rutile Surface Treated am And Zirconium Compounds				0 m (m/m)		>=0 %	<=0 %		Also	ortained in	~
	Additive (FILLER)		t Carbonate,Hydrocarb Og			471-34-1	0 % (w/w)		>=0 %	<=0 %		Also	certained in	0 Ca*
	Additive (DEAERATOR)	🕈 Tego Ai	rex 902 W.Polyether Siloxane				0 % (n/m)		>=0 %	<=0 %		Also	contained in	~
	Constituent	& Sliceou	a Earth - Silica And Kaolinite Sillitin			1318-74-7	0 = (w/w)		2=0 %	<=0 %		Also	contained in	

Figure 15. Example of a multicomponent material, provided via the composition data entry template

Material representation

The eNanoMapper database was originally designed as a chemical substance database, with a data model allowing to specify arbitrary compositions and component roles. Multicomponent materials can be represented by a set of components with defined roles, each of which is identified by its own identifiers (e.g. CAS number, name) and chemical structure (e.g. SMILES or InChI, which are the most popular and widely used linear notations for chemical structure representation).

Linear notations are methods for representation of chemical structure connectivity and other molecule features as a character string. Linear notations proved to be one of the most popular and



quite efficient tools in the field of chemoinformatics. Linear notations encode predominantly the CT (connection table) information, which can be enriched with additional atom or bond attributes. Currently SMILES and InChI are the most popular and widely used notations.

We have previously developed software library, Ambit-SLN, for processing of chemical objects via SYBYL Line Notation (SLN) [9] The SYBYL Line Notation is unambiguous, non-unique linear notation developed by TRIPOS Inc. SLN supports syntax for specification of molecules, substructure queries and reactions which cover the capabilities of SMILES, SMARTS and SMIRKS taken together. On top of the basic syntax, SLN includes other powerful features for specification of user defined attributes of atoms, bonds, structures and reactions, macro and Markush atoms for flexible and efficient definition of molecular fragments, search queries and structural libraries as well as 2D and 3D coordinates. All that is accomplished with a unified syntax within a single notation. These features make SLN suitable for database storage as well for data exchange between various programs.

SLN uses largely the same connection notation as SMILES. Also, the SLN specification of atom's and bond's attributes is organized in a similar manner to the SMILES/SMARTS syntax with logical expression of attributes defining chemical information. One of the advantages of the SLN is the syntax extension including comparison operations such as <, <=, >, >= and !=. SLN goes much beyond the capabilities of SMILES and SMARTS. The big "game changer" in the SLN syntax is the support for: user defined attributes; molecular attributes plus definition of 2D and 3D molecular coordinates; definition of macro atoms and Markush atoms which allows compact and efficient handling of large molecules, bio-macro molecules, polymers etc.; use of global and local dictionaries with definitions of macro or Markush atoms.

The InChI Trust works to develop and promote the use of the IUPAC InChI open-source chemical structure representation algorithm https://www.inchi-trust.org/. There is a InChI group dedicated to development of nanomaterial InChI (NInChI), where IDEA is represented. NInChI development is a collaborative effort of domain experts from different fields as well as requires collaboration with other InChi-trust groups such as RInChI (reaction InChI), MInChI (mixture InChI), PInChI (polymer InChI). There are many challenges and many questions. In the last two years a good progress is made identifying the essential NInChI features by an Iterative Prioritization Process [10]. The features are organized in several layers for capturing the NM structure and identity and consists of: core composition, surface topography, surface coatings, functionalization, doping with chemical, impurities, distributions of size, shape, composition and, surface properties, chemical linkages, crystallographic forms etc.

The identified nano data layers of by NInChI group [10] and the development of NInChI prototype are in a good agreement with the features and principles of the SLN. Therefore, IDEA is extending the Ambit-SLN open source package with support multicomponent materials. The software prototype will allow for configurable conversion of material description into a SLN string together with a feasible parallel serialization to NInChI notation (whenever the first official version of the NInChI syntax is released). User-defined SLN attributes will be used to serialize the eNanoMapper/Ambit data model components, while still adhering to the chemical logic defined by the NInChI semantic layers. While NInChI is still under discussion and development, computer readable representation of chemical substances and materials are important in the context of big data analysis.

Material annotation



In the beginning of the HARMLESS project manual annotation of advanced materials in the database was attempted (PN), according to the then available classification [5], which is helping with data gap analysis. The conclusion from this initial analysis is that with proper annotation there is a potential for viewing advanced materials and NAMs in the HARMLESS database.

However, manual annotation is time consuming, not scalable and prone to errors. Moreover, an agreed AdMa (advanced materials) definition is still under discussion, and the suggested description by the OECD Steering Group of Advanced Materials is not public yet. The list of advanced material categories by DAMADEI (project Design & Advanced Materials As a Driver of European Innovation) and MatSEEC (Materials Science and Engineering Expert Committee) are considered by HARMLESS partners as relevant, stressing that not all advanced materials are nano-enabled, and not all nanomaterials are advanced materials.

In a visionary scoping strategy, now nearly a decade old, the DAMADEI platform has structured the term "advanced materials" into several material categories, among them "nanomaterials", and a very similar list was provided by the ESF temporary committee "Materials Science and Engineering Expert Committee". DAMADEI 2013, MatSEEC 2015 The mostly consistent categories of the two sources can be easily merged:

- Active material (e.g. stimuli-responsive)
- composite (advanced if e.g. multi-structural)
- manufacturing (advanced if e.g. additive manufacturing or 3-D-printing)
- Textiles or Fibers (advanced if e.g. sensing)
- Biobased and/or biodegradable
- Nanomaterials
- Ceramic or cementitious
- Coating or targeted surface properties
- Foils and films
- Gels and foams
- Polymers (advanced if e.g. "high-performance")

In an attempt to automatize advanced materials recognition in a database, IDEA performed a feasibility study using text processing AI methods.

As there is no single agreed ontology of advanced materials, we performed two alternative annotations.

Material annotation with oekopol 2020 factsheets

First we used a text document - report on advanced materials, which consists of Factsheets on selected classes of advanced materials written in 2020 [11]. The document consists factsheet for the following classes of advanced materials: DNA-BASED BIOPOLYMERS, RNA-BASED BIOPOLYMERS, PROTEIN-BASED BIOPOLYMERS, SUGAR-BASED BIOPOLYMERS, LIPID-BASED BIOPOLYMERS, MACROSCOPIC COMPOSITES, HYBRIDS, FIBRE-REINFORCED COMPOSITES, PARTICLE REINFORCED COMPOSITES, **MICROPOROUS** MATERIALS, **MESOPOROUS** MATERIALS, MACROPOROUS MATERIALS, ELECTROMAGNETIC METAMATERIALS, ACOUSTIC METAMATERIALS, QUANTUM DOTS, SUPRAPARTICLES, NANOFLOWERS, GRAPHENE, ORGANIC FIBRES, CARBON-BASED FIBRES, INORGANIC FIBRES, ELECTRO-ACTIVE POLYMERS, SELF-REPAIRING POLYMERS, CO-POLYMERS, ADVANCED ALLOYS. Each factsheet consists of section with general information, applications, information on potential



risks, information on environmental impacts and material circularity, and uncertainties. The general information section includes subsections on synonyms, definition, building blocks, structural characteristics, intended change of the materials during use, properties and intended functionalities, other characteristics.

The oekopol list is a bit of a mixture of generic materials categories (which contain both advanced or conventional forms, e.g. *CO-POLYMERS, or PARTICLE REINFORCED COMPOSITES*) and very unique categories (e.g. *GRAPHENE or SELF-REPAIRING POLYMERS*).

The feasibility study was performed with a workflow implemented in Python. The document is parsed using the *pdftotext* package into json structure following the different sections. As an illustration, the text for the properties section is shown in Table 4.

Table 4. Example of the properties section of the advanced materials oekopol 2020 factsheets

DNA-BASED BIOPOLYMERS : DNA based biopolymers interact with their environment. They are mostly constructed to interact with other matter, e.g. as a carrier to deliver drugs they open when in contact with the targeted matter or as cleaning substances to an organic environment they close when in contact with the pollutant. Self-assembly is a further intended functionality.

RNA-BASED BIOPOLYMERS : Intended functionalities include passive, structure-related interaction on nanoscale and active interaction (like an enzymatic function). Also, combinations of RNA-based functionalities (riboswitches, ribozymes, interaction sites, and aptamers) may be intended.

PROTEIN-BASED BIOPOLYMERS : Protein-based biopolymers show outstanding mechanical properties, further they are degradable. A variety of other properties can be designed like superhydrophobicity.

SUGAR-BASED BIOPOLYMERS : Sugarbased biopolymers can be very durable and they are biodegradable. They also show adhesive properties. The combination of stability and biodegradability leads to a range of applications.

LIPID-BASED BIOPOLYMERS : Lipidbased biopolymers can be designed to be biocompatible and biodegradable. For medical purposes they can be designed to (passively) interact with their environment, e.g. for drug delivery and tissue engineering.

FIBRE-REINFORCED COMPOSITES : (Nano)fibre-reinforced composites combine the advantages of (nano-size) fibrous material and composite materials to achieve improved physical properties, like flexibility, catalytic activity, changing reflective index, mechanical strength.

PARTICLE REINFORCED COMPOSITES : Particle-reinforced composites combine the properties of the compounds to improve e.g. their interlaminar shear strength, fracture toughness or fracture energy. Reaction to external magnetic fields can be achieved. Their intended functionalities are often related to reduced delamination and fatigue resistance. MICROPOROUS MATERIALS : Specific conductivity for and/or absorption/isolation of heat or matter, gas transport and

partition due to high free volume. MESOPOROUS MATERIALS : Electronic conductivity, large surface area chemical and electrochemical stability high lifetime and coulombic efficiency

MACROPOROUS MATERIALS : Network strength, create anisotropy and directionality within the networks.

ELECTROMAGNETIC METAMATERIALS : Possible targeted properties are negative or non-linear refractive indices to create new electro-magnetic functionalities like negative permittivity and very high or negative magnetic permeability.

ACOUSTIC METAMATERIALS : Intended functionalities are vibration mitigation and isolation, impact absorption and wave guides.

QUANTUM DOTS : Tuneable optical and electrical characteristics (particle size controls bandgap which defines e.g. the fluorescence spectrum) as opposed to 'classical' semiconductors with fixed bandgap

SUPRAPARTICLES : Magneto-responsivity, dynamically changing electrical properties.

NANOFLOWERS : High surface to volume ratio.

GRAPHENE : Low density, high strength, high conductivity, high transparency.

ORGANIC FIBRES : High stiffness and/or high tensile strength, biocompatibility.

CARBON-BASED FIBRES : High stiffness and/or high tensile strength.

INORGANIC FIBRES : High stiffness and/or high tensile strength, added conductivity.

ELECTRO-ACTIVE POLYMERS : Shape change under an electrical field and vice versa.

SELF-REPAIRING POLYMERS : Selfrepairing of damage to the material with or without external stimulus.

CO-POLYMERS : Different polymer structures depending on mixture – targeted design is comparatively limited.

ADVANCED ALLOYS : Advanced intermetallic alloys (IMA): various, mainly increased strength elastic modulus, inertness and temperature stability, metallic semi-conductors. Shape memory alloys (SMA): one or two specific shape



configurations, which form depending on temperature. High entropy alloys (HEA): exceptional mechanical characteristics (high strength at high temperatures, while brittle at low), low diffusion coefficients.

For each section in each factsheet semantic embeddings were calculated using SBERT Sentence Transformers (<u>https://www.sbert.net/</u>). The semantic embeddings are multidimensional vectors (768 dimensions), and allow for calculation of similarity between arbitrary texts. Different similarity metrics can be used, we provide results with cosine similarity.

-			ADVANCES ALLO	 DNA-BASED BIOPOLYMERS RNA-BASED BIOPOLYMERS PROTEIN-BASED BIOPOLYMERS SUGAR-BASED BIOPOLYMERS LIPID-BASED BIOPOLYMERS MACROSCOPIC COMPOSITES HYBRIDS
FIBRE-REIN PARTICLE REI	DR&ED COMPOSITES ACOUSTIC M NFORCED COMPOSITES ELECTROM HYBRIDS	TAMATERIALS		FIBRE-REINFORCED COMPOSITES PARTICLE REINFORCED COMPOSIT MICROPOROUS MATERIALS MESOPOROUS MATERIALS MACROPOROUS MATERIALS ELECTROMAGNETIC METAMATERIA
-	MESOPOROLS MATERIALS	ORGANIG FIBRES INORGANIC FIBRES CARBON-BASED FIBRES GRABHENE	MACROPOROUS MATERIALS	ACOUSTIC METAMATERIALS QUANTUM DOTS SUPRAPARTICLES NANOFLOWERS GRAPHENE
RNA-BASED COPOLYMERS	CO-POURTMERS	IERS	MACROSCOPIO COMPOSITES	ORGANIC FIBRES
SUSAREWSENSED UPDUTHERS	SELF-REPAIRING POLYMERS	NANOFLOWER	SUPRAPHRTICLES	CARBUN-BASED FIBRES INORGANIC FIBRES ELECTRO-ACTIVE POLYMERS SELF-REPAIRING POLYMERS

Figure 16. Projection of the advanced material categories from [11] based on the semantic embeddings.

After the factsheets have been indexed with the semantic embeddings, we can use arbitrary text to query and find the most similar matches, which can then be utilized as an automated labeling of advanced materials categories. Figure 17 shows examples of querying the indexed factsheets with text describing WP6 materials (aerogels and imogolites) and the corresponding top 3 matches.

Query: Aerogels enable record-thin insula
top k: 3
Run Interact
Aerogels enable record-thin insulation on façades. They can be synthesized directly onto glass fiber mats, thus providing a multicomponent material The release of fragments can contain nanostructured particle aggregates and fibers.
<pre>0.33 MICROPOROUS MATERIALS [sector_construction] construction: Aerogels for heat/sound isolation 0.38 MICROPOROUS MATERIALS [applications] construction: Aerogels for heat/sound isolation energy: Metal-organic-frame 0.52 MICROPOROUS MATERIALS [subgroups] Amorphous Polymer Inorganic Amorphous Polymer Silica Organic Amorphous Polymer</pre>
Query: Modified Imogolites are developed
Run Interact
Modified Imogolites are developed for environmental plant protection. In the current state of development, the product contains multi-components (nanotubular framework, polymer, oxidative molect
0.5 NANOFLOWERS [synonyms] Nanobouquets, nanotrees, nanomeadow, organic-inorganic hybrid nanoflowers (HNFs). 0.51 DNA-BASED BIOPOLYMERS
[sector_agriculture] Agriculture: Tailored encapsulation for plant protection products and fertilizers Agriculture: 0.54 PARTICLE REINFORCED COMPOSITES

Figure 17. Examples of querying the indexed factsheets with text describing WP6 materials (aerogels and imogolites) and the top 3 matches.

