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Project Acronym: HARMLESS

Deliverable 1.1

HARMLESS database with extensions to handle advanced materials

Due date of Deliverable: 31.07.2022

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Lead beneficiary for this Deliverable: IDEA

Level of Dissemination: PU

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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 (Nano Environment, Health and Safety) 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 https://search.data.enanomapper.net/projects/harmless. 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)*

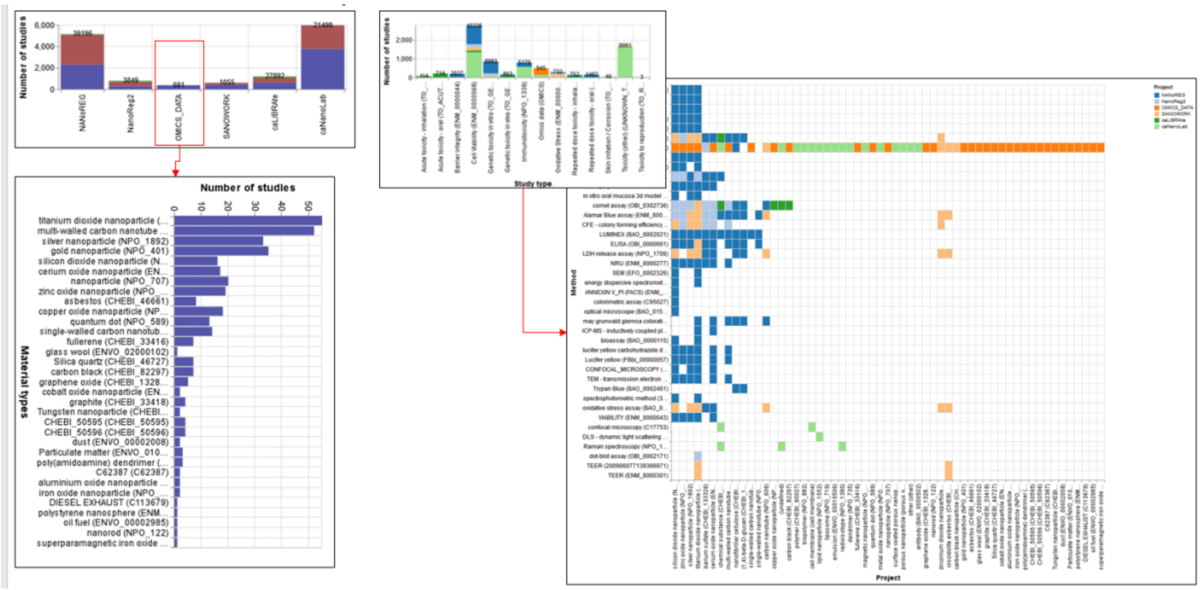


Figure 1. Example of visual gap analysis available in the Nanosafety Data Interface and HARMLESS database

Table 1. "Complexity" principles for advanced materials

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

			Silver NPs
Insulation	-	Nano-enabled insulation materials	-
Doped / Doping	Doped core [ENM_9000242]	Metal-doped imogolite nanotubes	**9 (”doping”) + 15 (”doped”) 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 ≥ 3:1, length ≥5 µm, and width ≤3 µm) and unlike other dusts are regulated by number per unit volume of air and not mass concentration per unit air [3].

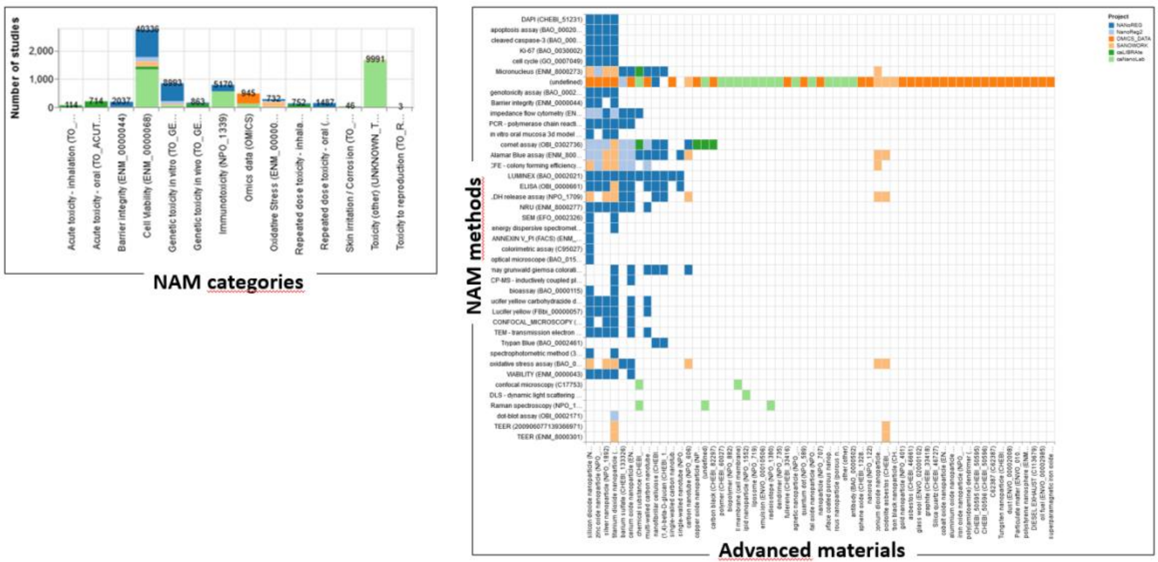
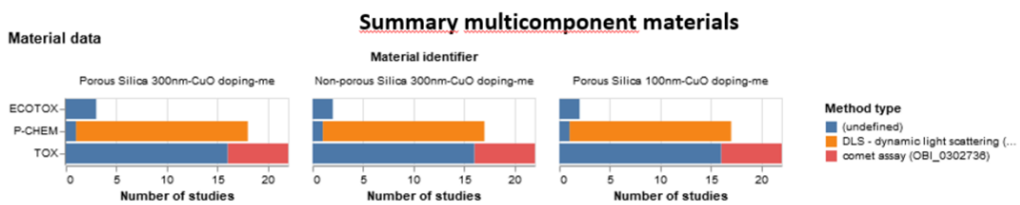


Figure 2. With proper annotation we have the potential for viewing advanced materials and NAMs in the HARMLESS database



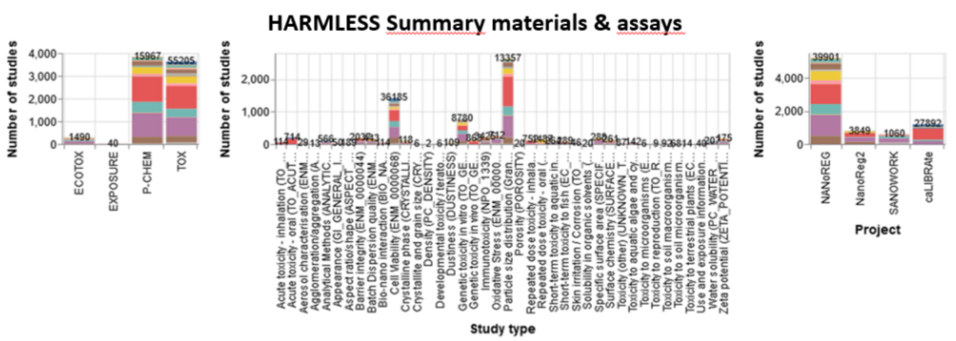


Figure 3. Example of the multicomponent materials in HARMLESS database (~2021)

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) https://www.mgi.gov/ 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 (https://materialsproject.org) (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.

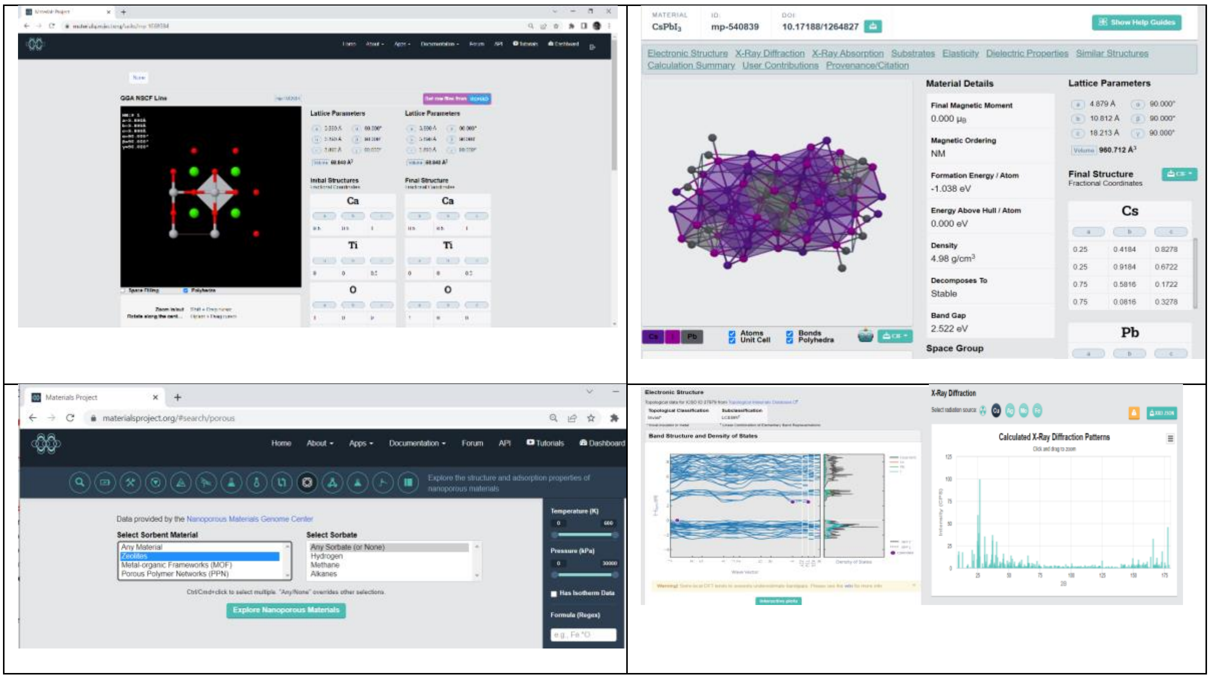


Figure 4. materialsproject.org. Example page showing perovskites

AFLOWlib http://aflowlib.org/ 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) http://oqmd.org/ 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 https://materialsdata.nist.gov/ 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 https://materials.registry.nist.gov/ MRR functions as a federated service, making the registered information from multiple institutions available for research to the materials community

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

The Materials Data Facility (MDF) https://materialsdatafacility.org/ 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 https://materials.nrel.gov/ 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 http://www.matweb.com/ contains over 130,000 metals, plastics, ceramics, and composites.

The NIMS Materials Database (MatNavi) https://mits.nims.go.jp/en/ 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

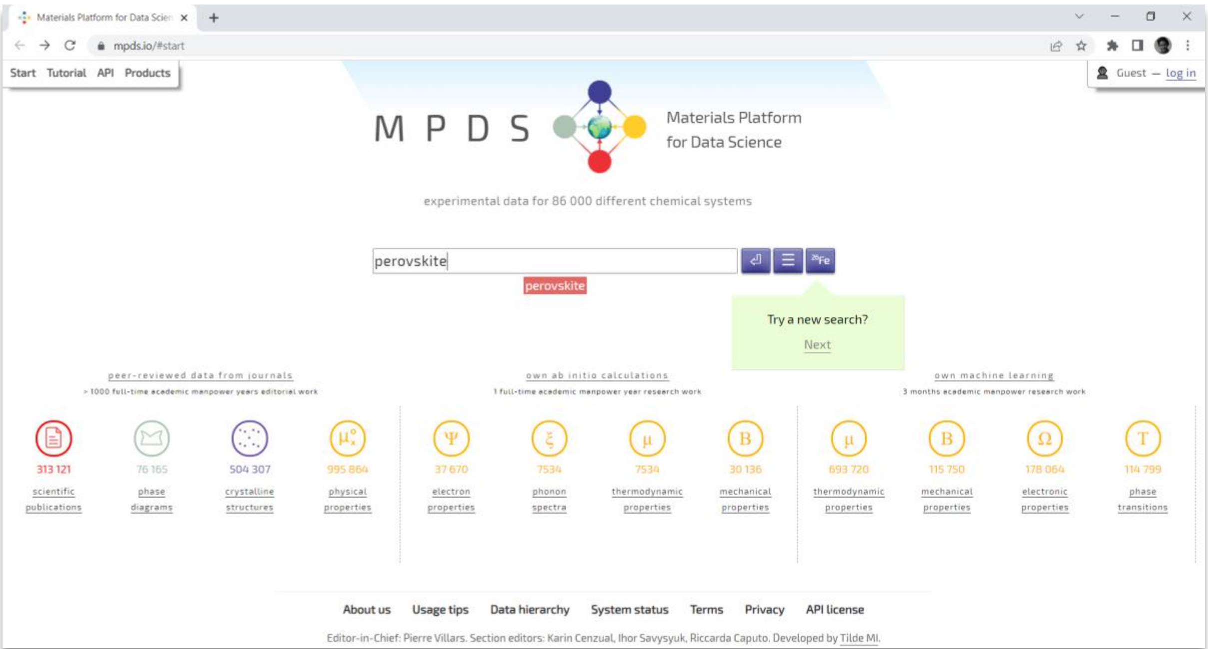


Figure 5. mdps.io

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

The NOMAD Repository and Archive (NOvel MAterials Discovery) https://nomad-lab.eu/ (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]

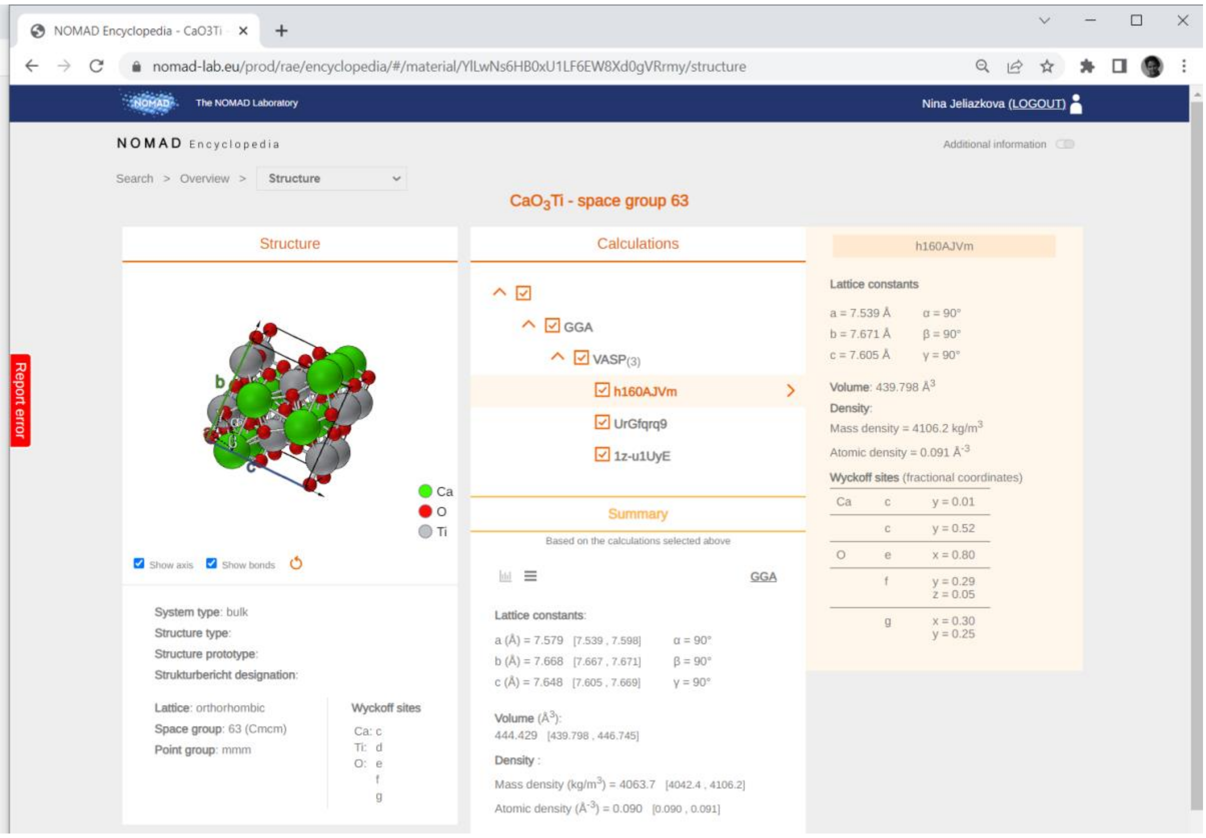


Figure 6. nomad-lab.eu

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).

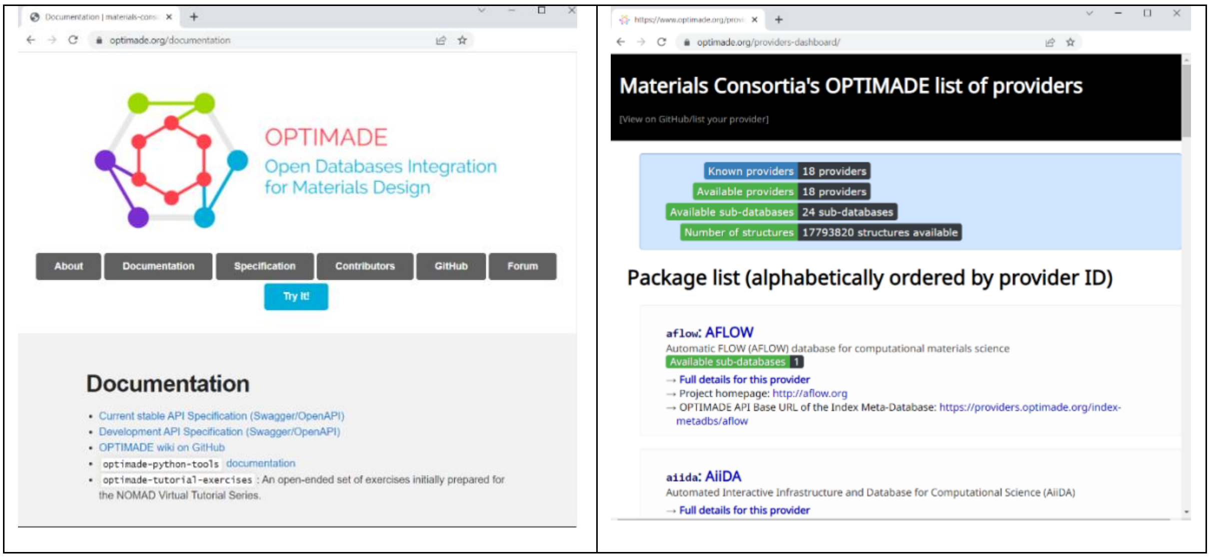


Figure 7. OPTIMADE - common API for materials databases

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 https://search.data.enanomapper.net/projects/harmless/ (Figure 8)