[sector_textiles] textiles: Surface modification of empty fruit bunch fibres of oil palm with Cu nanoparticles textil



Similarly, the semantic embeddings were used to predict advanced material annotation for materials from eNanoMapper database (text based on names and material type). Comparison of the results of manual annotation and predicted advanced material categories is shown in Table 5.

name	material	manual	tag1	dist	tag2	dist	tag3	dista
	туре	annotation		anc		ance		nces
	multi		EIDDE	ет	EIRDE	2		
	walled	advanced	FIDRE- REINEORCE		FIDRE- REINEORCE			
	carbon	fibros	D		D		FIBRE-	
	nanotub	carbon-	COMPOSITE		COMPOSITE			
MWCNT (Mitsui)		based fibres	S	0 / 9	S	0 / 9	COMPOSITES	0.50
	L.	buseu mores	SUGAR-	0.45	SUGAR-	0.45	00111 001120	0.50
AgNP (7–10 nm	silver	composite.	BASED		BASED		PARTICI F	
stabilized with	nanonar	hybrid	BIOPOLYME		BIOPOLYME		REINFORCED	
polvethylenimine)	ticle	material	RS	0.51	RS	0.51	COMPOSITES	0.53
AuNP	gold	composite.		0.01		0.01	001110	0.00
(Alkanethiol/lipid.	nanopar	hybrid	NANOFLOW		NANOFLOW		SUPRAPARTIC	
Custom made)	ticle	material	ERS	0.50	ERS	0.50	LES	0.51
	gold	composite.						
AuNP (Citrate.	nanopar	hvbrid	NANOFLOW		NANOFLOW		SUPRAPARTIC	
Custom made)	ticle	material	ERS	0.50	ERS	0.50	LES	0.52
AuNP			-		-		-	
(Poly(allylamine	gold	composite,						
hydrochloride),	nanopar	hybrid	NANOFLOW		NANOFLOW		SUPRAPARTIC	
Custom made)	ticle	material	ERS	0.51	ERS	0.51	LES	0.51
AuNP			SUGAR-		SUGAR-			
(Poly(allylamine	gold	composite,	BASED		BASED			
hydrochloride)/lipid	nanopar	hybrid	BIOPOLYME		BIOPOLYME		CO-	
, Custom made)	ticle	material	RS	0.49	RS	0.49	POLYMERS	0.50
AuNP	gold	RNA-based						
oligonucleotide	nanopar	biopolymer,	SUPRAPART		SUPRAPART		SUGAR-BASED	
complexes	ticle	biopolymer	ICLES	0.53	ICLES	0.53	BIOPOLYMERS	0.54
			MACROPOR		MACROPOR		PARTICLE	
Bentonite - Nano-	BENTON	particulate	OUS		OUS		REINFORCED	
clay	ITE	systems	MATERIALS	0.54	MATERIALS	0.54	COMPOSITES	0.54
	multi-		FIBRE-		FIBRE-			
	walled		REINFORCE		REINFORCE			
CNTSmall, CNT -	carbon		D		D		FIBRE-	
Carbon	nanotub	advanced	COMPOSITE		COMPOSITE		REINFORCED	
NRCWE-026	е	fibres	S	0.43	S	0.43	COMPOSITES	0.45
ENP (S-								
nitrosoglutathione			SUGAR-		SUGAR-			
(GSNO)-loaded		advanced	BASED		BASED			
Eudragit RL	nanopar	polymer,	BIOPOLYME		BIOPOLYME		SUPRAPARTIC	
nanoparticles)	ticle	co-polymer	RS	0.52	RS	0.52	LES	0.52
ENP (empty		advanced					PARTICLE	
Eudragit RL	nanopar	polymer,	SUPRAPART		SUPRAPART		REINFORCED	
nanoparticles)	ticle	co-polymer	ICLES	0.58	ICLES	0.58	COMPOSITES	0.59
		advanced						
		fibres,						
EPOCYL -		carbon-	SUPRAPART		SUPRAPART		QUANTUM	
NRCWE-036		based fibres	ICLES	0.57	ICLES	0.57	DOTS	0.60

Table 5. Comparison between manual annotation for advanced materials and automatic (tag1,tag2,tag3 columns)



		advanced						
		fibres,	CARBON-		CARBON-		MACROPORO	
EPOXY-CNT -		carbon-	BASED		BASED		US	
NRCWE-035		based fibres	FIBRES	0.54	FIBRES	0.54	MATERIALS	0.54
			FIBRE-		FIBRE-			
	multi-	advanced	REINFORCE		REINFORCE			
	walled	fibres,	D		D			
GO - Carbon	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
NRCWE-058	е	based fibres	S	0.57	S	0.57	BASED FIBRES	0.58
Graphene oxide		graphene,						
(NH2-	graphen	particulate					CARBON-	
functionalized)	e oxide	systems	GRAPHENE	0.45	GRAPHENE	0.45	BASED FIBRES	0.49
Graphene oxide		graphene,						
(pristine?) -	graphen	particulate					CARBON-	
GSE83516	e oxide	systems	GRAPHENE	0.50	GRAPHENE	0.50	BASED FIBRES	0.50
Graphene oxide		graphene,						
(pristine?) -	graphen	particulate					CARBON-	
GSE99929	e oxide	systems	GRAPHENE	0.50	GRAPHENE	0.50	BASED FIBRES	0.50
Graphene quantum	CdSe	graphene.						
dots (hvrdoxvl-	quantu	particulate	QUANTUM		QUANTUM		QUANTUM	
modified)	m dot	systems	DOTS	0.42	DOTS	0.42	DOTS	0.43
		advanced						
		fibres.						
Graphite (?) -		carbon-						
GSF92899	granhite	based fibres	GRAPHENE	0 48	GRAPHENE	0 48	GRAPHENE	0 51
00101000	Brapilite	advanced	0	0110	0	01.10	0	0.01
Graphite		fibres.	CARBON-		CARBON-			
(nanofibers Sigma-		carbon-	BASED		BASED		CARBON-	
Aldrich)	granhite	based fibres	FIBRES	0 43	FIBRES	0 43	BASED FIBRES	0 44
Iron oxide NPs	Brapinte		TIBRES .	0.15	TIDNE0	0.15	BROED FIDILES	0.11
(Custom made								
nolvalucose-	iron		SUGAR-		SUGAR-			
sorbitol-	oxide	composite.	BASED		BASED		PARTICI F	
carboxymethyether	nanonar	hybrid	BIOPOLYME		BIOPOLYME		REINFORCED	
(PSC) coated)	ticle	material	RS	0.49	RS	0.49	COMPOSITES	0.49
(multi-		FIBRE-	01.10	FIBRE-	01.15		01.15
	walled	advanced	REINEORCE		REINEORCE			
	carbon	fibres	D		D		FIBRF-	
MWCNT (?) - F-	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
TABM-679	P	based fibres	s	0 49	s	0 49	COMPOSITES	0.51
17(5)(1 075	multi-	buscu nores	EIBRE-	0.45	EIBRE-	0.45	00111 001120	0.51
	walled	advanced			REINEORCE			
	carbon	fibres	D		D			
MWCNT (2) -	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
GSF43515		based fibres	S	0 54	S	0 54	BASED FIBRES	0.55
03243313	multi-	buscu nores		0.54		0.54	DAGED HIDRES	0.55
	walled	advanced						
	carbon	fibres	D		D		FIRRE-	
MWCNT (Bayer	nanotub	carbon-	COMPOSITE		COMPOSITE			
material science)	e	based fibros	S S S S S S S S S S S S S S S S S S S	0⊿1	S S S S S S S S S S S S S S S S S S S	0 ⊿1	COMPOSITES	0 44
	multi-	NUSEU IIDIES	S FIRRE-	J.+1		0.41		5.44
	wallad	advanced	REINEORCE		REINEORCE			
	carbon	fibros	D		D			
	nanotub	carbon-	COMPOSITE		COMPOSITE		CARRON	
MMCNT (Raytuboc)		hased fibros	S	0 /6	S	0 16	RASEN EIDDES	050
ivivicivi (Baylubes)	e multi	based indies		0.40		0.40		0.50
	mulu-	advanced						
rosoarch)	carbon	fibros		0 4 4		0 4 4		0 47
research	Carbon	innes,	υ	0.44	U	0.44	CUIVIPUSITES	0.47



	nanotub	carbon-	COMPOSITE		COMPOSITE			
	е	based fibres	S		S			
	multi-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres.	D		D		FIBRE-	
MWCNT (Sigma-	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Aldrich)	e	based fibres	S	0.44	S	0.44	COMPOSITES	0.46
	multi-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres	D		D			
	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
MWCNT (carpet)	P	based fibres	S	0.43	S	0.43	BASED FIBRES	0.47
	multi-		FIBRE-		FIBRE-			••••
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres.	D		D		FIBRF-	
MWCNT 74 nm	nanotuh	carbon-	COMPOSITE		COMPOSITE		REINEORCED	
NRCWF-007	P	based fibres	s	0 58	s	0 58	COMPOSITES	0 58
	 multi-	bused libres	EIRRE-	0.50	EIRRE-	0.50	00111 001120	0.50
	walled	advanced	REINEORCE		REINEORCE			
MWCNT Chean	carbon	fibres	D		D			
Tubes 74 nm	nanotuh	carbon-	COMPOSITE		COMPOSITE		CARBON-	
		based fibres	composite	0.56	composite	0.56	BASED EIRRES	0.60
NRCVIL-007	cinglo	based libres		0.50		0.50	BASLD FIBRLS	0.00
	single-							
	walleu	fibros	REINFORCE		REINFORCE			
	carbon	nores,					CARRON	
NNA 411 Carban	nanotup		CONPOSITE	0.57	COMPOSITE	0.57		0.50
NW-411 - Carbon	е	based fibres	3	0.57	3	0.57	BASED FIBRES	0.58
NINI		composite,	MACKUPUK		MACKUPUK			
ININ -	allumin	nybria	UUS		UUS		NANOFLOWE	
				~				
Aluminosilicate clay	osilicate	material	MATERIALS	0.54	MATERIALS	0.54	RS	0.54
Aluminosilicate clay	osilicate	material	MATERIALS FIBRE-	0.54	MATERIALS FIBRE-	0.54	RS	0.54
Aluminosilicate clay	osilicate	material advanced	MATERIALS FIBRE- REINFORCE	0.54	MATERIALS FIBRE- REINFORCE	0.54	RS	0.54
Aluminosilicate clay	osilicate	material advanced fibres,	MATERIALS FIBRE- REINFORCE D	0.54	MATERIALS FIBRE- REINFORCE D	0.54	RS PARTICLE	0.54
Aluminosilicate clay	osilicate	material advanced fibres, carbon-	MATERIALS FIBRE- REINFORCE D COMPOSITE	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE	0.54	RS PARTICLE REINFORCED	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay	osilicate allumin osilicate	material advanced fibres, carbon- based fibres	MATERIALS FIBRE- REINFORCE D COMPOSITE S	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S	0.54	RS PARTICLE REINFORCED COMPOSITES	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL	osilicate allumin osilicate	material advanced fibres, carbon- based fibres advanced	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED	0.54	RS PARTICLE REINFORCED COMPOSITES	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric	osilicate allumin osilicate nanopar	material advanced fibres, carbon- based fibres advanced polymer,	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME	0.54	RS PARTICLE REINFORCED COMPOSITES	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles)	osilicate allumin osilicate nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles)	osilicate allumin osilicate nanopar ticle silicon	material advanced fibres, carbon- based fibres advanced polymer, co-polymer	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065,	osilicate allumin osilicate nanopar ticle silicon dioxide	material advanced fibres, carbon- based fibres advanced polymer, co-polymer	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar	material advanced fibres, carbon- based fibres advanced polymer, co-polymer	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067,	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS	0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS SUPRAPARTIC LES	0.54 0.57 0.54 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS SUPRAPARTIC LES	0.54 0.57 0.54 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069,	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS SUPRAPARTIC LES	0.54 0.57 0.54 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS	0.54 0.56 0.53 0.51	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU SUPRAPARTIC LES MESOPOROU	0.54 0.57 0.54 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU SMATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU SMATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica NRCWE#070, Porous Silica 100	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material porous material	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53 0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material porous material porous material advanced	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU SMATERIALS MESOPOROU SMATERIALS MESOPOROU SMATERIALS	0.54 0.57 0.54 0.53 0.53 0.54
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material porous material advanced alloys,	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS	0.54 0.56 0.53 0.51 0.52 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS MESOPOROU S MATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53 0.53
Aluminosilicate clay NN-etched - Aluminosilicate clay NP-ERL (Eudragit RL PO polymeric nanoparticles) NRCWE#065, Porous Silica 300 nm - Silica NRCWE#067, Porous Silica 100 nm - Silica NRCWE#069, Porous Silica 300 nm-CuO - Silica NRCWE#070, Porous Silica 100 nm-CuO - Silica	osilicate allumin osilicate nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle silicon dioxide nanopar ticle	material advanced fibres, carbon- based fibres advanced polymer, co-polymer porous material porous material porous material advanced alloys, intermetalli	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS FIBRE- REINFORCE	0.54 0.56 0.53 0.51 0.52 0.52	MATERIALS FIBRE- REINFORCE D COMPOSITE S LIPID-BASED BIOPOLYME RS QUANTUM DOTS QUANTUM DOTS QUANTUM DOTS QUANTUM FIBRE- REINFORCE	0.54 0.56 0.53 0.51 0.52 0.52	RS PARTICLE REINFORCED COMPOSITES CO- POLYMERS MESOPOROU S MATERIALS MESOPOROU S MATERIALS MESOPOROU S MATERIALS	0.54 0.57 0.54 0.53 0.53 0.54



			COMPOSITE		COMPOSITE			
			S		S			
			FIBRE-		FIBRE-			
		advanced	REINFORCE		REINFORCE			
		alloys,	D		D			
NRCWE-021	zinc	intermetalli	COMPOSITE		COMPOSITE		ADVANCED	
ZnFe2O4 30 nm	ferrite	C	S	0.61	S	0.61	ALLOYS	0.63
		-	FIBRF-		FIBRF-			
		advanced	REINFORCE		REINFORCE			
		allovs.	D		D			
NRCWE-022	nickel	intermetalli	COMPOSITE		COMPOSITE		CARBON-	
NiFe2O4 30 nm	ferrite	c	S	0.66	S	0.66	BASED FIBRES	0.68
	multi-	-	FIBRF-		FIBRF-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres.	D		D		FIBRF-	
NRCWF-040 -	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Carbon	e	based fibres	s	0 50	s	0 50	COMPOSITES	0 50
	 multi₋		EIBRE-	5.50	 FIBRF-	5.50	55 65.TE5	0.50
	walled	advanced	REINFORCE		REINFORCE			
	carhon	fibres	D		D		FIBRF-	
NRCWF-041 -	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Carbon	e	hased fibres	s s	0 52	ς ς	0 52	COMPOSITES	በፍን
	multi_	Sused IIDIES	S FIRRF-	0.02	 FIBRF-	0.02		0.52
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibros	D		D			
NRCW/F-042 -	nanotub	carbon-			COMPOSITE		CARBON	
Carbon		based fibres	controstite	0.53	controstre	0 5 3	BASED EIBRES	0.54
Carbon	multi_	Sascu IIDIES	J FIRRF-	0.00	 FIBRF-	0.00	DAJED HIBNES	0.54
	walled	advanced						
	carbon	fibros	D		D		FIBRE-	
	nanotub	carbon-	CONNECTIFE		CONNECCITE		REINEORCED	
Carbon		hasod fibres	S	0 52	S	052	COMPOSITES	050
	multi_	Sused IIDIES		5.52		0.52	CONTROSTES	0.52
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibros	nenvrukce		D			
	nanotub	carbon-	CONNECTIFE		CONNECCITE		CARRON	
Carbon		hased fibros	S	0 50	S	0 ⊑ว	RASEN EIPPES	0 50
Carbon	C			0.52		0.52	DAJLU FIDRES	0.52
	muiti-	advanced	FIDICE- REINICODOCE		REINEOPCE			
	carbon	fibros						
		corbon						
NACWE-045 -	nanotub	based fibres	convirusite	0 50	cUIVIPUSITE	0 50		0 51
Cal DUII	e	based fibres		0.50		0.50	CUIVIPUSITES	0.51
	muiti-	advanced						
	walled	advanced	REINFUKCE				EIDDE	
	Cdruon	nores,						
INKLWE-046 -	anotup	carbon-	CUIVIPUSITE	0 5 1	CONPOSITE	0.54	COMPOSITES	0 50
Carbon	e	based fibres	3	0.51	<u> </u>	0.51	COMPOSITES	0.52
	multi-	a duama a d	FIBRE-		FIBKE-			
	walled	advanced	REINFURCE		REINFURCE			
	carbon	TIDRES,					FIBRE-	
NKCWE-047 -	nanotub	carpon-	COMPOSITE	0.54	COMPOSITE	0.54	KEINFURCED	0 54
Carbon	e	based fibres	5	0.51	5	0.51	COMPOSITES	0.51
	multi-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	tibres,	D		D		FIBRE-	
		_						
NRCWE-048 -	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	