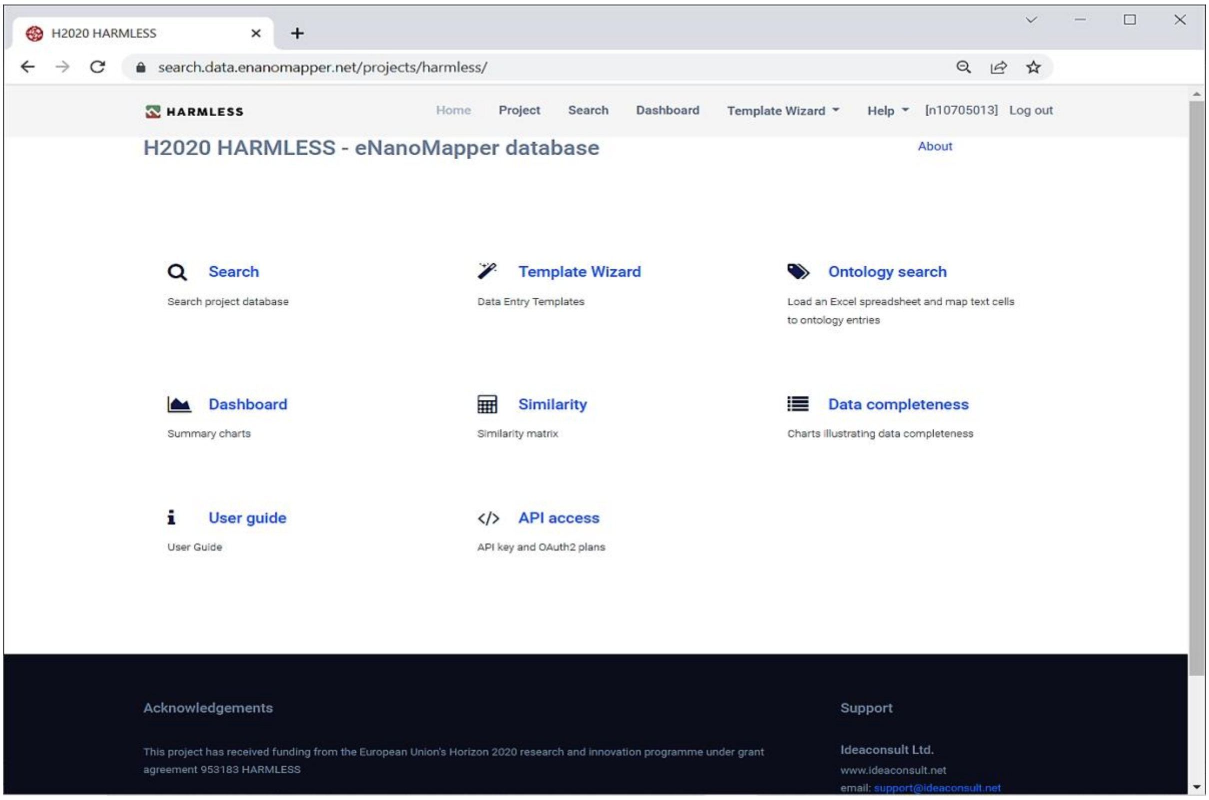


Figure 8. Main page of the HARMLESS eNanoMapper database. Each icon leads to a page with the corresponding functionality (search, Template Wizard, Dashboard, etc)

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 for data from previous EU projects available in HARMLESS eNanoMapper database***

eNanoMapper import	**Project**	**Materials**	**Studies**	**Data 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 https://api.ideaconsult.net), 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.

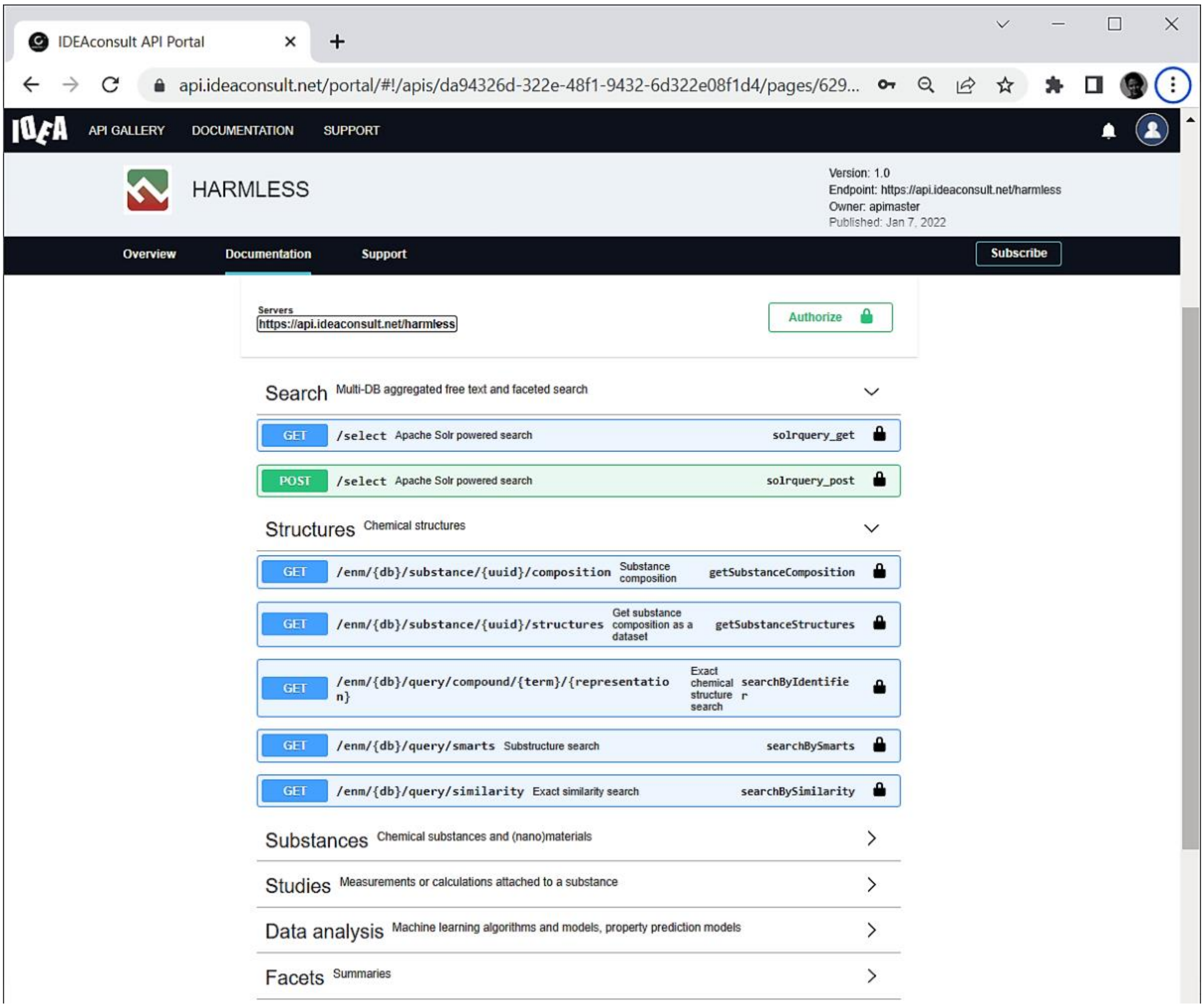


Figure 9. HARMLESS eNanoMapper database Application Programming Interface (API) interactive documentation

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.

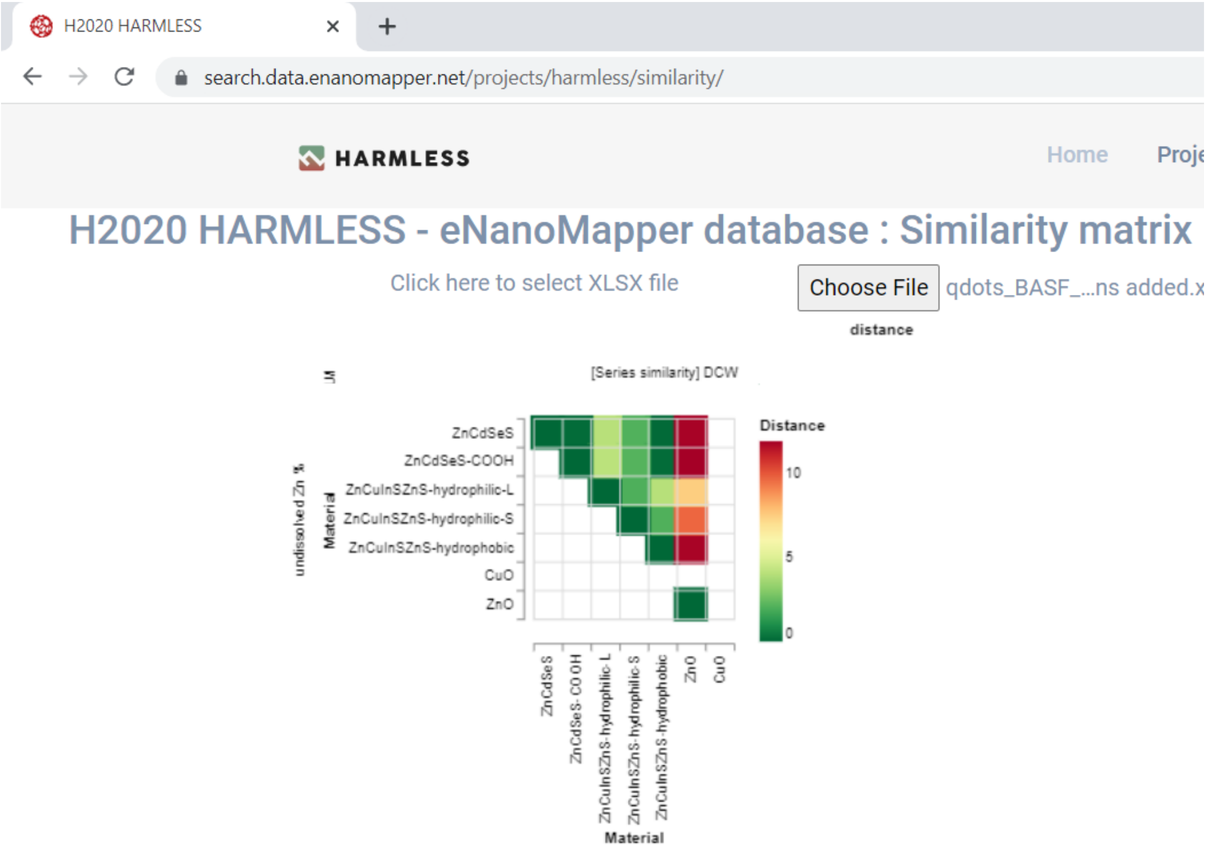


Figure 10. Screenshot of the online similarity assessment tool for dose response and/or time series

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)

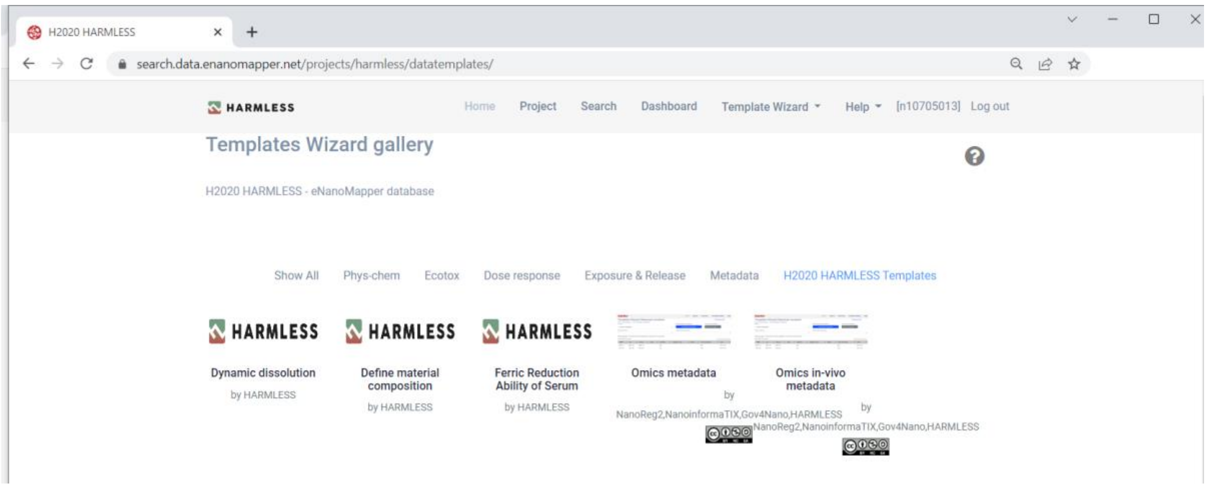


Figure 11. Overview of templates developed or updated by HARMLESS partners.

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.

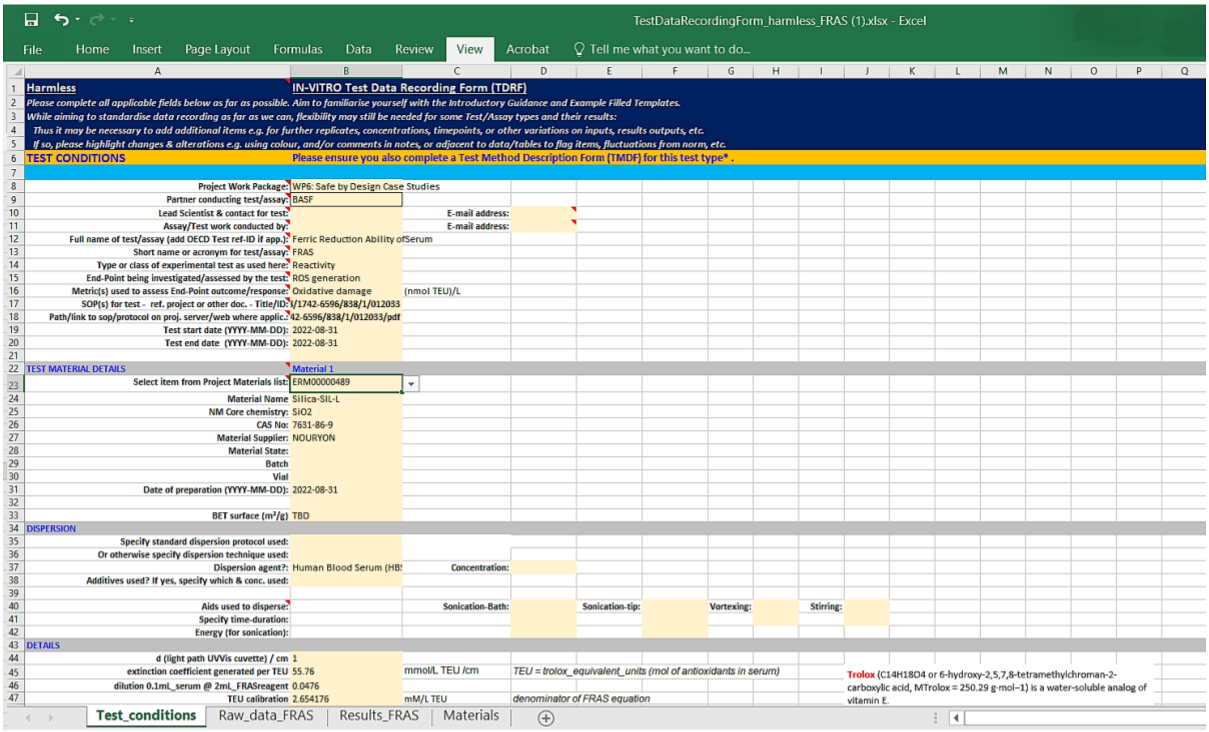


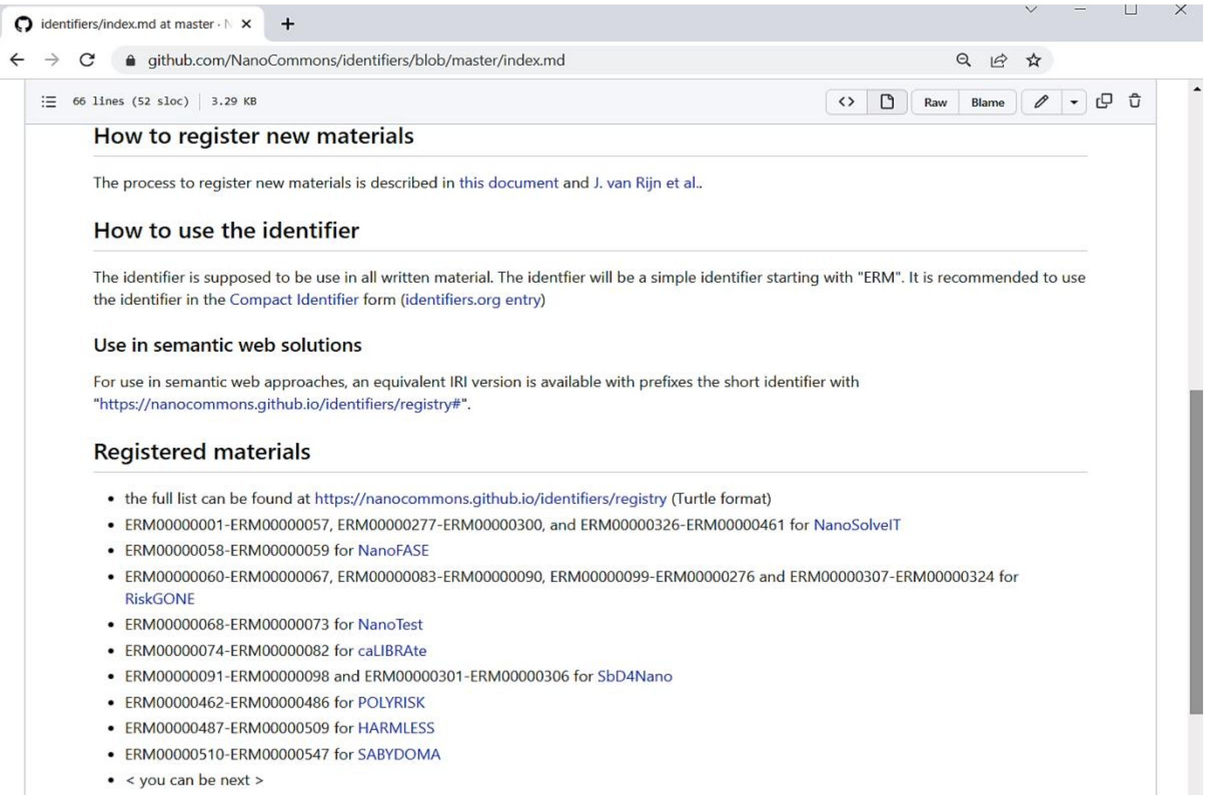
Figure 12. The list of materials is integrated in the Template Wizard and materials are selected via drop down box within the data entry template.

Table 3. ERM identifiers for WP6 case studies

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 https://github.com/NanoCommons/identifiers/blob/master/index.md (Figure 13).


identifiers/index.md at master · N

github.com/NanoCommons/identifiers/blob/master/index.md

66 lines (52 sloc) | 3.29 KB

Raw Blame

How to register new materials

The process to register new materials is described in this document and J. van Rijn et al..