	multi-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres.	D		D		FIBRE-	
NRCWF-049 -	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Carbon	P	based fibres	s	0 49	s	0 49	COMPOSITES	0 50
	single-	buscu marcs		0.15		0.15	00111 001120	0.50
	walled	advanced						
	carbon	fibros	D		D			
	carbon	nores,					CARRON	
Carbon	nanotub		COMPOSITE	0 5 4	CONPOSITE	0 5 4		0.54
Carbon	e	based libres		0.54		0.54	DASED FIDRES	0.54
	Single-	a du an aa d						
	walleu	fibree	REINFORCE		REINFORCE			
	Carbon	nores,					CARRON	
NKCWE-052 -	nanotub	carbon-	COMPOSITE	0.55	COMPOSITE	0.55		0.55
Carbon	е 	based fibres	5	0.55	5	0.55	BASED FIBRES	0.55
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,	D		D			
NRCWE-053 -	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
Carbon	е	based fibres	S	0.54	S	0.54	BASED FIBRES	0.54
	single-	. -	FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,	D		D			
NRCWE-054 -	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
Carbon	e	based fibres	S	0.53	S	0.53	BASED FIBRES	0.54
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,	D		D		FIBRE-	
NRCWE-055 -	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Carbon	е	based fibres	S	0.53	S	0.53	COMPOSITES	0.54
Carbon	e single-	based fibres	S FIBRE-	0.53	S FIBRE-	0.53	COMPOSITES	0.54
Carbon	e single- walled	based fibres advanced	S FIBRE- REINFORCE	0.53	S FIBRE- REINFORCE	0.53	COMPOSITES	0.54
Carbon	e single- walled carbon	based fibres advanced fibres,	S FIBRE- REINFORCE D	0.53	S FIBRE- REINFORCE D	0.53	COMPOSITES	0.54
Carbon NRCWE-056 -	e single- walled carbon nanotub	advanced fibres, carbon-	S FIBRE- REINFORCE D COMPOSITE	0.53	S FIBRE- REINFORCE D COMPOSITE	0.53	COMPOSITES FIBRE- REINFORCED	0.54
Carbon NRCWE-056 - Carbon	e single- walled carbon nanotub e	based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S	0.53	S FIBRE- REINFORCE D COMPOSITE S	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon	e single- walled carbon nanotub e single-	based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE-	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE-	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon	e single- walled carbon nanotub e single- walled	based fibres advanced fibres, carbon- based fibres advanced	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon	e single- walled carbon nanotub e single- walled carbon	based fibres advanced fibres, carbon- based fibres advanced fibres,	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE-	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 -	e single- walled carbon nanotub e single- walled carbon nanotub	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon-	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE-	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE-	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi-	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres,	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 -	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon-	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE	0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE	0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED FIBRE- REINFORCED	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi-	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE	0.53 0.53 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres,	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE	0.53 0.53 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.56	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi-	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE-	0.53 0.53 0.53 0.56 0.56	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.56	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES	0.54 0.53 0.56 0.58
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE	0.53 0.53 0.53 0.56	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE	0.53 0.53 0.53 0.56	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES	0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED	0.54 0.53 0.56 0.58
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon NRCWE-063 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES FIBRE- REINFORCED COMPOSITES	0.54 0.53 0.56 0.58 0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon NRCWE-063 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e multi-	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE S FIBRE- REINFORCE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.56 0.58 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54 0.53 0.56 0.58 0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon NRCWE-063 - Carbon NRCWE-063 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled carbon nanotub e multi- walled	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54 0.53 0.56 0.58 0.54
Carbon NRCWE-056 - Carbon NRCWE-057 - Carbon NRCWE-061 - Carbon NRCWE-062 - Carbon NRCWE-063 - Carbon NRCWE-063 - Carbon NRCWE-064 - Carbon	e single- walled carbon nanotub e single- walled carbon nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled nanotub e multi- walled carbon nanotub e multi- walled carbon	based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres advanced fibres, carbon- based fibres	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58 0.53	S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S FIBRE- REINFORCE D COMPOSITE S	0.53 0.53 0.53 0.56 0.58 0.53	COMPOSITES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES CARBON- BASED FIBRES FIBRE- REINFORCED COMPOSITES FIBRE- REINFORCED COMPOSITES	0.54 0.53 0.56 0.58 0.54



	nanotub	carbon-	COMPOSITE		COMPOSITE			
	е	based fibres	S		S			
		advanced						
		allovs.					FIBRF-	
NiFe2O4 30 nm	nickel	intermetalli	OUANTUM		OUANTUM		REINFORCED	
NRCWF-022	ferrite	c	DOTS	0.69	DOTS	0.69	COMPOSITES	0 70
	Territe	advanced	2013	0.05	2013	0.05	colum osiries	0.70
	nickol	allovs					FIRRE_	
Ni7nEo409.20 nm	zinc	intormotalli	OUANTUM		OUANTUM			
	forrito		QUANTON	0.66	QUANTON	0.66	COMPOSITES	0.60
INRCIVE-020	einele	L		0.00		0.00	CONPOSITES	0.09
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,					CARRON	
	nanotub		COMPOSITE	0.52	COMPOSITE	0.52		0.52
SWCNT (P2-SWNT)	e	based fibres	3	0.52	3	0.52	BASED FIBRES	0.53
	poly(am							
	idoamin							
	e)	advanced						
PAMAM dendrimer-	dendrim	polymer,	СО-		СО-		СО-	
NH2	er	co-polymer	POLYMERS	0.52	POLYMERS	0.52	POLYMERS	0.52
	poly(am							
	idoamin							
	e)	advanced						
PAMAM-NH2	dendrim	polymer,	СО-		СО-		MESOPOROU	
(Dendritech Inc.)	er	co-polymer	POLYMERS	0.55	POLYMERS	0.55	S MATERIALS	0.55
	poly(am							
	idoamin							
	e)	advanced						
PAMAM-OH	dendrim	polymer,	СО-		СО-		MESOPOROU	
(Dendritech Inc.)	er	co-polymer	POLYMERS	0.55	POLYMERS	0.55	S MATERIALS	0.55
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres.	D		D			
SWCNT (?) -	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
GSE83516	e	based fibres	S	0.49	S	0.49	BASED FIBRES	0.51
	single-		FIBRF-		FIBRF-			
	walled	advanced	REINEORCE		REINFORCE			
	carbon	fibres	D		D			
SWCNT (?) -	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
GSF83516	e	based fibres	s	0 49	s	0 49	BASED FIBRES	0 51
00100010	single-		EIBRE-	0.15	EIBRE-	0.15	BRIGEBTIBREG	0.51
	walled	advanced						
SWCNT (Carbon	carbon	fibros	D		D			
Nanotochnology	nanotub	nores,					CARRON	
CNII)		carbon-	CONPOSITE	0.44	CONPOSITE	0.44	CANDON-	0.47
CNI)	e	based fibres	5	0.44	3	0.44	BASED FIBRES	0.47
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
au (au = (a=a	carbon	fibres,	D		D			
SWCNT (SES	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
research)	e	based fibres	5	0.47	5	0.47	BASED FIBRES	0.47
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,	D		D		FIBRE-	
SWCNT (Sigma-	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
Aldrich)	е	based fibres	S	0.47	S	0.47	COMPOSITES	0.48
	single-		FIBRE-		FIBRE-		FIBRE-	
SWCNT (iron-	walled	advanced	REINFORCE		REINFORCE		REINFORCED	
enriched)	carbon	fibres,	D	0.46	D	0.46	COMPOSITES	0.47



	ماريخ معرم م	a a ult a u	COMPOCITE		COMPOCITE			
	nanotub	carbon-	CONPOSITE		CONPOSITE			
	e	based fibres	S		S			
	single-		FIBRE-		FIBRE-			
	walled	advanced	REINFORCE		REINFORCE			
	carbon	fibres,	D		D		FIBRE-	
	nanotub	carbon-	COMPOSITE		COMPOSITE		REINFORCED	
SWCNT (purified)	e	based fibres	S	0.46	S	0.46	COMPOSITES	0.47
					EIRRE_			••••
		ار مع برما م			FIDAL-			
		auvanceu	REINFURCE		REINFORCE			
	carbon	fibres,	D		D			
SWCNT 2 nm	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
NM-411	e	based fibres	S	0.53	S	0.53	BASED FIBRES	0.53
		advanced	PARTICLE		PARTICLE			
	silicon	polymer,	REINFORCE		REINFORCE			
Silica (2D	dioxide	electro-	D		D			
nanosilicates, a	nanopar	active	COMPOSITE		COMPOSITE		NANOFLOWF	
lavered clav)	ticle	nolymer	s	0 5 3	c	0 5 3	RS	0.54
layered clay	cilicon	polymer	5	0.55	5	0.55	10	0.54
	SIIICON	mesoporou			1456000000			
SIIICA NP (DMPC-	aioxide	s material,	MESUPORO		MESOPORO			
coated magnetic	nanopar	porous	US		US		SUGAR-BASED	
mesoporous)	ticle	material	MATERIALS	0.54	MATERIALS	0.54	BIOPOLYMERS	0.55
	silicon	mesoporou						
Silica NP (PEG-	dioxide	s material,	MESOPORO		MESOPORO			
coated magnetic	nanopar	porous	US		US		MESOPOROU	
mesonorous)	ticle	material	ΜΔΤΕΡΙΔΙS	0 50	ΜΔΤΕΡΙΔΙ S	0 50	S MATERIAI S	0 53
mesoporousy	cilicon	macanarau	NII (TENII (ES	0.50	NII (TENII (ES	0.50	5 10// (1 E1()/ (25	0.55
	shicon	mesoporou	45600000		145600000			
Silica NP (pristine	aloxide	s material,	MESOPORO		MESOPORO			
magnetic	nanopar	porous	US		US		SUGAR-BASED	
mesoporous)	ticle	material	MATERIALS	0.49	MATERIALS	0.49	BIOPOLYMERS	0.50
			PARTICLE		PARTICLE			
	titanium	advanced	REINFORCE		REINFORCE			
	dioxide	fibres,	D		D			
TiO2 nanobelts	nanopar	inorganic	COMPOSITE		COMPOSITE		SUPRAPARTIC	
(Custom made)	ticle	fibres	5	0 51	\$	0.51	IFS	0 52
(custom made)	tiele	libres		0.51		0.51	220	0.52
	t : t = = i	ار مع برما م						
	titanium	auvanceu	REINFURCE		REINFORCE			
102 nanotubes	dioxide	fibres,	D		D		PARTICLE	
(100nm, Custom	nanopar	inorganic	COMPOSITE		COMPOSITE		REINFORCED	
made)	ticle	fibres	S	0.53	S	0.53	COMPOSITES	0.53
			FIBRE-		FIBRE-			
	titanium	advanced	REINFORCE		REINFORCE			
TiO2 nanotubes	dioxide	fibres.	D		D			
(30nm Custom	nanonar	inorganic	COMPOSITE		COMPOSITE		SUPRAPARTIC	
(com) custom	ticle	fibros	s	0 54	s	054	IFS	054
maacy	titonium	advanced	5	0.94	5	0.54	LLJ	0.94
		auvanced						
	aioxide	fibres,						
	nanopar	inorganic	QUANTUM		QUANTUM		SUPRAPARTIC	
TiO2NF_1.1_NF	ticle	fibres	DOTS	0.57	DOTS	0.57	LES	0.58
	titanium	advanced						
	dioxide	fibres,						
TiO2NF 9,1 Sol B	nanopar	inorganic	QUANTUM		QUANTUM		NANOFLOWE	
M 15h	ticle	fibres	DOTS	0.53	DOTS	0.53	RS	0.53
··	titanium	advanced		2.00		2.00		2.55
	diovide	fibree						
	uioxide	indres,	CUIDD 4 5		CUDD 4 5			
	nanopar	inorganic	SUPRAPART		SUPRAPART		NANOFLOWE	
TiO2_1.1_NF	ticle	fibres	ICLES	0.55	ICLES	0.55	RS	0.59
	titanium	advanced	QUANTUM		QUANTUM		SUPRAPARTIC	
TiO2 11 Sil Sol	dioxide	fibres,	DOTS	0.55	DOTS	0.55	LES	0.55



	nanopar	inorganic						
	ticle	fibres						
	titanium	advanced						
	dioxide	fibres,						
	nanopar	inorganic	SUPRAPART		SUPRAPART		NANOFLOWE	
TiO2_9.1_NF	ticle	fibres	ICLES	0.57	ICLES	0.57	RS	0.60
	titanium	advanced						
	dioxide	fibres,					PARTICLE	
	nanopar	inorganic	SUPRAPART		SUPRAPART		REINFORCED	
TiO2_9.1_NF_BM	ticle	fibres	ICLES	0.57	ICLES	0.57	COMPOSITES	0.60
	titanium	advanced						
	dioxide	fibres,						
	nanopar	inorganic	QUANTUM		QUANTUM		MESOPOROU	
TiO2_9.1_sol_BM	ticle	fibres	DOTS	0.57	DOTS	0.57	S MATERIALS	0.59
	titanium	advanced						
	dioxide	fibres,					PARTICLE	
	nanopar	inorganic	SUPRAPART		SUPRAPART		REINFORCED	
TiO2_NF_BM_2h	ticle	fibres	ICLES	0.54	ICLES	0.54	COMPOSITES	0.55
	titanium	advanced						
	dioxide	fibres,						
	nanopar	inorganic	SUPRAPART		SUPRAPART		QUANTUM	
TiO2_NF_BM_4h	ticle	fibres	ICLES	0.54	ICLES	0.54	DOTS	0.55
	titanium	advanced						
	dioxide	fibres,					PARTICLE	
	nanopar	inorganic	SUPRAPART		SUPRAPART		REINFORCED	
TiO2_NF_BM_6h	ticle	fibres	ICLES	0.55	ICLES	0.55	COMPOSITES	0.55
	titanium	advanced						
	dioxide	fibres,						
	nanopar	inorganic	SUPRAPART		SUPRAPART		QUANTUM	
TiO2_NF_BM_9h	ticle	fibres	ICLES	0.55	ICLES	0.55	DOTS	0.56
		advanced						
		alloys,						
ZnFe2O4 30 nm	zinc	intermetalli	QUANTUM		QUANTUM		ADVANCED	
NRCWE-021	ferrite	C	DOTS	0.65	DOTS	0.65	ALLOYS	0.68
			SUGAR-		SUGAR-			
		advanced	BASED		BASED			
phage mimetic		fibres,	BIOPOLYME		BIOPOLYME		QUANTUM	
nanorods (PMN)	nanorod	organic	RS	0.52	RS	0.52	DOTS	0.53
			FIBRE-		FIBRE-			
	multi-	advanced	REINFORCE		REINFORCE			
	walled	fibres,	D		D			
rGO - Carbon	nanotub	carbon-	COMPOSITE		COMPOSITE		CARBON-	
NRCWE-059	е	based fibres	5	0.58	5	0.58	BASED FIBRES	0.59

Material annotation with InnoMat.Life AdMa categories

The InnoMat.Life categorisation (InnoMatLife D1.7, February 2022) is not yet published, but was made available to HARMLESS with approval of the InnoMat.Life concortium. In short, it proposed to categorise materials in three dimensions (Figure 18):

- Does the material consist of particles? (Particles of any aspect ratio: the original scheme does not differentiate spheroidal, elongated or platelet shape categories. This would be criteria of the risk screening that may be triggered)
- Is the material nano-enabled?



Manufacturing processes or materials considered as "advanced" are highlighted in red. The criteria are consistent with the OECD SG AdMa rationale that Advanced Materials are made by rational design, using precise control of its composition and internal structure, and/or are transformed through advanced manufacturing techniques. To be an AdMa, the material must have exceptional properties (mechanical, electric, optic, magnetic etc.) or specific functionalities that differentiate them from the rest of materials (e.g. self-repairing, shape change, ..., transformation of energy). The relative novelty is a qualifier, which will cease to qualify a material as "advanced" after some time.

A flow-scheme was developed by HARMLESS Task 4.2 to support the annotation, exemplified on the aerogel-fibre-mat case study (). This scheme only assigns materials to categories. Health and Safety may be the motivation, but is not actually delivered by this scheme. HARMLESS WP4 would need to add the identification of specific concerns, and assessment strategies.



Figure 18. InnoMat.Life categorisation of materials (conventional and advanced) with the assessment criteria.



Do we dea	il with particles	?			-												
Does particles (can also b	Me	Iting &	read	tion			does th particl	ne material c es (e.g. susp powder)	consist of ension or		yes –	▶ go to	second	column			
No	go to first colu	imn					No	go to the fi	rst column								
	go to moreon						it is a m ² r	mat contain	ing internally	norous an	rogel						
							itis a ili i		ing meenany	porous ac	logei						
	-							materialis	s composite								
								or formula	tion. (nice to								
								кп	iow)								
													-			 	
ls it a na (NEP)? Ap	ano-enabled propply the ISO def	oduct inition	yes I	In Strategy In Str	go to seco ower left o nano-en internal o struct	abled by or surface tures						is it your defin	a nanon regional nition (ir	naterial? by ly applicable n EU: REACH)	yes —	 go to secor right quadr is a nanom be asses	nd row = lower rant = material raterial, has to rsed as such.
No	▶ go to first quadrant: lin particles or	row = upper nited releva of nanostruc	left nce of tures									no —		go to first right quadra non-nano, dust issues consi	row = upper int: material is but general s need to be dered.		
											1						
						Is it an adva the OECD \	inced mate VPMN deso AdMa	rial? apply cription of		Yes	rational design, superior performa	document the ca in red color, document the reason	se study and <mark>AdMa</mark>				
											-						
						No	docu	ment case st	udy in black	color:							
								conventio	nal material								

Figure 19. InnoMat.Life flowchart on the example (yellow highlights) of aerogel-fibre-mats.

To apply the categorisation to the NRCWE materials, in comparison to the oekopol 2020 annotation, we combined the materials list of DAMADEI and MatSEEC (which are mutually compatible, but not identical), amended by additional classes, and tried to annotate for each an "advanced" version. Note that most of the classes are final products (potentially nano-enabled, potentially containing nanomaterials), whereas the nanomaterial classes are listed at the end of this list:

- 1) Final products (potentially nano-enabled, potentially containing nanomaterials)
 - Coatings
 - Advanced if e.g. self-healing
 - Paints
 - o Advanced if e.g. anti-soiling or based on dendrimers
 - Rubber
 - Advanced if e.g. low-wear tires
 - Ceramics
 - Glasses
 - Metal alloys
 - Advanced e.g. if shape-memory
 - One also notes the existence of the JRC "Institute for Advanced Materials (IAM)", 1755 ZG Petten, The Netherlands. Their research topics feature SiC-Ceramics for Aviation, Mechanical Characteristic of Cr-Ni Steels, and VVER-1000 Reactor Pressure Vessel. These topics are highly consistent with the "advanced alloy" and "ceramics" class in DAMADEI and MatSEEC schemes. But these materials are no nanomaterials by REACH [12] and are probably not even nanoenabled.
 - Plastics
 - o Advanced if e.g. biobased, traceable, recyclable, biodegrading,
 - 3D printed parts (the additive manufacturing process is advanced, not the resulting parts)
 - Metal (e.g. by SLS process (starting from micronised powder))
 - Polymer (e.g. by SLS process (starting from micronised powder), or by fused-filament process (starting from macroscopic filament)
 - Concrete (not by SLS process)



- Metamaterials (acoustic, radar)
- Textiles
 - o Advanced if e.g. sensing
- Battery electrodes
 - Advanced if e.g. fast-charging
- Solar cells, mostly conventional Si.
 - Advanced e.g. halide perovskites
- Fibre-reinforced Composites, (fibres have primarily mechanical reinforcement purpose)
 - conventional, e.g. Carbon-Fibre Reinforced Polymer (CFRP), Glass-Fibre Reinforced Polymer (GFRP)
 - o Adv. e.g. if recyclable, repairable
- Particle-filled Composites, (particles have not always mechanical reinforcement purpose)
 - conventional, incl. rubbers (CB, SAS in tires), coatings (e.g. transparent car coating)
 - o Advanced e.g. QLED[™] color converter or flexible display electrode, or dispersoid-pinned alloy
- Catalysts,
 - o conventional, e.g. three-way exhaust cleaning (TWC)
 - Advanced if e.g. five-way exhaust cleaning functionality (e.g. enabled by perovskites)
- Foams:
 - Conventional e.g. polymer foam
 - o Advanced: Aerogel insulation panels
- Sensor devices
 - Conventional: e.g. antibody-labeled Au NPs in pregnancy test; in analogy, also the covid tests, although a novel product & mass market, would be seen as incremental adaption only. [13]
- Advanced material for electrical power transmission: High-Temp. Superconductor cables
- Advanced material: Metal-Organic Framework, e.g. for CO₂ capture
- Advanced: Metamaterials (nano if for vis/NIR light, non-nano if for acoustic waves)
- 2) Nanomaterials by REACH criteria ("consisting of particles, etc")
 - Pigments & Fillers
 - not all nanomaterials are advanced materials, e.g. most grades of silica, pigments or Carbon Black are several decades old. Their nanoforms are now reported to the R-nano registry [14]. These materials rank high (ranks #1-5, 7, 9-12, 14-18) in the public list of production volumes above 100 tons to above 10,000 tons in France alone, which represents 3.4% of global GDP, allowing for a scaling to global production and comparison of use categories [15].
 - Advanced pigment e.g. Q-Dots
 - o Advanced filler e.g. graphenes, mwCNT, swCNT, TiO₂ cubes, TiO₂ fibers, Ag wires
 - Drug delivery formulation
 - Advanced e.g. if active vector (as focused on by the JRC workshop on advanced materials, [16] or if DNA-origami

Applying the above assessment, some advanced materials are nano-enabled, but still no nanomaterials by the REACH definition, and are not made via particles. E.g. aerogels are no nanomaterials by REACH, but the fragments that they potentially release during the lifecycle can be assessed by methods and tiered testing schemes developed for nanomaterials, with the above-listed limitation to respirable fractions [17][18].

Furthermore, some nanomaterials are advanced materials, e.g. quantum dots are still relatively novel and consist of NPs. Their unique properties enable advanced display technology [19][20][21]. We have thus annotated the NRCWE materials (Table 6).



Table 6. Manual annotation for advanced materials by InnoMat.Life criteria. A last column was added with the additional annotation to material classes, where the specific material could be contained as ingredient/component.

name	material class	Functionali ty	Could be used as ingredient in which final product material class?	Is there a benefit vs. conventional material? Which?	Consists of particle s/ fibres/ platelet s?	Advance d ?	Nano- material or nano- enabled ?
NRCWE-006 MWCNT (Mitsui)	multi- walled carbon nanotube	mechanical modulus	FIBRE- REINFORCE D COMPOSIT ES	Compare CFRP	Yes	yes	Yes (borderlin e to non- nano)
AgNP (7–10 nm, stabilized with polyethylenimi ne)	silver nanoparticl e	Biocidal activity	PARTICLE REINFORCE D COMPOSIT ES	Compare other food packaging	Yes	Yes (due to targeted structure)	Yes
AuNP (Alkanethiol/lip id, Custom made)	gold nanoparticl e	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	No (due to highly establish ed market)	yes
AuNP (Citrate, Custom made)	gold nanoparticl e	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	No (due to highly establish ed market)	yes
AuNP (Poly(allylamine hydrochloride), Custom made)	gold nanoparticl e	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	No (due to highly establish ed market)	yes
AuNP (Poly(allylamine hydrochloride)/ lipid, Custom made)	gold nanoparticl e	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	No (due to highly establish ed market)	yes
AuNP oligonucleotide complexes	gold nanoparticl e	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	No (due to highly establish ed market)	yes
Bentonite - Nano-clay	BENTONITE	Barrier properties, adsorption properties	PARTICLE REINFORCE D COMPOSIT ES, food processing aid	Established as clarifier in winemaking (by adsorption, flocculation)	Yes	No	Yes
CNTSmall, CNT - Carbon NRCWE-026	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Compare CFRP	Yes	yes	Yes



ENP (S- nitrosoglutathi one (GSNO)- loaded Eudragit RL nanoparticles)	Polymer nanoparticl e	Taste masking and encapsulati on during stomach phase	Drug delivery	Co-Polymer class is used since 1950ies	Yes	Yes (targeted structure)	Yes
ENP (empty Eudragit RL nanoparticles)	Polymer nanoparticl e	Taste masking and encapsulati on during stomach phase	Drug delivery	Co-Polymer class is used since 1950ies	yes	Yes (targeted structure)	Yes
EPOCYL - NRCWE-036	multi- walled nanotube suspended in liquid epoxy precursor	mechanical modulus	FIBRE- REINFORCE D COMPOSIT ES	Compare CFRP	No (NM contain ed)	yes	Yes
EPOXY-CNT - NRCWE-035	multi- walled nanotube in epoxy	mechanical modulus	FIBRE- REINFORCE D COMPOSIT ES	Compare CFRP	No (NM contain ed)	yes	Yes
GO - Carbon NRCWE-058	graphene oxide	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (targeted structure	Yes
Graphene oxide (NH2- functionalized)	graphene oxide	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (targeted structure	Yes
Graphene oxide (pristine?) - GSE83516	graphene oxide	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (targeted structure	Yes
Graphene oxide (pristine?) - GSE99929	graphene oxide	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (targeted structure	Yes
Graphene quantum dots (hyrdoxyl- modified)	Carbon particle	luminescen ce	PARTICLE COMPOSIT ES	No heavy metals	Yes	yes	yes
Graphite (?) - GSE92899 Graphite (nanofibers, Sigma-Aldrich)	graphite graphite						
Iron oxide NPs (Custom made, polyglucose-	iron oxide nanoparticl e	Heats up in AC	Hyper- thermia	Other cancer therapies	yes	Yes (due to medical	yes



sorbitol- carboxymethye ther (PSC)		magnetic field	therapy of tumours			applicat on only)	i
MWCNT (?) - E- TABM-679	multi- walled carbon nanotube?	Mechanical modulus, conductivit y?	FIBRE- REINFORCE D COMPOSIT ES?		Yes	yes	Yes
MWCNT (?) - GSE43515	multi- walled carbon nanotube?	Mechanical modulus, conductivit y?	FIBRE- REINFORCE D COMPOSIT ES?		Yes	yes	Yes
MWCNT (Bayer material science)	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT (Baytubes)	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT (SES research)	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT (Sigma-Aldrich)	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT (carpet)	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT 74 nm NRCWE-007	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
MWCNT Cheap Tubes 74 nm NRCWE-007	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NM-411 - Carbon	multi- walled	Mechanical modulus,	FIBRE- REINFORCE	Can achieve conductivity at	Yes	yes	Yes



	carbon nanotube	conductivit y	D COMPOSIT ES	lower loading than w/ CB. Mechanics: compare CFRP			
NN - Aluminosilicate clay	alluminosili cate	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (due to targeted structure	Yes
NN-etched - Aluminosilicate clay	alluminosili cate	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (due to targeted structure	Yes
NP-ERL (Eudragit RL PO polymeric nanoparticles)	Polymer nanoparticl e	Taste masking and encapsulati on during stomach phase	Drug delivery	Co-Polymer class is used since 1950ies	yes	Yes (due to targeted structure	Yes
NRCWE#065, Porous Silica 300 nm - Silica	silicon dioxide nanoparticl e		Drug delivery	Compare similar aggregated grades of SiO2	Yes	borderlin e	Νο
NRCWE#067, Porous Silica 100 nm - Silica	silicon dioxide nanoparticl e		Drug delivery	Compare similar aggregated grades of SiO2	Yes	borderlin e	Borderlin e
NRCWE#069, Porous Silica 300 nm-CuO - Silica	silicon dioxide nanoparticl e	Delayed release of biocide	Drug delivery	Compare similar aggregated grades of SiO2	Yes	Yes, (multi- compone nt)	No
NRCWE#070, Porous Silica 100 nm-CuO - Silica	silicon dioxide nanoparticl e	Delayed release of biocide	Drug delivery	Compare similar aggregated grades of SiO2	Yes	Yes, (multi- compone nt)	Borderlin e
NRCWE-020 NiZnFe4O8 30 nm	nickel-zinc ferrite			Cannot tell. R&D material, not for specific use	Yes		Yes
NRCWE-021 ZnFe2O4 30 nm	zinc ferrite			Cannot tell. R&D material, not for specific use	Yes		Yes
NRCWE-022 NiFe2O4 30 nm	nickel ferrite			Cannot tell. R&D material, not for specific use	yes		Yes
NRCWE-040 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit Y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-041 - Carbon	multi- walled	Mechanical modulus,	FIBRE- REINFORCE D	Can achieve conductivity at lower loading	Yes	yes	Yes



	carbon	conductivit	COMPOSIT	than w/ CB.			
	nanotube	У	ES	wiechanics:			
	multi-	Mechanical	FIBRE-	conductivity at			
NRCW/F-042 -	walled	modulus	REINFORCE	lower loading			
Carbon	carbon	conductivit	D	than w/ CB	Yes	yes	Yes
carbon	nanotube	v	COMPOSIT	Mechanics:			
		,	ES	compare CFRP			
				Can achieve			
	multi-	Mechanical	FIBRE-	conductivity at			
NRCWE-043 -	walled	modulus,	REINFORCE	lower loading			
Carbon	carbon	conductivit	D	than w/ CB.	Yes	yes	Yes
	nanotube	У	COMPOSIT	Mechanics:			
			ES	compare CFRP			
			EIDDE	Can achieve			
	multi-	Mechanical	FIBRE-	conductivity at			
NRCWE-044 -	walled	modulus,	D	lower loading	Voc	Vac	Vac
Carbon	carbon	conductivit	COMPOSIT	than w/ CB.	165	yes	163
	nanotube	У	FS	Mechanics:			
			20	compare CFRP			
			FIBRE-	Can achieve			
	multi-	Mechanical	REINFORCE	conductivity at			
NRCWE-045 -	walled	modulus,	D	lower loading	Yes	ves	Yes
Carbon	carbon	conductivit	COMPOSIT	than w/ CB.		,	
	nanotube	У	ES	Mechanics:			
			-	compare CFRP			
			FIBRE-	Can achieve			
	multi-	Mechanical	REINFORCE	conductivity at			
NRCWE-046 -	walled	modulus,	D	lower loading	Yes	yes	Yes
Carbon	carbon	conductivit	COMPOSIT	than w/ CB.			
	nanotube	У	ES	Mechanics:			
				Compare CFRP			
	multi	Machanical	FIBRE-	conductivity at			
	multi-	modulus	REINFORCE				
Carbon	carbon	conductivit	D	than w/ CB	Yes	yes	Yes
Carbon	nanotube	v	COMPOSIT	Mechanics:			
	hanotabe	У	ES	compare CFRP			
				Can achieve			
	multi-	Mechanical	FIBRE-	conductivity at			
NRCWE-048 -	walled	modulus.	REINFORCE	lower loading			
Carbon	carbon	conductivit	D	than w/ CB.	Yes	yes	Yes
	nanotube	У	COMPOSIT	Mechanics:			
		-	ES	compare CFRP			
				Can achieve			
	multi-	Mechanical	FIBKE-	conductivity at			
NRCWE-049 -	walled	modulus,		lower loading	Vor	Vec	Vec
Carbon	carbon	conductivit	COMPOSIT	than w/ CB.	163	yes	103
	nanotube	У	FS	Mechanics:			
			LJ	compare CFRP			
			FIBRF-	Can achieve			
	multi-	Mechanical	REINFORCE	conductivity at			
NRCWE-051 -	walled	modulus,	D	lower loading	Yes	Ves	Yes
Carbon	carbon	conductivit	_ COMPOSIT	than w/ CB.		<i>y</i> c 5	
	nanotube	У	ES	Mechanics:			
				compare CFRP			



NRCWE-052 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-053 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-054 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-055 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-056 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-057 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-061 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-062 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-063 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	yes	Yes
NRCWE-064 - Carbon	multi- walled carbon nanotube	Mechanical modulus, conductivit y	FIBRE- REINFORCE D	Can achieve conductivity at lower loading than w/ CB.	Yes	yes	Yes



			COMPOSIT	Mechanics:			
			ES	compare CFRP			
			Cannot tell.				
NiEo2O4 20 pm	nickol		R&D				
	forrito		material,		Yes		Yes
INRCOVE-022	lenne		not for				
			specific use				
			Cannot tell.				
NiZnFe4O8 30	nickal zina		R&D				
nm	forrito		material,		Yes		Yes
NRCWE-020	lenne		not for				
			specific use				
	singlo		FIBRE-	Can achiovo			
	single-	conductivit	REINFORCE				
	carbon	v	D	lower loading	yes	yes	yes
500101	nanotube	y	COMPOSIT	than w/ CB			
	nanotube		ES	than wy cb.			
	nolv(amido	Tunahle		Conolymer is	No <i>,</i>		No (single
PAMAM	amine)	responsive	Drug	stimuli-	single	VPS	molecules
dendrimer-NH2	dendrimer	ness	delivery	responsive	molecul	yes	are no
	dendrimer	11633		responsive	е		NM)
	nolv(amido	Tunahle		Copolymer is	No,		No (single
(Dendritech	amine)	responsive	Drug	stimuli-	single	Ves	molecules
	dendrimer	ness	delivery	responsive	molecul	yes	are no
inc.)	dentarimer	ness		responsive	е		NM)
ραμαμ-ομ	nolv(amido	Tunable		Conolymer is	No,		No (single
(Dendritech	amine)	responsive	Drug	stimuli-	single	VPS	molecules
	dendrimer	ness	delivery	responsive	molecul	yes	are no
inc.)	uchannel	11035		responsive	е		NM)
	single-		FIBRE-				
SWCNT (?) -	walled		REINFORCE				
GSE83516	carbon		D				
	nanotube?		COMPOSIT				
			ES?				
	single-		FIBRE-				
SWCNT (?) -	walled		REINFORCE				
GSE83516	carbon		D				
	nanotube?		COMPOSIT				
			ES?				
	single-		FIBRE-	Can achieve			
SWCNT (Carbon	walled	conductivit	REINFORCE	conductivity at			
Nanotechnolog	carbon	у	D	lower loading	yes	yes	yes
y, CNI)	nanotube		COMPOSIT	than w/ CB.			
			ES				
	single-		FIBRE-	Can achieve			
SWCNT (SES	walled	conductivit	REINFORCE	conductivity at			
research)	carbon	У		lower loading	yes	yes	yes
	nanotube		CUMPUSII	than w/ CB.			
	single-		FIBKE-	Can achieve			
SWCNT (Sigma- Aldrich)	walled	conductivit	REINFURCE	conductivity at	100	1100	1/00
	carbon	У		lower loading	yes	yes	yes
	nanotube		EC	than w/ CB.			
	cingle		ES	Con ochieve			
SWCNT /irea	single-	conductivit	FIBRE-	can achieve			
enriched)	walleu	v	REINFORCE	lower loading	yes	yes	yes
ennuneu)	carbon y	D	than w/ CP				
	nanocube			than w/ CB.			