How to use the identifier

The identifier is supposed to be use in all written material. The identfier will be a simple identifier starting with "ERM". It is recommended to use the identifier in the Compact Identifier form (identifiers.org entry)

Use in semantic web solutions

For use in semantic web approaches, an equivalent IRI version is available with prefixes the short identifier with "https://nanocommons.github.io/identifiers/registry#".

Registered materials

- the full list can be found at https://nanocommons.github.io/identifiers/registry (Turtle format)
- ERM00000001-ERM00000057, ERM00000277-ERM00000300, and ERM00000326-ERM00000461 for NanoSolveIT
- ERM00000058-ERM00000059 for NanoFASE
- ERM00000060-ERM00000067, ERM00000083-ERM00000090, ERM00000099-ERM00000276 and ERM00000307-ERM00000324 for RiskGONE
- ERM00000068-ERM00000073 for NanoTest
- ERM00000074-ERM00000082 for caLIBRAte
- ERM00000091-ERM00000098 and ERM00000301-ERM00000306 for SbD4Nano
- ERM00000462-ERM00000486 for POLYRISK
- ERM00000487-ERM00000509 for HARMLESS
- ERM00000510-ERM00000547 for SABYDOMA
- < you can be next >

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 (https://search.data.enanomapper.net/projects/harmless/datatemplates/pchem/index.html?template=COMPOSITION). Figure 14 illustrates an example with composition data for silica paper, provided by partner.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1		Material			Component									
2	Identifiers				Comp	Component	FUNCTION	Component identifiers					Proportion	
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	O		
5	EXAMPLE1	example1	NPO_1373	NOURYON	2	HAS_ADDITIVE	DISPERSANT			sodium salt of a maleic anl	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_MODIFIER			hydrophobically modified	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	O		
13	EXAMPLE2	example2	NPO_1373	NOURYON	2	HAS_ADDITIVE	COUPLING_AID	252-104-2	34590-94-8	Dipropylene glycol mono p	Dowanol DPnP	CCC(O)OCCCOC		
14	EXAMPLE2	example2	NPO_1373	NOURYON	3	HAS_ADDITIVE	BINDER			acrylic copolymer dispersic	Alberdingk AC 2019 VP			
15	EXAMPLE2	example2	NPO_1373	NOURYON	4	HAS_ADDITIVE	RHEOLOGY_MODIFIER			hydrophobically modified	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	Substance Type	Public name	Reference substance UUID	Owner	Info
- 1 -	EXAMPLE1	HRMZ-ce6fafaf-...	NPO_1373	EXAMPLE1	XLSX-0a05544c-...	HARMLESS	Supplier = NOURYON

Composition name: Siliceous Earth - Silica And Kaolinite,Sillitin Z 89 (0 % (w/w))
Composition UUID: HRMZ-1a0807f2-7c0d-3e69-9197-61a941d8230d
Purity of IUC Substance:

Type	Name	EC No.	CAS No.	Typical concentration	Concentration ranges			Structure
Additive (SOLVENT)	Water		7732-18-5	0 % (w/w)	>=0 %	<=0 %	Also contained in...	H_2O
Additive (DISPERSANT)	Orotan 731,Sodium Salt Of A Maleic Anhydride Copolymer			0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Additive (DEFOAMER)	Tego Foamex 810,Polyether Siloxane			0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Additive (RHEOLOGY_MODIFIER)	Aquaflow Nls-205,Hydrophobically Modified Polyacetal Polyether			0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Additive (PIGMENT)	Kronos 2190,Tio2 - Rutile Surface Treated W Aluminium And Zirconium Compounds			0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Additive (FILLER)	Calcium Carbonate,Hydrocarb Og		471-34-1	0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Additive (DEAERATOR)	Tego Airex 902 W,Polyether Siloxane			0 % (w/w)	>=0 %	<=0 %	Also contained in...	
Constituent	Siliceous Earth - Silica And Kaolinite,Sillitin		1318-74-7	0 % (w/w)	>=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 life-time 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 (https://www.sbert.net/). 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.

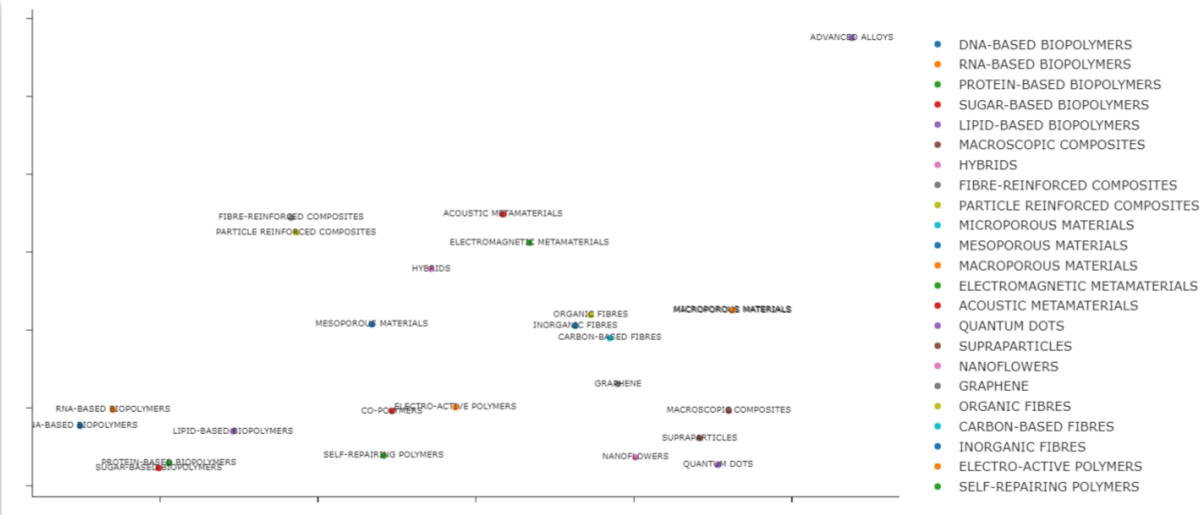


Figure 16. Projection of the advanced material categories from [11] *based on the semantic embeddings.*

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.

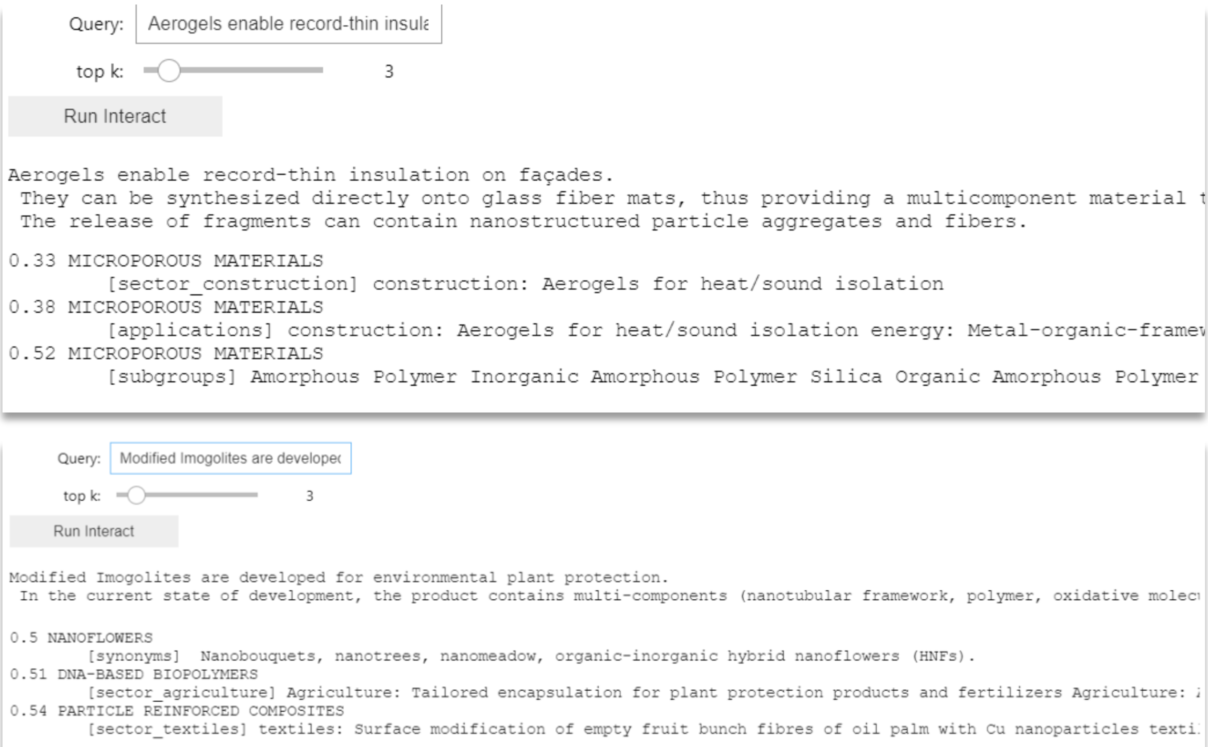


Figure 17. Examples of querying the indexed factsheets with text describing WP6 materials (aerogels and imogolites) and the top 3 matches.

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.

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

name	material type	manual annotation	*tag1*	distance1	*tag2*	distance2	*tag3*	distance3
NRCWE-006 MWCNT (Mitsui)	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.50
AgNP (7–10 nm, stabilized with polyethylenimine)	silver nanoparticle	**composite, hybrid material**	*SUGAR-BASED BIOPOLYMERS*	0.51	*SUGAR-BASED BIOPOLYMERS*	0.51	*PARTICLE REINFORCED COMPOSITES*	0.53
AuNP (Alkanethiol/lipid, Custom made)	gold nanoparticle	**composite, hybrid material**	*NANOFLOWERS*	0.50	*NANOFLOWERS*	0.50	*SUPRAPARTICLES*	0.51
AuNP (Citrate, Custom made)	gold nanoparticle	**composite, hybrid material**	*NANOFLOWERS*	0.50	*NANOFLOWERS*	0.50	*SUPRAPARTICLES*	0.52
AuNP (Poly(allylamine hydrochloride), Custom made)	gold nanoparticle	**composite, hybrid material**	*NANOFLOWERS*	0.51	*NANOFLOWERS*	0.51	*SUPRAPARTICLES*	0.51
AuNP (Poly(allylamine hydrochloride)/lipid , Custom made)	gold nanoparticle	**composite, hybrid material**	*SUGAR-BASED BIOPOLYMERS*	0.49	*SUGAR-BASED BIOPOLYMERS*	0.49	*CO-POLYMERS*	0.50
AuNP oligonucleotide complexes	gold nanoparticle	**RNA-based biopolymer, biopolymer**	*SUPRAPARTICLES*	0.53	*SUPRAPARTICLES*	0.53	*SUGAR-BASED BIOPOLYMERS*	0.54
Bentonite - Nano-clay	BENTONITE	**particulate systems**	*MACROPOROUS MATERIALS*	0.54	*MACROPOROUS MATERIALS*	0.54	*PARTICLE REINFORCED COMPOSITES*	0.54
CNTSmall, CNT - Carbon NRCWE-026	multi-walled carbon nanotube	**advanced fibres**	*FIBRE-REINFORCED COMPOSITES*	0.43	*FIBRE-REINFORCED COMPOSITES*	0.43	*FIBRE-REINFORCED COMPOSITES*	0.45
ENP (S-nitrosoglutathione (GSNO)-loaded Eudragit RL nanoparticles)	nanoparticle	**advanced polymer, co-polymer**	*SUGAR-BASED BIOPOLYMERS*	0.52	*SUGAR-BASED BIOPOLYMERS*	0.52	*SUPRAPARTICLES*	0.52
ENP (empty Eudragit RL nanoparticles)	nanoparticle	**advanced polymer, co-polymer**	*SUPRAPARTICLES*	0.58	*SUPRAPARTICLES*	0.58	*PARTICLE REINFORCED COMPOSITES*	0.59
EPOCYL - NRCWE-036		**advanced fibres, carbon-based fibres**	*SUPRAPARTICLES*	0.57	*SUPRAPARTICLES*	0.57	*QUANTUM DOTS*	0.60

EPOXY-CNT - NRCWE-035		**advanced fibres, carbon-based fibres**	*CARBON-BASED FIBRES*	0.54	*CARBON-BASED FIBRES*	0.54	*MACROPOROUS MATERIALS*	0.54
GO - Carbon NRCWE-058	multi-walled nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.57	*FIBRE-REINFORCED COMPOSITES*	0.57	*CARBON-BASED FIBRES*	0.58
Graphene oxide (NH2-functionalized)	graphene oxide	**graphene, particulate systems**	*GRAPHENE*	0.45	*GRAPHENE*	0.45	*CARBON-BASED FIBRES*	0.49
Graphene oxide (pristine?) - GSE83516	graphene oxide	**graphene, particulate systems**	*GRAPHENE*	0.50	*GRAPHENE*	0.50	*CARBON-BASED FIBRES*	0.50
Graphene oxide (pristine?) - GSE99929	graphene oxide	**graphene, particulate systems**	*GRAPHENE*	0.50	*GRAPHENE*	0.50	*CARBON-BASED FIBRES*	0.50
Graphene quantum dots (hyrdoxyl-modified)	CdSe quantum dot	**graphene, particulate systems**	*QUANTUM DOTS*	0.42	*QUANTUM DOTS*	0.42	*QUANTUM DOTS*	0.43
Graphite (?) - GSE92899	graphite	**advanced fibres, carbon-based fibres**	*GRAPHENE*	0.48	*GRAPHENE*	0.48	*GRAPHENE*	0.51
Graphite (nanofibers, Sigma-Aldrich)	graphite	**advanced fibres, carbon-based fibres**	*CARBON-BASED FIBRES*	0.43	*CARBON-BASED FIBRES*	0.43	*CARBON-BASED FIBRES*	0.44
Iron oxide NPs (Custom made, polyglucose-sorbitol-carboxymethyether (PSC) coated)	iron oxide nanoparticle	**composite, hybrid material**	*SUGAR-BASED BIOPOLYMERS*	0.49	*SUGAR-BASED BIOPOLYMERS*	0.49	*PARTICLE REINFORCED COMPOSITES*	0.49
MWCNT (?) - E-TABM-679	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.51
MWCNT (?) - GSE43515	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.54	*FIBRE-REINFORCED COMPOSITES*	0.54	*CARBON-BASED FIBRES*	0.55
MWCNT (Bayer material science)	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.41	*FIBRE-REINFORCED COMPOSITES*	0.41	*FIBRE-REINFORCED COMPOSITES*	0.44
MWCNT (Baytubes)	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.46	*FIBRE-REINFORCED COMPOSITES*	0.46	*CARBON-BASED FIBRES*	0.50
MWCNT (SES research)	multi-walled carbon	**advanced fibres,**	*FIBRE-REINFORCED D*	0.44	*FIBRE-REINFORCED D*	0.44	*FIBRE-REINFORCED COMPOSITES*	0.47

	nanotube	**carbon-based fibres**	*COMPOSITES*		*COMPOSITES*			
MWCNT (Sigma-Aldrich)	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.44	*FIBRE-REINFORCED COMPOSITES*	0.44	*FIBRE-REINFORCED COMPOSITES*	0.46
MWCNT (carpet)	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.43	*FIBRE-REINFORCED COMPOSITES*	0.43	*CARBON-BASED FIBRES*	0.47
MWCNT 74 nm NRCWE-007	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.58	*FIBRE-REINFORCED COMPOSITES*	0.58	*FIBRE-REINFORCED COMPOSITES*	0.58
MWCNT Cheap Tubes 74 nm NRCWE-007	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.56	*FIBRE-REINFORCED COMPOSITES*	0.56	*CARBON-BASED FIBRES*	0.60
NM-411 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.57	*FIBRE-REINFORCED COMPOSITES*	0.57	*CARBON-BASED FIBRES*	0.58
NN - Aluminosilicate clay	alluminosilicate	**composite, hybrid material**	*MACROPOROUS MATERIALS*	0.54	*MACROPOROUS MATERIALS*	0.54	*NANOFLOWERS*	0.54
NN-etched - Aluminosilicate clay	alluminosilicate	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.56	*FIBRE-REINFORCED COMPOSITES*	0.56	*PARTICLE REINFORCED COMPOSITES*	0.57
NP-ERL (Eudragit RL PO polymeric nanoparticles)	nanoparticle	**advanced polymer, co-polymer**	*LIPID-BASED BIOPOLYMERS*	0.53	*LIPID-BASED BIOPOLYMERS*	0.53	*CO-POLYMERS*	0.54
NRCWE#065, Porous Silica 300 nm - Silica	silicon dioxide nanoparticle	**porous material**	*QUANTUM DOTS*	0.51	*QUANTUM DOTS*	0.51	*MESOPOROUS MATERIALS*	0.53
NRCWE#067, Porous Silica 100 nm - Silica	silicon dioxide nanoparticle	**porous material**	*QUANTUM DOTS*	0.52	*QUANTUM DOTS*	0.52	*SUPRAPARTICLES*	0.53
NRCWE#069, Porous Silica 300 nm-CuO - Silica	silicon dioxide nanoparticle	**porous material**	*QUANTUM DOTS*	0.52	*QUANTUM DOTS*	0.52	*MESOPOROUS MATERIALS*	0.54
NRCWE#070, Porous Silica 100 nm-CuO - Silica	silicon dioxide nanoparticle	**porous material**	*QUANTUM DOTS*	0.52	*QUANTUM DOTS*	0.52	*MESOPOROUS MATERIALS*	0.53
NRCWE-020 NiZnFe4O8 30 nm	nickel-zinc ferrite	**advanced alloys, intermetallic**	*FIBRE-REINFORCED*	0.64	*FIBRE-REINFORCED*	0.64	*QUANTUM DOTS*	0.64

			COMPOSITES		*COMPOSITES*			
NRCWE-021 ZnFe2O4 30 nm	zinc ferrite	**advanced alloys, intermetallic**	*FIBRE-REINFORCED COMPOSITES*	0.61	*FIBRE-REINFORCED COMPOSITES*	0.61	*ADVANCED ALLOYS*	0.63
NRCWE-022 NiFe2O4 30 nm	nickel ferrite	**advanced alloys, intermetallic**	*FIBRE-REINFORCED COMPOSITES*	0.66	*FIBRE-REINFORCED COMPOSITES*	0.66	*CARBON-BASED FIBRES*	0.68
NRCWE-040 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.50
NRCWE-041 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52
NRCWE-042 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*CARBON-BASED FIBRES*	0.54
NRCWE-043 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52
NRCWE-044 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52	*CARBON-BASED FIBRES*	0.52
NRCWE-045 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.51
NRCWE-046 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.51	*FIBRE-REINFORCED COMPOSITES*	0.51	*FIBRE-REINFORCED COMPOSITES*	0.52
NRCWE-047 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.51	*FIBRE-REINFORCED COMPOSITES*	0.51	*FIBRE-REINFORCED COMPOSITES*	0.51
NRCWE-048 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.50	*FIBRE-REINFORCED COMPOSITES*	0.51