			COMPOSIT FS				
SWCNT (purified)	single- walled carbon nanotube	conductivit Y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB.	yes	yes	yes
SWCNT 2 nm NM-411	carbon nanotube	conductivit Y	FIBRE- REINFORCE D COMPOSIT ES	Can achieve conductivity at lower loading than w/ CB.	yes	yes	yes
Silica (2D nanosilicates, a layered clay)	silicon dioxide nanoparticl e	Barrier & adsorption properties	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
Silica NP (DMPC-coated magnetic mesoporous)	silicon dioxide nanoparticl e	Filler		Cannot tell. R&D material, not for specific use	yes	Yes (multico mponent)	yes
Silica NP (PEG- coated magnetic mesoporous)	silicon dioxide nanoparticl e	Filler		Cannot tell. R&D material, not for specific use	yes	Yes (multico mponent)	yes
Silica NP (pristine magnetic mesoporous)	silicon dioxide nanoparticl e	Filler		Cannot tell. R&D material, not for specific use	yes	Yes (multico mponent)	yes
TiO2 nanobelts (Custom made)	titanium dioxide nanoparticl e	Filler		Cannot tell. R&D material, not for specific use	yes	Yes (targeted structure	yes
TiO2 nanotubes (100nm, Custom made)	titanium dioxide nanoparticl e	Filler	Particle- reinforced composite	Paint, paper, plastics,	yes	no	borderline
TiO2 nanotubes (30nm, Custom made)	titanium dioxide nanoparticl e		Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2NF_1.1_NF	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2NF_9,1_Sol _BM_15h	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_1.1_NF	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_11_Sil_So I	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	Cannot tell by name



TiO2_9.1_NF	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_9.1_NF_B M	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_9.1_sol_B M	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	Cannot tell by name
TiO2_NF_BM_2 h	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_NF_BM_4 h	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_NF_BM_6 h	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
TiO2_NF_BM_9 h	titanium dioxide nanoparticl e	pigment	Particle- reinforced composite	Paint, paper, plastics,	yes	no	yes
ZnFe2O4 30 nm NRCWE-021	zinc ferrite	Filler		Cannot tell. R&D material, not for specific use	yes	Yes (multico mponent)	yes
phage mimetic nanorods (PMN)	nanorod						
rGO - Carbon NRCWE-059	graphene (via reduction of GO)	Barrier properties	PARTICLE REINFORCE D COMPOSIT ES	Laminate structures, other 2D fillers	Yes	Yes (graphen e is much younger than GO)	Yes

The textminning approach is difficult to apply to the InnoMat.Life classification above provided by partners, because it only lists categories and provided a few terse examples, without sufficient text description the texmining requires. Therefore, we augment our approach, by relying on recent AI developments, namely Generative Pre-trained Transformer 3 (GPT-3) language model [22], as exposed by OpenAI API (<u>https://openai.com/api/</u>). The OpenAI provides a range of functionalities, e.g. question and answer (Figure 20) or parsing unstructured data (Figure 22, Figure 24). While the figures below are screenshots of the browser playground provided for illustration of the capabilities, we have used the OpenAI API programmatically via Python notebooks, which allows to automatically send large number of queries and obtain the responses in machine readable form.



Playground - OpenAl API × +		~ -	
← → C		<i>È</i> ☆	:
Overview Documentation Examples Playground	🗲 Upgra	ade 🕐 Help N	Personal
Playground OSA × ~	Save	View code Share	
I am a highly intelligent question answering bot. If you ask me a question that is rooted in truth, I will give you the answer. If you ask me a question the is nonsense, trickery, or has no clear answer, I will respond with "Unknown". Q: Please list properties of fast charging battery electrodes? A: Fast charging battery electrodes typically have high electrical conductivity, high surface area, low internal resistance, and high capacity. O: Please list functionality of anti-soling paints? A: Anti-soling paints are designed to prevent the formation of soles on the surface of a material. They are typically used to protect surfaces from corrosion, abrasion, and other forms of wear and tear. They also provide a protective barrier against water, oil, and other liquids. O: Definition of active vector materials used in drug delivery formulations? A: Active vector materials are substances used in drug delivery formulations to transport therapeutic agents to specific sites in the body. These materials can be natural or synthetic polymers, lipids, or other molecules that can be used to encapsulate and protect the drug, target it to a specific site, and control its release. Examples of active vector materials include polymers, liposomes, micelles, and nanocarriers.	at 🍨	Mode Temperature Maximum length Stop sequences Enter sequence and press I w x Top P	
Looking for ChatGPT? Try it now	×	Frequency penalty	0
Submit O & O	273	Presence penalty	0

Figure 20. Screenshot of OpenAI playground for question answering. The user provides the question (Q:) and the OpenAI generates the answer. The same Q&A functionality can be requested programmatically.

We have arranged the suggested InnoMat.Life classification as three columns (Query, class and advanced) – the first three shaded columns on Figure 21, in a total of 60 rows. Then we programmatically queried the OpenAI Q&A for definition, composition, property, functionality and applications, based only on the query column (e.g. 'Q: property of shape-memory metal alloys'). The rest of the columns Figure 21 are filled by the OpenAI responses. We also provide the results as a separate file for examination by the experts.

G1	2 • i X v fr Shape-memory metal alloys are typically composed of nickel-titanium (NiTi), copper-aluminum-nickel (CuAINi), and iron-manganese-silicon (FeMnSi).														
_	A	В	C	F	G	Н		J	К	L	M	N	0	Р	1
1	query	class	advanced	definition	composition	property	functionality	pplications							
2	coatings	coatings	FALSE	Coatings are thin	Coatings are typically co	Properties of coatings car	Coatings are used to provide	e Coatings ar	e used in	a variety o	f applicatio	ns, includin	g automotiv	/e, aerosp	ace
3	self-healing coatings	coatings	TRUE	Self-healing coat	Self-healing coatings typ	Self-healing coatings typic	Self-healing coatings are coa	a Self-healing	g coatings	s have a wid	de range of	application	s, including		<u> </u>
4	paints	paints	FALSE	Paints are pigme	Paint is typically compo-	Properties of paint includ	Paint is a liquid or mastic co	n Paints are u	used for a	variety of	application	s, including	interior and	exterior	val
5	anti-soiling paints	paints	TRUE	Anti-soiling paint	Anti-soiling paints typica	Anti-soiling paints are des	Anti-soiling paints are design	Anti-soiling	paints ar	e used in a	variety of a	pplications	, including:		
6	paints based on dendrimers	paints	TRUE	Paints based on o	Paints based on dendrin	Dendrimer-based paints of	Paints based on dendrimers	c Dendrimers	s are a typ	be of nanor	naterial tha	t can be us	ed to create	e paints w	thu
7	rubber	rubber	FALSE	Rubber is a mate	Rubber is composed of	Rubber is a highly elastic i	Rubber is a material with a v	Rubber is u	sed in a w	vide variety	of applicat	ions, includ	ing tires, se	als, gasket	s, h
8	low-wear tires	rubber	TRUE	Low-wear tires a	Low-wear tires are typic	Low-wear tires typically h	Low-wear tires are designed	Low-wear t	tires are c	commonly u	used in appli	ications wh	ere long tir	e life is de	sire
9	ceramics	ceramics	FALSE	Ceramics are a t	Ceramics are typically o	Ceramics are typically har	Ceramics are materials mad	e Ceramics h	ave a wid	le range of	application	s, including:			
10	glasses	glasses	FALSE	Glasses are fram	Glasses are typically cor	Optical properties, scratc	The primary function of glas	s Glasses are	common	nly used to (correct visio	on, such as	nearsighted	lness, farsi	ght
11	metal alloys	metal alloys	FALSE	Metal alloys are	Metal alloys are compo	Metal alloys typically hav	Metal alloys are combinatio	r Metal alloy	s are use	d in a wide	variety of a	pplications	, including a	utomotiv	9 CC
12	shape-memory metal alloys	metal alloys	TRUE	Shape-memory r	Shape-memory metal a	Shape-memory metal allo	Shape-memory metal alloys	Shape-men	nory meta	al alloys are	e used in a v	ariety of ap	oplications,	including I	nec
13	plastics	plastics	FALSE	Plastics are synth	Plastics are typically cor	Plastics are lightweight, d	Plastics are versatile materia	a Plastics are	used in a	wide varie	ty of applic	ations, incl	uding packa	ging, cons	truc
14	biobased plastics	plastics	TRUE	Biobased plastic:	Biobased plastics are ty	Biobased plastics have pr	Biobased plastics are plastic	s Biobased p	lastics ha	ve a wide r	ange of app	lications, ir	cluding pac	kaging, au	ton
15	traceable plastics	plastics	TRUE	Traceable plastic	Traceable plastics are ty	Traceable plastics typical	Traceable plastics are plasti	c Traceable p	plastics ar	e used in a	variety of a	pplications	, including r	nedical de	vice
16	recyclable plastics	plastics	TRUE	Recyclable plasti	Recyclable plastics are t	The main property of rec	Recyclable plastics are mate	r Recyclable	plastics c	an be used	to make a v	ariety of p	roducts, inc	luding pac	kag
17	biodegrading plastics	plastics	TRUE	Biodegrading pla	Biodegrading plastics ar	Biodegradable plastics ar	Biodegrading plastics are pla	a: Biodegradi	ng plastic:	s can be use	ed in a varie	ty of applic	ations, incl	uding pacl	tagi
18	Fused Deposition Modeling (FDM	3D printed parts process	TRUE	Fused Deposition	Fused Deposition Mode	Fused Deposition Modelin	Fused Deposition Modeling	(F Fused Depo	sition Mo	odeling (FDI	M) is a 3D p	rinting tech	nology that	is used to	cre
19	Stereolithography (SLA)	3D printed parts process	TRUE	Stereolithograph	Stereolithography (SLA)	Stereolithography (SLA) is	Stereolithography (SLA) is a	f Stereolitho	graphy (S	LA) is a 3D	printing tecl	nology use	ed to create	parts and	pre
20	Selective Laser Sintering (SLS)	3D printed parts process	TRUE	Selective Laser S	Selective Laser Sintering	Selective Laser Sintering (Selective Laser Sintering (SL	Selective La	aser Sinte	ring (SLS) is	a 3D printir	ng technolo	gy that use	s a laser te	o fu
21	Digital Light Processing (DLP)	3D printed parts process	TRUE	Digital Light Proc	Digital Light Processing	Digital Light Processing (D	Digital Light Processing (DLP) DLP techno	logy is us	ed in a vari	ety of appli	cations, inc	luding proje	ectors, 3D	prir
22	Multi Jet Fusion (MJF)	3D printed parts process	TRUE	Multi Jet Fusion (MJF) is a 3D printing tech	Multi Jet Fusion (MJF) is a	Multi Jet Fusion (MJF) is a 30	O Multi Jet Fu	usion (MJI	F) is a 3D pr	inting techn	ology that	uses a com	bination o	f fu
23	textiles or fibers	textiles or fibres	FALSE	Textiles or fibers	Textiles and fibers are c	Properties of textiles or fi	Textiles and fibers are used	f Textiles and	d fibers ha	ave a wide	range of ap	plications, i	ncluding clo	othing, hor	ne
24	sensing textiles or fibers	textiles or fibres	TRUE	Sensing textiles c	Sensing textiles or fibers	Tactility.	Sensing textiles or fibers can	Sensing tex	tiles or fil	bers can be	used in a vi	ariety of ap	plications, i	including r	ned
25	battery electrodes	battery electrodes	FALSE	Battery electrod	Battery electrodes are t	The properties of battery	Battery electrodes are the c	c Battery ele	ctrodes a	re used in a	a variety of	application	s, including	portable e	lec
26	fast charging battery electrodes	battery electrodes	TRUE	Fast charging bat	Fast charging batteries t	Fast charging battery elec	Fast charging battery electro	Fast charging	ng battery	electrode:	s can be use	d in a varie	ty of applic	ations, ind	lud
27	solar cells	solar cells	FALSE	Solar cells are de	Solar cells are typically of	Solar cells have the prope	Solar cells are devices that o	Solar cells h	have a wi	de range of	application	is, including	powering	nomes and	l bu
28	solar cells based on halide perove	solar cells	TRUE	Solar cells based	Solar cells based on hali	Halide perovskite solar ce	Halide perovskite solar cells	a Halide pero	ovskite so	lar cells hav	ve a wide ra	nge of app	lications, in	cluding po	wei
29	solar cells based on perovskites	solar cells	TRUF	Solar cells based	Solar cells based on per	Some of the properties of	Solar cells based on perovsk	ir Solar cells b	based on	perovskites	s can be use	d in a varie	tv of applic	ations. inc	ludi ▼

Figure 21. Screenshot of automatic augmentation of InnoMat.Life classification based on OpenAI (GPT-3) query answering.

While free text responses can be used in a similar manner as the text mining approach described earlier, the option of parsing unstructured data allows for requesting further details. The screenshot at Figure 22 illustrates how we can ask for examples of specific class of materials (metal-organic framework in this case).





Figure 22. Screenshot of OpenAI playground for unstructured data parsing. The user provides the question and a table template and the OpenAI generates the answer, filling in the table. The same functionality can be requested programmatically.

Using the same 60 queries representing InnoMat.Life classification, we asked for examples of each class of materials, resulting on overall 223 examples, structured as in Figure 23. Note that there is specific column whether material is nanoenabled, not nano, or nanomaterial, and another column specifying if the material is made of particles, platelets or fibres. Since the advanced material concept is not well defined at the moment, we decided to ask for how long the material has known applications (column J, *application_since*).

1	A	В	C	D	E	F	G	Н	1	J	К	L
1	query_s	productclass_s	advanced_s	material_s	materialclass_ss	functionality_ss	productclass_ss	benefits_ss	is_particle_s	lications_sinc	isnano_s	synonyms_ss
2	coatings	coatings	FALSE	Titanium dioxide	Inorganic compound	UV protection, self-clear	Paint, coating, plastic	Improved durability, scra	Particles	1970s	Nanomaterial	TiO2, Titania
3	coatings	coatings	FALSE	Zinc oxide	Inorganic compound	UV protection, anti-fouli	Paint, coating, plastic	Improved durability, scra	Particles	1970s	Nanomaterial	ZnO, Zincite
4	coatings	coatings	FALSE	Silver	Metal	Anti-bacterial, anti-foulir	Paint, coating, plastic	Improved durability, scra	Particles	1990s	Nanomaterial	Ag, Argentum
5	coatings	coatings	FALSE	Graphene	Carbon allotrope	Anti-corrosion, anti-fouli	Paint, coating, plastic	Improved durability, scra	Platelets	2000s	Nanomaterial	Graphite, Carbon
6	self-healing coatings	coatings	TRUE	Polyurethane	Polymer	Self-healing	Paint, coating, adhesive	Longer lasting, improved	Particles	2000s	Nanoenabled	Polyurethane-based
7	self-healing coatings	coatings	TRUE	Polysiloxane	Polymer	Self-healing	Paint, coating, adhesive	Improved flexibility, impr	Particles	2000s	Nanoenabled	Polysiloxane-based
8	self-healing coatings	coatings	TRUE	Polyurea	Polymer	Self-healing	Paint, coating, adhesive	Improved durability, imp	Particles	2000s	Nanoenabled	Polyurea-based self-
9	self-healing coatings	coatings	TRUE	Polydopamine	Polymer	Self-healing	Paint, coating, adhesive	Improved adhesion, impr	Particles	2010s	Nanomaterial	Polydopamine-based
10	paints	paints	FALSE	Titanium dioxide	Pigment	Opacity	Paint, coating, ink, plastic	High hiding power, UV pr	Particles	1950s	Nanomaterial	TiO2, Titania
11	paints	paints	FALSE	Acrylic	Resin	Binding	Paint, coating, ink, plastic	High flexibility, durability	Particles	1950s	Nanomaterial	Polymethyl methacr
12	paints	paints	FALSE	Silica	Pigment	Opacity	Paint, coating, ink, plastic	High hiding power, UV pr	Particles	1950s	Nanomaterial	Silicon dioxide
13	paints	paints	FALSE	Alkyd	Resin	Binding	Paint, coating, ink, plastic	High flexibility, durability	Particles	1950s	Nanomaterial	Polyester resin
14	anti-soiling paints	paints	TRUE	Silica	Inorganic	Anti-soiling	Paint	Improved durability, wat	Particles	1980s	Nanoenabled	Silicon dioxide, quar
15	anti-soiling paints	paints	TRUE	Titanium dioxide	Inorganic	Anti-soiling	Paint	Improved durability, wat	Particles	1980s	Nanoenabled	Titanium oxide, titar
16	anti-soiling paints	paints	TRUE	Zinc oxide	Inorganic	Anti-soiling	Paint	Improved durability, wat	Particles	1980s	Nanoenabled	Zincite, zinc white
17	anti-soiling paints	paints	TRUE	Polytetrafluoroethyle	Polymer	Anti-soiling	Paint	Improved durability, wat	Fibres	1950s	None	Teflon, PTFE
18	paints based on dendrim	epaints	TRUE	Dendrimers	Polymers	Antimicrobial, UV protec	Paints, coatings, adhesiv	Improved durability, bett	Particles	1990s	Nanomaterial	Starburst molecules
19	rubber	rubber	FALSE	Natural rubber	Polymer	Elasticity	Footwear, tires, hoses, b	More elasticity, better sh	Particles	Ancient time	None	Caoutchouc, India n
20	rubber	rubber	FALSE	Styrene-butadiene rul	Polymer	Elasticity	Footwear, tires, hoses, b	More elasticity, better sh	Particles	1930s	None	SBR, Buna-S
21	rubber	rubber	FALSE	Nitrile rubber	Polymer	Oil resistance	Hoses, gaskets, seals, etc	Better oil resistance, bet	Particles	1940s	None	Buna-N, NBR
22	low-wear tires	rubber	TRUE	Silica	Inorganic	Low-wear	Tire rubber	Increased wear resistance	Particles	1970s	Nanoenabled	Silicon dioxide
23	low-wear tires	rubber	TRUE	Carbon black	Inorganic	Low-wear	Tire rubber	Increased wear resistance	Particles	1970s	Nanoenabled	Lamp black, acetyle
24	low-wear tires	rubber	TRUE	Polytetrafluoroethyle	Polymer	Low-wear	Tire rubber	Increased wear resistance	Fibres	1970s	None	Teflon, Fluon
25	low-wear tires	rubber	TRUE	Polyurethane	Polymer	Low-wear	Tire rubber	Increased wear resistance	Platelets	1970s	None	Polyether, Polyester
26	ceramics	ceramics	FALSE	Alumina	Ceramic	Wear resistance	Refractory material	High temperature resista	Particles	1950s	None	Aluminum oxide
27	ceramics	ceramics	FALSE	Zirconia	Ceramic	High strength	Refractory material	High temperature resista	Particles	1950s	None	Zirconium oxide
28	ceramics	ceramics	FALSE	Silicon Carbide	Ceramic	High hardness	Refractory material	High temperature resista	Particles	1950s	None	Carborundum
29	ceramics	ceramics	FALSE	Mullite	Ceramic	High thermal shock resist	Refractory material	High temperature resista	Particles	1950s	None	3Al2O3.2SiO2
30	glasses	glasses	FALSE	Glass	Inorganic	Transparent	Window frames, lenses,	Durable, heat resistant, l	Platelets	Ancient time	None	Silica, quartz, soda-l

Figure 23. Results of automatic augmentation of the Innomat.Life classification. The columns Query, class and advanced are arranged based on the Innomat.Life classification. The rest of the columns are filled in with OpenAI responces. The annotation column is filled by asking OpenAI API to parse unstructured data queryinto a table with columns : material, material class, functionality, potential ingredient in which final product material class, benefit over convential material, does it consist of particles or fibres or platelets, since when it is used in applications, is it nanomaterial or nanoenabled or none and synonyms.

Therefore, we have amended the terse InnoMat.Life classification with both free text description (related to the ones we found in OEKOPOL factsheets) and structured data table with example



materials. Feedback from expert on the validity of the automated annotation is welcome. The output does not have the goal of directly assigning the AdMa class, but have sufficient information to be used as a supporting tool for searching if a material of interest is similar to the ones in the table, and considering the columns B (AdMa class) and C (advanced material yes or no). Integrating both the structured and unstructured similarity search in eNanoMapper database is ongoing.



Figure 24. Screenshot of OpenAl playground for unstructured data parsing. The user provides the question and a table template and the OpenAl generates the answer, filling in the table. (The color code relates to the uncertainty of the prediction of particular letters – green – high confidence, red – lower confidence). The same functionality can be requested programmatically.

Similarly, we can ask for structured data of specific material (Figure 24) and performed this programmatically for over 2000 materials in eNanoMapper HARMLESS database (this number includes caNanoLab), resulting in a table of 2269 rows. Excerpts of the annotation are shown in Figure 25, the annotation of NRCWE materials (same materials as in Table 6) is shown in **Error! Reference source not found.**



H10	04 🔹 i 🗙 🗸	f _x High streng	th, low density, bio	odegradability,	renewable, nor	i-toxic, etc.								*
	۵	в		c	D	F	F	G	н			ĸ		
1	name he v	publicname b	e zubstance		material e v	materialclass s	 functionality r 		benefite r v	is particle T	applications since y	ispano. s		
38	NM-402 MW/CNT 12.7 pm	IRCNM04002a	multi-wall	ed carbon r Mi	WCNT 12.7 pm	Carbon Nanotub	a Conductive The	Bohmer Ceramic	High Strength	Sibrer	2000	Nanomaterial	Multiaug	lled Carb
41	MW/CNT 20-20 pm	IRCNM40002a	multi-wall	led carbon r Mi	WCNT 12.7 IIII	Carbon Nanotub	e Conductive, The	m Flactronics Aaross	High Strength,	Fibrer	2000	Nanomaterial	Multi-wa	lled Carb
42	MWCNT 20-30 nm	IRCNM40005a	multi-wall	led carbon r Mi	WCNT	Carbon Nanotub	e Conductive, The	m Electronics, Aeros	High Strength,	Fibrer	2000	Nanomaterial	Multi-wa	lled Carb
42	MWCNT 20-30 nm	IRCNM40000a	multi-wall	led carbon r Mi	WCNT	Carbon Nanotub	e Conductive, The	m Electronics, Aeros	High Strength,	Fibrer	2000	Nanomaterial	Multi-wa	lled Carb
55	MWCNT <9 pm	IRCNM40004a	multi-wall	led carbon r Mi	WCNT < 9 nm II	Carbon nanotub	Conductive, The	m Bolymor composity	High strength,	Fibrer	2000	Nanomaterial	Multi-wa	lled carb
56	MW/CNT < 9 nm	IRCNM40010a	multi-wall	led carbon r Mi	WCNT <8 nm li	Carbon nanotub	Conductive, The	m Conductive materi	High electrical	Fibres	2000	Nanomaterial	Multi-wa	lled carb
84	2-budromethal collulore	TVLOSE HS 6000 VP2	multi-wai	2.k	weren so him a	Polymer	Thickening agent	Cormetic pharma	Non-toxic bio	Fibres	1050c	None	TYLOSE	
104	AS (-COOH) - Nanocellulose	LIPM BIOFIBBILS AS		lar cellulose LC	OOH)	Nanocellulose	LIPM BIOFIBRIES	Ecod cosmetics n	High strength	Fibres	Since the early 2000s	Nanomaterial	Nanofibr	illar cellu
144	CNE 90 NM WI 20161026.1	CANANOLAR 716063	nanonorm	ar cellulose (-C	IE RO NIM W/L2	Carbon nanofibr	Conductive The	Pobu, cosmetics, p	High strength,	Fibres	3016	Nanomaterial	Carbon	anofibro
154	AsslaniVThan JHU EBrasslar	CANANOLAB_710503	20 Pior polymor	Acc	looiYThor IHU	Dohmor	Nonfunctional	DLCA DEC AVTOSO	Improved mar	Fibres	2010	Nanoenabled	Aloha5 fi	bril of the
186	BROWN STANFORD-HI colN	ICANANOLAB_078023	539 Bior biopolyme	ASC Bio	apolymer penti	Biopolymer	Biodegradable	Biodegradable play	Biodegradable	Fibres	2008	Nanoenabled	Rolynent	ide polyr
189	BROWN STANFORD-IVIEIAC	CANANOLAB_107000	7 Biony biopolyma	ar Bic	polymer pepti	Polymer	Biodegradable	Biodegradable plat	Renewable bi	Fibres	2008	Nanoenabled	Polypept	ide Poly
218	Bleached birch pulp	BI FACHED BIRCH PU	IP (14)-beta-	D-glucan Ble	ached birch or	Cellulose	Thickening agent	Ecod pharmaceut	Non-toxic bio	Fibres	1950	None	14-beta	D-glucan
242	AsclaniXThar, HUL-EBrasslar	LCANANOLAB 696320	06 Bior biopolyme	ar Asc	leniXTher HIL	Biopolymer pent	ide AYT050	Bionolymer	Improved mer	Fibres	2018	Nanoenabled	CANANC	1 48 696
243	AsclepiXTher_HULEBressler	ICANANOLAB_696320	07 Bior biopolyme	ar Asc	lepiXTher_HU	Biopolymer pept	ide AXT050	Biopolymer	Improved mer	Fibres	2018	Nanoenabled	CANANC	LAB 696
245	CGU CGMH CGUST MCUT-	CANANOLAB_090320	192 dox antibody	er Asc	hole Antibody	Brotein	Antibody	Drug Delivery	Increased bior	Fibres	2018	Nanoenabled	Antibody	1740_090
266	CNE-SONM-WI 20161026-1	CANANOLAB_608613	209	CN	IE-SONM-W/L20	Carbon nanofiba	re Conductive The	m Bolymer composity	High strength	Fibres	2016	Nanoenabled	Carbon	anofiber
257	CNT-COOH-birth - Carbon	N M DAR 3	multi-wall	led papotuk Ca	rhop N M PAR	CNT-COOH-birth	High strength old	of Composites polym	High strength,	Fibres	2000	Nanomaterial	Carbon r	anotuba
250	CNT-Long - Carbon	N.M. PAR J	multi-wall	led nanotuk CN	IT-Long	Carbon N M	PAP 1 multi-walk	d Composite materi	High strength,	Fibros	1000	Nanomaterial	Carbon	anotube
200	CNT-Short - Carbon	N.M. PAR 1	multi-wall	led nanotuk CN	IT-Short	Carbon N.M.	PAR 1 multi-walk	d Composite materia	High strength,	Fibros	19905	Nanomaterial	Carbon	anotube
269	CWRLL RWTH-Aachen-DLeN	CANANOLAB 622592	200 Bior biopolyme	er Po	tato virus X bic	Biopolymer	Other	Could be used as a	Biodegradable	Fibres	Since 2017	Nanoenabled	PVX bion	olymer
205	CWRU RWTH-Aachen-DLeN	CANANOLAB_022392	07 Bio biopolyme	er Po	tato virus X bic	Biopolymer	Other	Could be used as a	Biodogradable	Fibros	Since 2017	Nanoenabled	PVX biop	olymer
271	CWRU RWTH-Aachen-DLeN	CANANOLAB_613416	598 Bio biopolyme	er Po	tato virus X bic	Biopolymer	Other	Could be used as a	Biodegradable	Fibres	Since 2017	Nanoenabled	PVX biop	olymer
272		C 1 1 NT	carbon na	notube Ca	rhon nanotube	Nanomaterial	Conductive then	Electronics aeros	High strength	Fibres	10000	Nanomaterial	CNT Full	erene Co
273	C 3.1 Pol NP EG	C 3.1 POL NP EG	carbon na	notube Ca	rhon Nanotube	Nanomaterial	Conductive The	m Electronics, Aeros	High Strength	Fibres	1990¢	Nanomaterial	CNT Full	erene Co
274	C 3.1 Pol NP EG	C 3.1 POL NP EG	carbon na	notube Ca	rhon Nanotube	Nanomaterial	Conductive, The	m Electronics, Aeros	High Strength	Fibres	1990¢	Nanomaterial	CNT Full	erene
275			carbon na	notube Ca	rhon Nanotube	Nanomaterial	Conductive, The	m Electronics, Aeros	High Strength	Fibres	1990s	Nanomaterial	CNT Nat	otube E
C / J	C_4.1_101_141_30	C_4.1_10L_11_30	carbon na	motuoc cu	10011 Hullottube	Nulloinateriai	conductive, men	In Electronics, Acros	mgn strength,	110103	13303	Nulloinateria	CIVI, IV0	iotube, i
276	C 4.1 Pol NP SD	C 4.1 POL NP SD	carbon na	notube Ca	rhon Nanotube	Nanomaterial	Conductive Ther	m Electronics Aeros	High Strength	Fibres	1990s	Nanomaterial	CNT Car	hon Nan
276	C_4.1_Pol_NP_SD Caltech-HHanBC2013-11	C_4.1_POL_NP_SD	carbon na	notube Ca	rbon Nanotube	Nanomaterial Biopolymer	Conductive, Ther	m Electronics, Aeros Pharmaceuticals	High Strength, Biodegradable	Fibres Fibres	1990s	Nanomaterial Nanoenabled	CNT, Car Hercenti	bon Nand
276	C_4.1_Pol_NP_SD Caltech-HHanBC2013-11 annotated (C_4.1_POL_NP_SD CANANOLAB 460062 +	carbon na 198 Bior biopolyme	er Bic	rbon Nanotube poolvmer nenti	Nanomaterial Biopolymer	Conductive, Ther Antibody	m Electronics, Aeros Pharmaceuticals	High Strength, Biodegradable	Fibres Fibres	1990s 1990s	Nanomaterial Nanoenabled	CNT, Car Hercepti	bon Nan n. Trastuz 🍷
276	C_4.1_Pol_NP_SD Caltech-HHanBC2013-11 annotated	C_4.1_POL_NP_SD CANANOLAB_460067 +	carbon na 198 Bior biopolyme	er Bic	rbon Nanotube poolvmer nenti	Nanomaterial Biopolymer	Conductive, Ther Antibody	m Electronics, Aeros Pharmaceuticals : 4	High Strength, Biodegradable	Fibres Fibres	1990s 1990s	Nanomaterial Nanoenabled	CNT, Car Hercepti	bon Nan n. Trastua ▼ ▶
276	C_4.1_Pol_NP_SD Caltech-HHanBC2013-11 annotated (C_4.1_POL_NP_SD CANANOLAB_460062 € C	carbon na 298 Bior biopolyme D	er Bic	rbon Nanotube poolymer nepti	Nanomaterial Biopolymer	Conductive, Ther Antibody G H	m Electronics, Aerosp Pharmaceuticals : 4	High Strength, Biodegradable	Fibres Fibres	1990s 1990s K	Nanomaterial Nanoenabled L	CNT, Car Hercepti	bon Nan n. Trastua M *
276	C_4.1_Pol_NP_SD Caltech_HHanRC2013-11 annotated (B publicname_hs	C_4.1_POL_NP_SD CANANOLAB_460062 + C ubstanceType_na	carbon na 298 Bioc bionolyme D material_s *	er Bio E materialclass	rbon Nanotube poolvmer pepti i	Nanomaterial Bionolymer Bionolymer	G Hutclass_e benefit	m Electronics, Aeross Pharmaceuticals : • • • • • • • •	High Strength, Biodegradable	Fibres Fibres J	1990s 1990s K • isnano_s •	Nanomaterial Nanoenabled L synonym	CNT, Car Hercepti	bon Nan n. Trastuz ¥ M ▲
276 288 1 5	C_4.1_Pol_NP_SD Caltech-HHanRC2013-11 annotated (B publicname_hs CANANOLAB_11337790 Em	C_4.1_POL_NP_SD CANANOLAB_460062 + C ubstanceType_ne *	carbon na 298 Bior biopolyme D material_s * Emulsion	er Bic E Materialdess Emulsion	rbon Nanotube poolvmer nenti I suspensi	Nanomaterial Biopolymer Hality_t Produced In of drop Food,	G H Antibody G H Antibody G H Antibody G H Antibody G H Antibody G H Antibody	Electronics, Aerosy Pharmaceuticals : • • • • • • • • • • • • • • • • • • •	High Strength, Biodegradable le_s T app 1950	Fibres Fibres J lications_since_ Is	1990s 1990s K • isnano_s •	Nanomaterial Nanoenabled L synonym Emulsifier, Emuls	CNT, Car Hercepti Is_5s * ifying agent	bon Nan n. Trastuz M
276 288 1 5 6	C 4.1. Pol_NP_SD Caltech-HHanBC2013-11 annotated B publicname_hs CANANOLAB_11337790 Em 0.9% NACL (W/V) IN MILLQ V	C_4.1_POL_NP_SD CANANOLAB_460062 CANANOLAB_460062 C ubstanceType_na * remulsion chemical substance	carbon na 298 Bior biopolyme D material_s * Emulsion 0.9% NaCl (w/v) i	er Bic E E E E Emulsion Chemical subs	rbon Nanotube poolvmer penti I Suspensi itance None	Nanomaterial Biopolymer Hality_e • produ on of drop Food, None	G H actoless_c * beneficosmetics, p Improv None	Electronics, Aerosp Pharmaceuticals I I I I I I I I I I I I I I I I I I I	High Strength, Biodegradable le_s IY app 1950 None	Fibres Fibres j lications_since_ is a	1990s 1990s • K • isnano_s • None None	Nanomaterial Nanoenabled L synonym Emulsifier, Emuls 0.9% NACL (W/V	CNT, Car Hercepti Is_ss * ifying agent) IN MILIQ W	M ANNU ANNU ANNU ANNU ANNU ANNU ANNU ANN
276 288 1 5 6 8	CALL POL NP SD Caltech-HHANRC2013-11 annotated publicname_hs CANANOLAB_11337790 Em 0.9% NACL (W/V) IN MILIQ V CONTROL TNF-A	C_4.1_POL_NP_SD CANANOLAB_460062 C ubstanceType_nc cemulsion chemical substance chemical substance	Carbon na 298 Biot bionolyme D material_s * Emulsion 0.9% NaCl (w/v) i CONTROL TNF-α	E E E E E Emulsion Chemical subs Chemical subs	rbon Nanotube poolymer peoti i function Suspensi stance None stance Anti-infla	Nanomaterial Biopolymer Hality * produ on of drog. Food, None mmatory Pharm	G H G H Intibiody G H Intibiody G H Intibiody None accuticals Reduce	Electronics, Aerosp Pharmaceuticals i a is a is partic ed stat: Droplets None ed side None	High Strength, Biodegradable Ie_s Y app 1950 None 1990	Fibres Fibres J lications_since_ Is a Is	1990s 1990s K None None None	Nanomaterial Nanoenabled L synonym Emulsifier, Emuls 0.9% NACL (W/V Tumor necrosis f	CNT, Car Hercepti IS_SS • ifying agent) IN MILIQ W/ actor alpha in	M ATER hibitor
276 288 1 5 6 8 10	CALLON IN SO Caltech-HHANRC2013-11 annotated (B publiconing hs CANANOLAB_11337790 Em 0.9% NACL (W/V) IN MILLQ V CONTROL TNF-A NRCWE-036	C_4.1_POL_NP_5D CANANOI AB_460062 ⊕ C ubstanceType_nc v chemical substance chemical substance	carbon na 298 Biot bionolyme D material_s * Emulsion 0.9% NaCl (w/v) i CONTROL TNF-α EPOCYL - NRCWF	E E Emulsion Chemical subs Polymer	rbon Nanotube poolvmer penti	Nanomaterial Bionolymer Hality • produ on of drog: Food, None Immatory Pharm Adhesi	G Conductive, Ther Antibody G F rttdPss_t bent cosmetics, p Improv None aceuticals Reduce yes High et	M Electronics, Aerosy Pharmaceuticals i 4 is_e* None d side None rength. None	High Strength, Biodegradable le_s 7 app 1950 None 1990	Fibres Fibres J lications_since is s s motive, constru-	1990s 1990s • K • isnano_s • None None None	Nanomaterial Nanoenabled L synonym Emulsifier, Emuls 0.9% NACL (W/V Tumor necrosis f Polymer adhesivy	CNT, Car Herceoti ifying agent) IN MILIQ W/ actor alpha in e	M AND
276 288 1 5 6 8 10 11	C.4.1.Pol_NP_SD Caltech-HimaRC013-11 annotated B BUBICNAME AND AND CONTROL TNF-A NRCWE-036 MMC	C 4.1 POL NP 5D CANANOI AR 450062 ⊕ C UbstanceType ne • emulsion chemical substance chemical substance	Carbon na 298 Bioc bionolyme D material_s - Emulsion 0.9% NaCl (w/v) i CONTROL TNF-cu EPOCYL - NRCWE Mitromycin C	er Bic E materialclass Emulsion Chemical subs Polymer Chemical subs	rbon Nanotub poolvmer penti suppolvmer penti function Suspensi stance None stance Anti-infla Adhesive stance Anti-infla	Nanomaterial Biopolymer hality_c produ on of drop Food, None mmatory Pharm Adhesi	Conductive, Ther Antibody G H Ittclass e benef cosmetics, p Improv None aceuticals Reduct ves High st Antipode More	M Electronics, Aerosy Pharmaceuticals i 4 its_v is_partic ed stat Droplets None d side None ffective None	High Strength, Biodegradable 1950 None 1990 Auto	Fibres Fibres J lications_since_ s s motive, constru- s	1990s 1990s • K • isnano_s • None None None Ctit None	Nanomaterial Nanoenabled L synonym Emulsifier, Emuls 0.9% NACL (W/V Tumor necrosis f Polymer adhesive MMC	CNT, Car Hercenti ifying agent) IN MILIQ W/ actor alpha in e	M A
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Figure 25. Screenshots of automated annotation of eNanoMapper materials. Full list is available in appendix. Only the name and substance type columns are used as queries, the rest of the columns are automatically filled in.