NRCWE-049 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.50
NRCWE-051 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.54	*FIBRE-REINFORCED COMPOSITES*	0.54	*CARBON-BASED FIBRES*	0.54
NRCWE-052 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.55	*FIBRE-REINFORCED COMPOSITES*	0.55	*CARBON-BASED FIBRES*	0.55
NRCWE-053 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.54	*FIBRE-REINFORCED COMPOSITES*	0.54	*CARBON-BASED FIBRES*	0.54
NRCWE-054 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*CARBON-BASED FIBRES*	0.54
NRCWE-055 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.54
NRCWE-056 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.54
NRCWE-057 - Carbon	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53
NRCWE-061 - Carbon	multi-walled nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.56	*FIBRE-REINFORCED COMPOSITES*	0.56	*FIBRE-REINFORCED COMPOSITES*	0.56
NRCWE-062 - Carbon	multi-walled nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.58	*FIBRE-REINFORCED COMPOSITES*	0.58	*CARBON-BASED FIBRES*	0.58
NRCWE-063 - Carbon	multi-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.54
NRCWE-064 - Carbon	multi-walled carbon	**advanced fibres,**	*FIBRE-REINFORCED*	0.52	*FIBRE-REINFORCED*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.54

	nanotube	carbon-based fibres	*COMPOSITES*		*COMPOSITES*			
NiFe2O4 30 nm NRCWE-022	nickel ferrite	**advanced alloys, intermetallic**	*QUANTUM DOTS*	0.69	*QUANTUM DOTS*	0.69	*FIBRE-REINFORCED COMPOSITES*	0.70
NiZnFe4O8 30 nm NRCWE-020	nickel-zinc ferrite	**advanced alloys, intermetallic**	*QUANTUM DOTS*	0.66	*QUANTUM DOTS*	0.66	*FIBRE-REINFORCED COMPOSITES*	0.69
SWCNT (P2-SWNT)	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.52	*FIBRE-REINFORCED COMPOSITES*	0.52	*CARBON-BASED FIBRES*	0.53
PAMAM dendrimer-NH2	poly(amidoamine) dendrimer	**advanced polymer, co-polymer**	*CO-POLYMERS*	0.52	*CO-POLYMERS*	0.52	*CO-POLYMERS*	0.52
PAMAM-NH2 (Dendritech Inc.)	poly(amidoamine) dendrimer	**advanced polymer, co-polymer**	*CO-POLYMERS*	0.55	*CO-POLYMERS*	0.55	*MESOPOROUS MATERIALS*	0.55
PAMAM-OH (Dendritech Inc.)	poly(amidoamine) dendrimer	**advanced polymer, co-polymer**	*CO-POLYMERS*	0.55	*CO-POLYMERS*	0.55	*MESOPOROUS MATERIALS*	0.55
SWCNT (?) - GSE83516	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.49	*CARBON-BASED FIBRES*	0.51
SWCNT (?) - GSE83516	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.49	*FIBRE-REINFORCED COMPOSITES*	0.49	*CARBON-BASED FIBRES*	0.51
SWCNT (Carbon Nanotechnology, CNI)	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.44	*FIBRE-REINFORCED COMPOSITES*	0.44	*CARBON-BASED FIBRES*	0.47
SWCNT (SES research)	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.47	*FIBRE-REINFORCED COMPOSITES*	0.47	*CARBON-BASED FIBRES*	0.47
SWCNT (Sigma-Aldrich)	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.47	*FIBRE-REINFORCED COMPOSITES*	0.47	*FIBRE-REINFORCED COMPOSITES*	0.48
SWCNT (iron-enriched)	single-walled carbon	**advanced fibres,**	*FIBRE-REINFORCED D*	0.46	*FIBRE-REINFORCED D*	0.46	*FIBRE-REINFORCED COMPOSITES*	0.47

	nanotube	**carbon-based fibres**	*COMPOSITES*		*COMPOSITES*			
SWCNT (purified)	single-walled carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.46	*FIBRE-REINFORCED COMPOSITES*	0.46	*FIBRE-REINFORCED COMPOSITES*	0.47
SWCNT 2 nm NM-411	carbon nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*CARBON-BASED FIBRES*	0.53
Silica (2D nanosilicates, a layered clay)	silicon dioxide nanoparticle	**advanced polymer, electro-active polymer**	*PARTICLE REINFORCED COMPOSITES*	0.53	*PARTICLE REINFORCED COMPOSITES*	0.53	*NANOFLOWERS*	0.54
Silica NP (DMPC-coated magnetic mesoporous)	silicon dioxide nanoparticle	**mesoporous material, porous material**	*MESOPOROUS MATERIALS*	0.54	*MESOPOROUS MATERIALS*	0.54	*SUGAR-BASED BIOPOLYMERS*	0.55
Silica NP (PEG-coated magnetic mesoporous)	silicon dioxide nanoparticle	**mesoporous material, porous material**	*MESOPOROUS MATERIALS*	0.50	*MESOPOROUS MATERIALS*	0.50	*MESOPOROUS MATERIALS*	0.53
Silica NP (pristine magnetic mesoporous)	silicon dioxide nanoparticle	**mesoporous material, porous material**	*MESOPOROUS MATERIALS*	0.49	*MESOPOROUS MATERIALS*	0.49	*SUGAR-BASED BIOPOLYMERS*	0.50
TiO2 nanobelts (Custom made)	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*PARTICLE REINFORCED COMPOSITES*	0.51	*PARTICLE REINFORCED COMPOSITES*	0.51	*SUPRAPARTICLES*	0.52
TiO2 nanotubes (100nm, Custom made)	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*FIBRE-REINFORCED COMPOSITES*	0.53	*FIBRE-REINFORCED COMPOSITES*	0.53	*PARTICLE REINFORCED COMPOSITES*	0.53
TiO2 nanotubes (30nm, Custom made)	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*FIBRE-REINFORCED COMPOSITES*	0.54	*FIBRE-REINFORCED COMPOSITES*	0.54	*SUPRAPARTICLES*	0.54
TiO2NF_1.1_NF	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*QUANTUM DOTS*	0.57	*QUANTUM DOTS*	0.57	*SUPRAPARTICLES*	0.58
TiO2NF_9,1_Sol_BM_15h	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*QUANTUM DOTS*	0.53	*QUANTUM DOTS*	0.53	*NANOFLOWERS*	0.53
TiO2_1.1_NF	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.55	*SUPRAPARTICLES*	0.55	*NANOFLOWERS*	0.59
TiO2_11_Sil_Sol	titanium dioxide	**advanced fibres,**	*QUANTUM DOTS*	0.55	*QUANTUM DOTS*	0.55	*SUPRAPARTICLES*	0.55

	nanoparticle	**inorganic fibres**						
TiO2_9.1_NF	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.57	*SUPRAPARTICLES*	0.57	*NANOFLOWERS*	0.60
TiO2_9.1_NF_BM	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.57	*SUPRAPARTICLES*	0.57	*PARTICLE REINFORCED COMPOSITES*	0.60
TiO2_9.1_sol_BM	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*QUANTUM DOTS*	0.57	*QUANTUM DOTS*	0.57	*MESOPOROUS MATERIALS*	0.59
TiO2_NF_BM_2h	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.54	*SUPRAPARTICLES*	0.54	*PARTICLE REINFORCED COMPOSITES*	0.55
TiO2_NF_BM_4h	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.54	*SUPRAPARTICLES*	0.54	*QUANTUM DOTS*	0.55
TiO2_NF_BM_6h	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.55	*SUPRAPARTICLES*	0.55	*PARTICLE REINFORCED COMPOSITES*	0.55
TiO2_NF_BM_9h	titanium dioxide nanoparticle	**advanced fibres, inorganic fibres**	*SUPRAPARTICLES*	0.55	*SUPRAPARTICLES*	0.55	*QUANTUM DOTS*	0.56
ZnFe2O4 30 nm NRCWE-021	zinc ferrite	**advanced alloys, intermetallic**	*QUANTUM DOTS*	0.65	*QUANTUM DOTS*	0.65	*ADVANCED ALLOYS*	0.68
phage mimetic nanorods (PMN)	nanorod	**advanced fibres, organic**	*SUGAR-BASED BIOPOLYMERS*	0.52	*SUGAR-BASED BIOPOLYMERS*	0.52	*QUANTUM DOTS*	0.53
rGO - Carbon NRCWE-059	multi-walled nanotube	**advanced fibres, carbon-based fibres**	*FIBRE-REINFORCED COMPOSITES*	0.58	*FIBRE-REINFORCED COMPOSITES*	0.58	*CARBON-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.

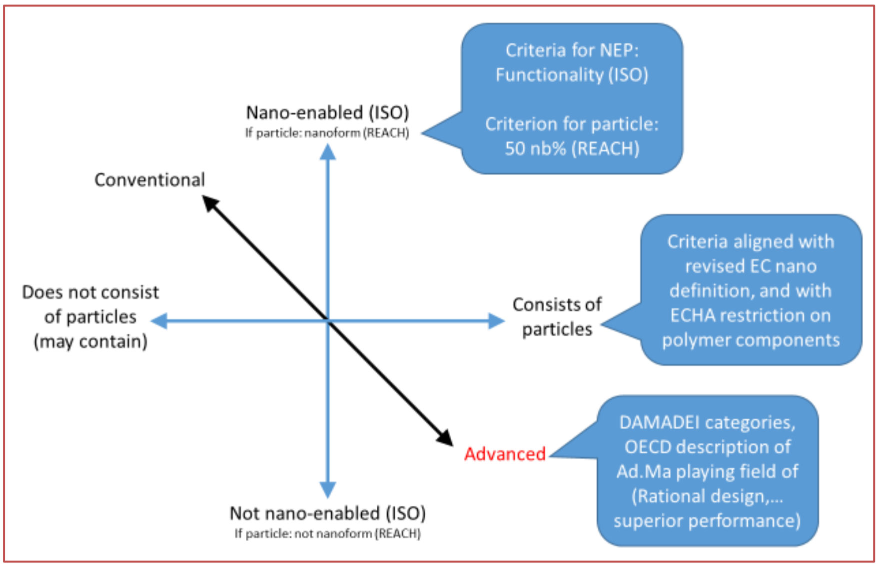


Figure 18. InnoMat.Life categorisation of materials (conventional and advanced) with the assessment criteria.