Note the output does not directly assigning the AdMa class, but have sufficient information to be used searching if a material or material class of interest is similar to the ones in the InnoMat.Life annotated table(Figure 23), and considering the columns B (AdMa class) and C (advanced material yes or no). Integrating both the structured and unstructured similarity search in eNanoMapper database is ongoing.

Table 7. Automated annotation of functionality, ingredient, benefit over conventional material, industrial usage and nanomaterial indicators (usig OpenAI Completion API and text-davinci-003 (GPT3 model). The automated annotation is based only on columns name and material class, which are always present in the eNanoMapper database.

name	material class	Functiona lity	Could be used as ingredient in which final product material class	benefit over convential material	does it consist of particle s or fibres	industrial usage since	is it nano or nanoen abled
NRCWE-006 MWCNT (Mitsui) AgNP (7–10	multi-walled carbon nanotube	Conductiv e, Thermal, Mechanic al	Conductive polymers, composites, coatings, etc. Textiles, plastics,	Higher conductivity, thermal and mechanical properties Higher	Particles	2000	Nanom aterial
nm, stabilized with	silver nanoparticle	Antimicro bial	paints, coatings, etc.	antimicrobial activity,	Particles	2000s	Nanom aterial



polyethylenim ine)				improved durability, and better color retention			
AuNP (Alkanethiol/li pid, Custom made)	gold nanoparticle	Antimicro bial, catalytic, optical, and electrical properties	Cosmetics, pharmaceuticals, food, and medical devices	Improved performance, enhanced properties, and cost savings	Particles	2000s	Nanom aterial
AuNP (Citrate, Custom made)	gold nanoparticle	Antimicro bial, catalytic, optical, and electrical properties	Cosmetics, pharmaceuticals, food, and medical devices	Improved performance, enhanced properties, and cost savings	Particles	2000s	Nanom aterial
AuNP (Poly(allylami ne hydrochloride), Custom made)	gold nanoparticle	Antimicro bial	Cosmetics, pharmaceuticals, food, etc.	Increased antimicrobial activity, improved solubility, and enhanced stability	Particles	Since 2000s	Nanom aterial
(Poly(allylami ne hydrochloride)/lipid, Custom made)	gold nanoparticle	Antimicro bial	Cosmetics, pharmaceuticals, food, etc.	antimicrobial activity, improved solubility, and enhanced stability	Particles	2000s	Nanom aterial
AuNP oligonucleotid e complexes	gold nanoparticle	Antibacter ial	Pharmaceuticals, cosmetics, food, and other consumer products	increased stability, improved solubility, and enhanced bioavailability	Particles	2000	Nanom aterial
Bentonite - Nano-clay	BENTONITE	Adsorptio n, Absorptio n, Cation Exchange	Cosmetics, Pharmaceuticals, Paints, Drilling Fluids	High adsorption capacity, Low cost, Non- toxic	Particles	1950s	Nanoen abled
CNTSmall,	multi-walled	Conductiv e, Thermal,	Plastics, rubbers,	High strength, high thermal			
CNT - Carbon NRCWE-026 ENP (S- nitrosoglutath ione (GSNO)- loaded	carbon nanotube	Mechanic al	coatings, composites, etc.	conductivity, low weight	Particles	2000	Nanom aterial
Eudragit RL nanoparticles)	Polymer nanoparticle	Drug delivery	Pharmaceuticals	Improved drug delivery	Particles	Since 2000s	Nanom aterial



				Improved drug solubility, increased			
ENP (empty Eudragit RL nanoparticles)	Polymer nanoparticle	Drug delivery	Pharmaceuticals	bioavailability, improved stability improved mechanical properties, increased	Particles	2000	Nanom aterial
EPOCYL - NRCWE-036	multi-walled nanotube suspended in liquid epoxy precursor	Reinforce ment	composite materials	thermal conductivity, improved electrical conductivity	particles	since 2000	nanom aterial
	multi-walled			Increased strength and stiffness, improved thermal and			
EPOXY-CNT - NRCWE-035	nanotube in epoxy	Reinforce ment	Epoxy resin	electrical conductivity High electrical conductivity, high thermal conductivity, high	Particles	Since 2000	Nanom aterial
			Polymers.	mechanical strength, high			
		Conductiv	composites,	chemical			
GO - Carbon NRCWE-058	graphene oxide	e, barrier, adsorptive	coatings, films, etc.	stability, low cost	Platelets	Since 2010	Nanoen abled
		Adsorptio		High surface			
Graphene		n,		area, high			
oxide (NH2-		filtration,	Polymers,	electrical			
functionalized	graphene oxide	catalysis, etc.	composites,	conductivity, etc.	Particles	Since 2010	Nanom aterial
,				Higher conductivity.			
Graphene		Conductiv	Electronics,	strength, and			
oxide		e, strong,	batteries,	flexibility than			
(pristine?) - GSE83516	graphene oxide	lightweigh t	composites,	conventional materials	Platelets	Unknown	Nanoen abled
05205510	ONICE	L.	coutings, etc.	High	Thatelets	Chikitown	usicu
Graphene		Conductiv		conductivity,			
oxide		e, barrier,	Electronics,	high strength,			
(pristine?) - GSE99929	graphene oxide	adsorptive , etc.	batteries, coatings, etc.	low weight, etc.	Particles	Since 2010	Nanoen abled
		Conductiv		High			
Graphene		e,	Electronics,	conductivity,			
quantum dots (hyrdoxyl-	Carbon	iuminesce	patteries, coatings naints	nign surface			Nanoen
modified)	particle	catalytic	etc.	cost	Particles	2018	abled



Graphite (?) - GSE92899	graphite	Conductiv e	Electronics	Higher conductivity, lower cost	Particles	Unknown	None
Graphite				Higher conductivity,			
(nanofibers,		Conductiv	Battery	higher		Cinco	Nanaan
Aldrich)	granhite	e, merman	cells sensors	insulation	Fibres	2000s	abled
Iron oxide	Braphice	mountion		Higher	TIBLES	20003	ubicu
NPs (Custom				magnetic			
made,				properties,			
polyglucose-				better			
sorbitol-			Magnatic fluida	stability, and			
carboxymetny	iron ovido		Magnetic fluids,	Improved biocompatibili		Sinco	Nanom
coated)	nanonarticle	Magnetic	lubricants etc	tv	Particles	2000s	aterial
couteuy	nanopurtiere	Magnetic		Higher	i di ticico	20003	aterial
		Conductiv		electrical			
		e,		conductivity,			
		thermal,		thermal			
		and	Conductive	conductivity,			
	multi-walled	mechanic	polymers,	and			Nanam
IVIVVCINI (?) -	carbon	di properties	composites, and	strength	Particles	2000	Nanom
	hanotabe	properties	coatings	Higher	1 di ticico	2000	ateriai
				conductivity,			
				heat			
				resistance,			
		Conductiv	Conductive	and strength			
	multi-walled	e, heat	materials,	than			Nanom
GSF43515	nanotube	strong	coatings etc	materials	Particles	2000s	aterial
002 10010	hanotabe	511 0115	courings, etc.	High	i ul ticles	20003	aterial
				strength, light			
		Conductiv		weight, high			
MWCNT		e,		electrical			
(Bayer	multi-walled	thermal,	Plastics, rubbers,	conductivity,			Newser
material	carbon	mechanic al ontical	coatings,	nign thermai	Particles	2000	Nanoen
science	nanotube	al, optical	composites, etc.	conductivity	r al ticles	2000	ableu
		Conductiv		Higher			
		e,		strength,			
		thermal,		lighter weight,			
		and		better			
	multi-walled	mechanic	composites	thermal			Nanom
(Bavtubes)	nanotube	properties	coatings, etc.	conductivity	Particles	2000	aterial
(F F		,			
		Conductiv					
		e,		l lieb c ::			
		conductiv		nigner strength			
		e. and		lighter weight.			
		electricall		and improved			
	multi-walled	у	Plastics, rubbers,	electrical and			
MWCNT (SES	carbon	conductiv	coatings, and	thermal			Nanom
research)	nanotube	e	composites	conductivity	Particles	2000	aterial



MWCNT (Sigma-	multi-walled carbon	Conductiv e, thermal, mechanic	Plastics, rubbers, coatings,	High strength, light weight, high electrical conductivity, high thermal			Nanom
Aldrich)	nanotube	al, optical Conductiv	composites, etc.	conductivity	Particles	2000	aterial
		e, thermal, and	Conductive	conductivity, thermal			
	multi-walled	mechanic	materials,	stability, and			
MWCNT	carbon	al	plastics, rubbers,	mechanical			Nanom
(carpet)	nanotube	properties	coatings, etc.	strength Higher	Particles	2000s	aterial
		Conductiv		conductivity,			
		е,	Conductive	thermal			
MWCN1 74	multi-walled	Thermal,	polymers,	stability,			
nm NRCWE-	carbon	Mechanic	composites,	mechanical	Doutidoo	2000	Nanom
	nanotube	ai Conductiv	coatings, etc.	strength	Particles	2000	ateriai
	multi wallad	e, Thormol	plactics rubbars	Increased			
74 nm	multi-walled	Mochanic	plastics, rubbers,	durability and			Nanom
NRCWE-007	nanotube	al	composites, etc.	flexibility	Particles	2000	aterial
		Conductiv		strength, high			
		e.	Polvmer	thermal			
	multi-walled	Thermal.	composites.	conductivity.			
NM-411 -	carbon	Mechanic	coatings.	high electrical			Nanom
Carbon	nanotube	al	adhesives, etc.	conductivity	Particles	2000	aterial
				mechanical			
				properties,			
				Increased			
		Adsorptio		thermal			
		n, .		stability,			
NN -		Absorptio	Polymers,	Improved			
Aluminosilicat	alluminosilicat	n,	Plastics, Coatings,	barrier			Nanoen
e clay	е	Filtration	Paints, Adhesives	properties	Particles	1990s	abled
				High surface			
				area, high			
		Adsorptio		adsorption			
NN-etched -		n,		capacity, high			
Aluminosilicat	alluminosilicat	filtration,	Polymer, ceramic,	thermal		Since	Nanoen
e clay	е	catalysis	composite	stability	Particles	2000s	abled
				Improved			
				drug delivery,			
NP-ERL				improved			
(Eudragit RL			Pharmaceuticals,	stability,			
PO polymeric	Polymer	Controlled	food, cosmetics,	improved			Nanom
nanoparticles)	nanoparticle	release	agrochemicals	solubility	Particles	2000	aterial
			Pharmaceuticals,	surface area,			
NRCWE#065,		Adsorptio	cosmetics, food,	improved			
Porous Silica	attice and the set	n, filterette	paints, coatings,	adsorption,		C :	N
500 nm -	silicon dioxide	nitration,	adnesives,	improved	Deutst-L-	SINCE	ivanom
SIIICd	nanoparticle	catalysis	sediditts, etc.	nitration,	Particles	2000	aterial



NRCWE#067, Porous Silica		Adsorptio n,	Pharmaceuticals, cosmetics, food, paints, coatings,	improved catalysis Increased surface area, improved adsorption, improved filtration,			
100 nm - Silica	silicon dioxide nanoparticle	filtration, catalysis	adhesives, sealants, etc.	improved catalysis	Particles	Since 2000	Nanom aterial
		Adsorptio		High surface			
NRCWE#069,		n, Catalysis	Pharmaceuticals,	area, high			
300 nm-CuO -	silicon dioxide	Separatio	Agriculture,	reactivity, low			Nanom
Silica	nanoparticle	n	Environmental	cost	Particles	2000	aterial
		Adsorptio					
Porous Silica		n, Catalysis	Pharmaceuticals	area High			
100 nm-CuO -	silicon dioxide	Separatio	Cosmetics, Food,	porosity, High			Nanom
Silica	nanoparticle	n .	Agriculture	reactivity	Particles	2000	aterial
				High			
NRCWE-020				coercivity and			
NiZnFe4O8 30	nickel-zinc	Magnotic	Magnetic	saturation	Particlos	2000	Nanom
	lente	wagnetic	materials	High	Particles	2000	ateriai
NRCWE-021				coercivity and		C :	N
ZnFe2O4 30	zinc ferrite	Magnetic	Magnetic	saturation	Particles	Since	Nanom
	Zinchernite	Magnetic	materials	Higher	Faiticles	2000	ateriai
NRCWE-022				coercivity and		C :	N
nm	nickel ferrite	Magnetic	magnetic	saturation	Particles	2000s	Nanom
	mekerreritte		materials	High	r di ticies	20003	ateriai
		Conductiv	Plastics	strength, nigh			
	multi-walled	C, Thermal.	composites.	conductivity.			
NRCWE-040 -	carbon	Mechanic	coatings,	high electrical			Nanom
Carbon	nanotube	al	elastomers, etc.	conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
		е,		thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			
NRCWE-041 -	carbon	Mechanic	composites,	high electrical			Nanom
Carbon	nanotube	al	coatings, etc.	conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
	االمنتقابيم	e, Theres	Diactics	thermal			
	multi-walled	i nermai, Mechanic	riastics,	high electrical			Nanom
Carbon	nanotube	al	coatings, etc.	conductivity	Particles	2000	aterial
		-		High			
		Conductiv		strength, high			
		e,		thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			•.
NRCWE-043 -	carbon	Mechanic	composites,	nigh electrical	Darticlas	2000	Nanom
Carbon	nanotube	dl	coatings, etc.	conductivity	Particles	2000	aterial



		Conductiv		High strength, high			
		e,	- 1	thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			
NRCWE-044 -	carbon	Mechanic	composites,	high electrical			Nanom
Carbon	nanotube	al	coatings, etc.	conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
		e,	Polymer	thermal			
	multi-walled	Thermal,	composites,	conductivity,			
NRCWE-045 -	carbon	Mechanic	coatings,	high electrical			Nanom
Carbon	nanotube	al	adhesives, etc.	conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
		e,	Diantina	thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			N
NRCWE-046 -	carbon	wiechanic	composites,	nign electrical	B I	2000	Nanom
Carbon	nanotube	al	coatings, etc.	Conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
	اممالمنا فالمعا	e, The model		thermal			
	multi-walled	Thermal,	Plastics, rubbers,	conductivity,			Nonom
NRCWE-047 -	carbon	Niechanic	coatings,	nigh electrical	Darticlas	2000	nanom
Carbon	nanotube	ai	composites, etc.	High	Particles	2000	aterial
		Conductiv	Dalamaan	strength, high			
	اممالمنا فالمعا	e, The medial	Polymer	thermal			
	multi-walled	Thermal,	composites,	conductivity,			N
NKCWE-048 -	carbon	wiechanic	coatings,	nign electrical	Dortioloc	2000	Nanom
Carbon	nanotube	dl	aunesives, etc.	High	Particles	2000	ateriai
		Conductiv	Dolumor	strengtn, nign			
	multi wallad	e, Thormol	Polymer	unermai			
	carbon	Mochanic	contings	bigh electrical			Nanom
Carbon	nanotubo	al	adhasiyas atc	conductivity	Particlos	2000	atorial
Carbon	Hallotube	ai	aunesives, etc.	High	Faiticles	2000	ateriai
		Conductiv		strengtn, nign			
	multi wallad	e, Thormol	Diactics	electrical			
	multi-walleu	Machania	Plastics,	bigh thermal			Nonom
Carbon	nanotubo		contings atc	conductivity	Particlos	2000	atorial
Carbon	nanotube		coatings, etc.	High	Faiticies	2000	ateriai
		Conductiv		strength, high			
		e,	- 1	thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			
NRCWE-052 -	carbon	Mechanic	composites,	high electrical	B I	2000	Nanom
Carbon	nanotube	al	coatings, etc.	conductivity High	Particles	2000	aterial
		Conductiv		strength, high			
		e,		thermal			
	multi-walled	Thermal,	Plastics,	conductivity,			
NRCWE-053 -	carbon	Mechanic	composites,	high electrical	.	2000	Nanom
Carbon	nanotube	al	coatings, etc.	conductivity High	Particles	2000	aterial
			Plastics,	strength, high			
	multi-walled	Conductiv	composites,	thermal			
NRCWE-054 -	carbon	e,	coatings,	conductivity,	_		Nanom
Carbon	nanotube	Thermal,	elastomers, etc.	nigh electrical	Particles	2000	aterial



SWCNT (P2- SWNT)	carbon nanotube	conductiv e,	coatings, composites, etc.	electrical and thermal	Fibres	2000	Nanom aterial
	single-walled	Conductiv e, thermally	Plastics, rubbers,	strength, lighter weight, better			
nm NRCWE- 020	nickel-zinc ferrite	Magnetic	Magnetic materials	saturation magnetization Higher	Particles	Since 2018	Nanom aterial
NiZnFe4O8 30				High coercivity and high			
nm NRCWE- 022	nickel ferrite	Magnetic	magnets, motors, and generators	saturation magnetization	Particles	Since 2000s	Nanom aterial
NiFe2O4 30	nanotube	aı	Magnetic Materials, such as	Higher coercivity and	rai licies	2000	ateridi
NRCWE-064 -	multi-walled carbon	Conductiv e, Thermal, Mechanic	Plastics, composites,	strength, high thermal conductivity, high electrical	Darticlas	2000	Nanom
Carbon	nanotube	al	coatings, etc.	conductivity High	Particles	2000	aterial
NRCWE-063 -	multi-walled carbon	Conductiv e, Thermal, Mechanic	Plastics, composites,	High strength, high electrical conductivity, high thermal			Nanom
NRCWE-062 - Carbon	multi-walled carbon nanotube	Thermal, Mechanic al	Plastics, composites, coatings, etc.	conductivity, high electrical conductivity	Particles	2000	Nanom aterial
		Conductiv e,		High strength, high thermal			
Carbon	nanotube	al	coatings, etc.	conductivity	Particles	2000	aterial
NRCWE-061 -	multi-walled	Conductiv e, Thermal, Mechanic	Plastics,	High strength, high electrical conductivity, high thermal			Nanom
NRCWE-057 - Carbon	multi-walled carbon nanotube	Conductiv e, Thermal, Mechanic al	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanom aterial
NRCWE-056 - Carbon	multi-walled carbon nanotube	Conductiv e, Thermal, Mechanic al	Plastics, composites, coatings, etc.	High strength, high electrical conductivity, high thermal conductivity	Particles	2000	Nanom aterial
NRCWE-055 - Carbon	multi-walled carbon nanotube	al Conductiv e, Thermal, Mechanic al	Polymer composites, coatings, adhesives, etc.	low weight High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanom aterial
		Mechanic		conductivity,			



		optically active		conductivity, higher chemical stability			
PAMAM dendrimer- NH2	poly(amidoam ine) dendrimer	Adsorptio n, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, biocompatibili ty, and solubility	Particles	1990s	Nanoen abled
PAMAM-NH2 (Dendritech Inc.)	poly(amidoam ine) dendrimer	Adsorptio n, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, high solubility, biocompatibili ty, etc.	Particles	2000	Nanoen abled
PAMAM-OH (Dendritech Inc.)	poly(amidoam ine) dendrimer	Adsorptio n, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, high solubility, biocompatibili ty, etc.	Particles	2000	Nanoen abled
SWCNT (?) - GSE83516	single-walled carbon nanotube	Conductiv e, thermally conductiv e, optically active	Conductive polymers, composites, coatings	Higher conductivity, thermal conductivity, optical activity	Particles	2000	Nanom aterial
SWCNT (?) - GSE83516	single-walled carbon nanotube	Conductiv e, thermally conductiv e, optically active	Conductive polymers, composites, coatings	Higher conductivity, thermal conductivity, optical activity	Particles	2000	Nanom aterial
SWCNT (Carbon Nanotechnolo	single-walled carbon	Conductiv e, thermally conductiv e, optically	Electronics, batteries, composites,	High strength, light weight, high electrical and thermal conductivity, high surface			Nanom
gy, CNI)	nanotube single-walled	active Conductiv e, thermally conductiv e,	coatings, etc. Plastics, rubbers.	area High strength, light weight, high electrical and thermal conductivity,	Particles	2000	aterial
SWCNT (SES research)	carbon nanotube	optically active	coatings, composites	high surface area	Particles	2000	Nanom aterial



SWCNT	single-walled	Conductiv e, Thermal,	Plastics,	High strength, High electrical conductivity,			
(Sigma-	carbon	Mechanic	Composites,	High thermal			Nanom
Aldrich)	nanotube	al	Coatings	conductivity	Particles	2000	aterial
SWCNT (iron-	single-walled carbon	Conductiv e, thermally and electricall	Conductive polymers, composites,	High electrical and thermal conductivity, high strength,			Nanom
enriched)	nanotube	у	coatings, etc.	lightweight	Particles	2000	aterial
	single-walled	Conductiv e, thermally conductiv	Conductive	Higher conductivity, thermal conductivity, and optical activity than			
SWCNT	carbon	optically	composites.	conventional			Nanom
(purified)	nanotube	active	coatings, etc.	materials High strength, high	Fibres	2000s	aterial
SWCNT 2 nm	carbon	e, thermal, mechanic	aerospace, automotive, energy, medical,	electrical conductivity, high thermal conductivity,			Nanom
NM-411	nanotube	al, optical	etc.	low weight Improved performance,	Particles	2000	aterial
Silica (2D		Adsorptio	cosmetics,	properties			
nanosilicates.	silicon dioxide	Filtration.	adhesives.	improved		Since	Nanom
a layered clay)	nanoparticle	Catalysis	sealants, etc.	durability, etc.	Particles	2000s	aterial
Silica NP (DMPC- coated magnetic mesoporous)	silicon dioxide nanoparticle	Adsorptio n, catalysis, drug delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	Higher surface area, improved reactivity, etc.	Particles	2000s	Nanom aterial
Silica NP		Adsorptio n, catalysis,		Increased			
(PEG-coated		drug	Pharmaceuticals,	surface area,			Newswa
magnetic mesonorous)	silicon dioxide	delivery,	etc	solubility etc	Particles	2000s	Nanom
	nanoparticle	ele.	Pharmaceuticals,	Improved	r al ticles	20003	aterial
Inristing		Magnetic	naints coatings	solubility			
magnetic	silicon dioxide	mesoporo	adhesives.	stability, and			Nanom
mesoporous)	nanoparticle	us	sealants, etc.	bioavailability Higher photocatalytic	Particles	2000s	aterial
TiO2				activity,			
nanobelts	titanium	-	Paint, coating,	better UV		<i>.</i>	
(Custom made)	dioxide nanoparticle	Photocata lyst	plastics, paper, etc.	protection, better	Particles	Since 2010	Nanom aterial



TiO2 nanotubes (100nm, Custom made)	titanium dioxide nanoparticle	photocata lyst UV protection	paints, coatings, plastics, textiles, etc.	thermal stability improved UV protection, increased durability, improved optical properties	particles	since 2000s	nanom aterial
TiO2 nanotubes (30nm, Custom made)	titanium dioxide nanoparticle	, photocata lysis, antibacter ial, antifoulin g	Cosmetics, paints, coatings, plastics, textiles, etc.	Improved UV protection, photocatalysis , antibacterial, antifouling properties	Particles	2000s	Nanom aterial
TiO2NF_1.1_ NF	titanium dioxide nanoparticle	protection , whitening, anti- bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties	Particles	2000	Nanom aterial
TiO2NF_9,1_S ol_BM_15h	titanium dioxide nanoparticle	protection , whitening, anti- bacterial UV	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties	Particles	2000s	Nanom aterial
TiO2_1.1_NF	titanium dioxide nanoparticle	protection , whitening, anti- bacterial UV	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties Improved UV	Particles	2000s	Nanom aterial
TiO2_11_Sil_S ol	titanium dioxide nanoparticle	protection , whitening, anti- bacterial UV	Cosmetics, paints, coatings, plastics, paper, food, etc.	protection, whitening, and anti- bacterial properties	Particles	Since 2000s	Nanom aterial
TiO2_9.1_NF	titanium dioxide nanoparticle	protection , whitening, anti- bacterial UV	Cosmetics, paints, coatings, plastics, paper, food, pharmaceuticals	Improved UV protection, whitening, anti-bacterial properties Improved UV	Particles	2000s	Nanom aterial
TiO2_9.1_NF_ BM	titanium dioxide nanoparticle	protection , whitening, anti- bacterial UV	Cosmetics, paints, coatings, plastics, paper, food, etc. Cosmetics,	protection, whitening, and anti- bacterial properties Improved UV	Particles	2000s	Nanom aterial
TiO2_9.1_sol_ BM	titanium dioxide nanoparticle	protection , whitening,	paints, coatings, plastics, paper, food, etc.	protection, whitening, and anti-	Particles	2000s	Nanom aterial

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		anti-		bacterial			
		bacterial		properties			
		UV		Improved UV			
		protection		protection,			
		,	Cosmetics,	whitening,			
	titanium	whitening,	paints, coatings,	and anti-			
TiO2_NF_BM	dioxide	anti-	plastics, paper,	bacterial			Nanom
_2h	nanoparticle	bacterial	food, etc.	properties	Particles	2000	aterial
		UV		Improved UV			
		protection		protection,			
		,	Cosmetics,	whitening,			
	titanium	whitening,	paints, coatings,	and anti-			
TiO2_NF_BM	dioxide	anti-	plastics, paper,	bacterial			Nanom
_4h	nanoparticle	bacterial	food, etc.	properties	Particles	2000s	aterial
		UV		Improved UV			
		protection		protection,			
		,	Cosmetics,	whitening,			
	titanium	whitening,	paints, coatings,	and anti-			
TiO2_NF_BM	dioxide	anti-	plastics, paper,	bacterial			Nanom
_6h	nanoparticle	bacterial	food, etc.	properties	Particles	2000s	aterial
		UV		Improved UV			
		protection		protection,			
		,	Cosmetics,	whitening,			
	titanium	whitening,	paints, coatings,	and anti-			
TiO2_NF_BM	dioxide	anti-	plastics, paper,	bacterial			Nanom
_9h	nanoparticle	bacterial	food, etc.	properties	Particles	2000s	aterial
				High			
ZnFe2O4 30				coercivity and			
nm NRCWE-		Magnetic	Magnetic	saturation		Since	Nanom
021	zinc ferrite	properties	materials	magnetization	Particles	2018	aterial
			-	High			
phage			Pharmaceuticals,	antimicrobial			
mimetic		.	cosmetics, food,	activity, low		c :	
nanorods		Antimicro	and medical	toxicity, and	Dantialaa	Since	Nanom
(PIVIN)	nanorod	biai	devices	IOW COST	Particles	2018	aterial
				Higher			
		Conduction	Floatronics	conductivity,			
	granhana (sia		electronics,	flovibility there			
rCO Carbon	graphene (Via	e, strong,	contings			Sinco	Nanom
		+	battorios etc	matorials	Distalata	2010	inditutti
INFCARE-028	GU)	ι	balleries, etc.	materials	Platelets	2010	aterial

Data sharing

In order to accommodate a recent requirement for dataset-level protection (instead of project level data sharing) IDEA has installed a modern open source identity management solution (Keycloak [11], at iam.ideaconsult.net), implemented support for Bearer token authorization in eNanoMapper database instances and the NanoSafety Data Interface. The updated NanoSafety Interface is online at https://search.data.enanomapper.net/projects/harmless . The redesign also includes ability to



convert and store the data as HDF5¹ datasets with ontology annotations (HDF5 is a widely used open scientific format optimized for data matrices), which will help with handling the massive quantities of data expected by HTS, HCA and omics methods and will be reported in T1.4 . Last but not least, an open source electronic notebook (eLabFTW) is installed at https://elab.ideaconsult.net , and integrated with the single sign on (users can log with the same credentials as for the eNanoMapper database). The lab notebook will be promoted to partners for storing the data templates with additional annotation and links to SOP (instead of the current storage on a shared drive). The FAIRification workflow [23] is being updated to automatically read the files from the lab notebook and populate the eNanoMapper database.

Conclusion

WP1 launched HARMLESS - eNanoMapper database, populated with data from several previous projects and partner contributions. Data entry is streamlined through online Template Wizard, and new templates were created to support WP6 use cases and complex compositions. An electronic lab notebook was installed to store templates with additional metadata and links to SOPs. The Nanosafety Interface was redesigned with a modern identity management solution to enable data sharing with more precise access rights. The redesign also included the ability to convert and store data as HDF5, a binary format optimized for large data sets.

Computer readable representation of chemical substances and materials are important in the context of big data analysis. The multicomponent materials in eNanoMapper are represented as a set of components with defined roles (annotated by ontology terms). In addition to existing representations IDEA is developing a software prototype for configurable conversion of material description into a Sybyl Line Notation string together with a parallel serialization to NInChI notation (subject to availability, NInChI is still under discussion and development).

Manual annotation of advanced materials in the database was performed at the beginning of the project (by KI) to help with gap analysis. Since manual annotation is time consuming, and an agreed AdMa (advanced materials) definition is still under discussion, IDEA performed feasibility study for automatic annotation based on text analysis of a document containing factsheets for selected classes of advanced materials. Using semantic embedding and similarity search we are able to suggest meaningful categories based on the name and type of the materials in the database. Comparison with the manual annotation is provided. Upon partner suggestion, the unpublished InnoMat.Life classification was provided by partners. While sufficient amount of text to perform text mining was not available, IDEA have performed feasibility study using a recent large language model (GPT-3) for information extraction. We are able to augment the Innomat.Life classification with both textual descriptions and structured information and examples of materials. The same approach was performed to annotate materials in eNanoMapper database. We decided to take a two-phase approach instead of directly assigning the AdMa class. This approach involves augmenting the classification scheme and database with the same structured information as well as with textual descriptions. The automatic annotation provides to be used searching if a material or material class of interest is similar to the ones in the InnoMat.Life annotated table and considering the AdMa class and whether it is considered an advanced material. Integration of both the structured and unstructured similarity search in eNanoMapper database is ongoing as well as the implementation of user interface.

¹ <u>https://www.hdfgroup.org/solutions/hdf5/</u>



The benefit of this approach is that it can be tailored to utilize various classification systems, and it can still extract structured data even if the classification document does not provide enough information.



Appendix. Outputs from automated annotation

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