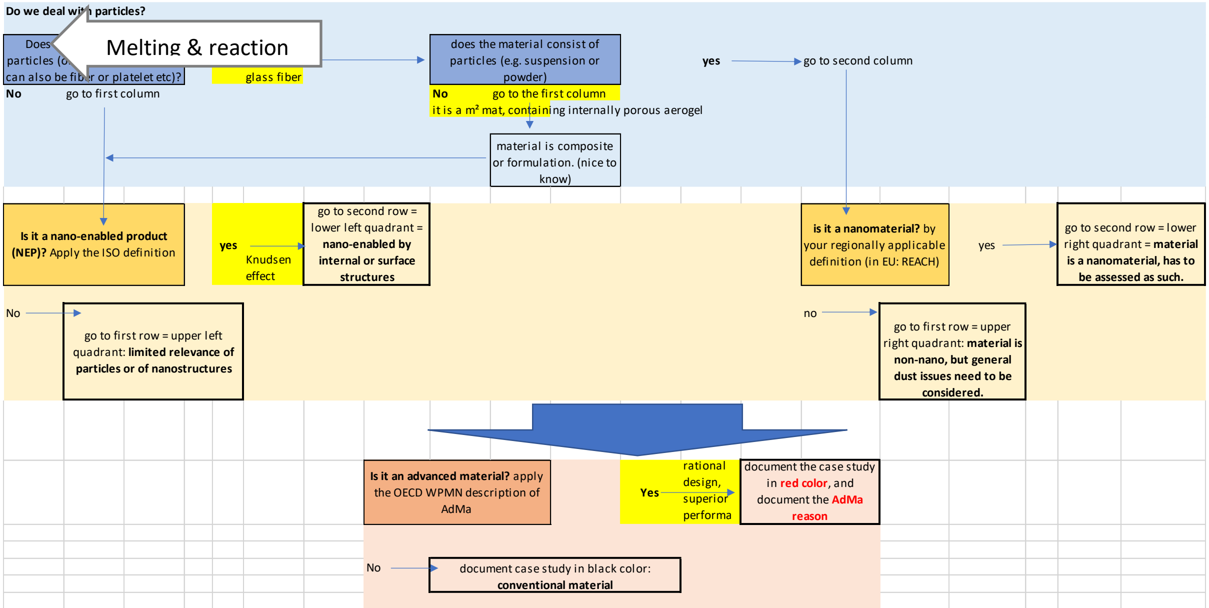


Figure 19. InnoMat.Life flowchart on the example (yellow highlights) of aerogel-fibre-mats.

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
     - 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 nano-enabled.
   - Plastics
     - 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
  - 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)
  - 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)
  - Advanced e.g. QLED™ color converter or flexible display electrode, or dispersoid-pinned alloy
- Catalysts,
  - 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
  - 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 CO_2 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
  - Advanced filler e.g. graphenes, mwCNT, swCNT, TiO_2 cubes, TiO_2 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	Functionality	*Could be used as ingredient in which final product material class?*	Is there a benefit vs. conventional material? Which?	Consists of particles/ fibres/ platelets?	*Advanced ?*	*Nano-material or nano-enabled ?*
NRCWE-006 MWCNT (Mitsui)	multi-walled carbon nanotube	mechanical modulus	*FIBRE-REINFORCED COMPOSITES*	Compare CFRP	Yes	*yes*	*Yes (borderline to non-nano)*
AgNP (7–10 nm, stabilized with polyethylenimine)	silver nanoparticle	Biocidal activity	*PARTICLE REINFORCED COMPOSITES*	Compare other food packaging	Yes	*Yes (due to targeted structure)*	*Yes*
AuNP (Alkanethiol/lipid, Custom made)	gold nanoparticle	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	*No (due to highly established market)*	*yes*
AuNP (Citrate, Custom made)	gold nanoparticle	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	*No (due to highly established market)*	*yes*
AuNP (Poly(allylamine hydrochloride), Custom made)	gold nanoparticle	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	*No (due to highly established market)*	*yes*
AuNP (Poly(allylamine hydrochloride)/ lipid, Custom made)	gold nanoparticle	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	*No (due to highly established market)*	*yes*
AuNP oligonucleotide complexes	gold nanoparticle	Visible marker particle	Sensors	Routine in pregnancy test, adapted in mass-covid test	yes	*No (due to highly established market)*	*yes*
Bentonite - Nano-clay	BENTONITE	Barrier properties, adsorption properties	*PARTICLE REINFORCED COMPOSITES, 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, conductivity	*FIBRE-REINFORCED COMPOSITES*	Compare CFRP	Yes	*yes*	*Yes*

ENP (S-nitrosoglutathione (GSNO)-loaded Eudragit RL nanoparticles)	Polymer nanoparticle	Taste masking and encapsulation during stomach phase	Drug delivery	Co-Polymer class is used since 1950ies	Yes	*Yes (targeted structure)*	*Yes*
ENP (empty Eudragit RL nanoparticles)	Polymer nanoparticle	Taste masking and encapsulation 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-REINFORCED COMPOSITES*	Compare CFRP	No (NM contained)	*yes*	*Yes*
EPOXY-CNT - NRCWE-035	multi-walled nanotube in epoxy	mechanical modulus	*FIBRE-REINFORCED COMPOSITES*	Compare CFRP	No (NM contained)	*yes*	*Yes*
GO - Carbon NRCWE-058	graphene oxide	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (targeted structure*	*Yes*
Graphene oxide (NH2-functionalized)	graphene oxide	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (targeted structure*	*Yes*
Graphene oxide (pristine?) - GSE83516	graphene oxide	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (targeted structure*	*Yes*
Graphene oxide (pristine?) - GSE99929	graphene oxide	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (targeted structure*	*Yes*
Graphene quantum dots (hyrdoxyl-modified)	Carbon particle	luminescence	*PARTICLE COMPOSITES*	No heavy metals	Yes	*yes*	*yes*
Graphite (?) - GSE92899	graphite						
Graphite (nanofibers, Sigma-Aldrich)	graphite						
Iron oxide NPs (Custom made, polyglucose-	iron oxide nanoparticle	Heats up in AC	Hyper-thermia	Other cancer therapies	yes	*Yes (due to medical*	*yes*

sorbitol-carboxymethyether (PSC) coated)		magnetic field	therapy of tumours			*applicati on only)*	
MWCNT (?) - E-TABM-679	multi-walled carbon nanotube?	Mechanical modulus, conductivity?	*FIBRE-REINFORCED COMPOSITES?*		Yes	*yes*	*Yes*
MWCNT (?) - GSE43515	multi-walled carbon nanotube?	Mechanical modulus, conductivity?	*FIBRE-REINFORCED COMPOSITES?*		Yes	*yes*	*Yes*
MWCNT (Bayer material science)	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
MWCNT (Baytubes)	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
MWCNT (SES research)	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
MWCNT (Sigma-Aldrich)	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
MWCNT (carpet)	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	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, conductivity	*FIBRE-REINFORCED COMPOSITES*	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, conductivity	*FIBRE-REINFORCED COMPOSITES*	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	conductivity	*D COMPOSITES*	lower loading than w/ CB. Mechanics: compare CFRP			
NN - Aluminosilicate clay	alluminosilicate	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (due to targeted structure*	*Yes*
NN-etched - Aluminosilicate clay	alluminosilicate	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (due to targeted structure*	*Yes*
NP-ERL (Eudragit RL PO polymeric nanoparticles)	Polymer nanoparticle	Taste masking and encapsulation 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 nanoparticle		*Drug delivery*	Compare similar aggregated grades of SiO2	Yes	*borderline*	*No*
NRCWE#067, Porous Silica 100 nm - Silica	silicon dioxide nanoparticle		*Drug delivery*	Compare similar aggregated grades of SiO2	Yes	*borderline*	*Borderline*
NRCWE#069, Porous Silica 300 nm-CuO - Silica	silicon dioxide nanoparticle	Delayed release of biocide	*Drug delivery*	Compare similar aggregated grades of SiO2	Yes	*Yes, (multi-component)*	*No*
NRCWE#070, Porous Silica 100 nm-CuO - Silica	silicon dioxide nanoparticle	Delayed release of biocide	*Drug delivery*	Compare similar aggregated grades of SiO2	Yes	*Yes, (multi-component)*	*Borderline*
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, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-041 - Carbon	multi-walled	Mechanical modulus,	*FIBRE-REINFORCED*	Can achieve conductivity at lower loading	Yes	*yes*	*Yes*

	carbon nanotube	conductivity	*COMPOSITES*	than w/ CB. Mechanics: compare CFRP			
NRCWE-042 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-043 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-044 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-045 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-046 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-047 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-048 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-049 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*
NRCWE-051 - Carbon	multi-walled carbon nanotube	Mechanical modulus, conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB. Mechanics: compare CFRP	Yes	*yes*	*Yes*

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

			COMPOSITES	Mechanics: compare CFRP			
NiFe2O4 30 nm NRCWE-022	nickel ferrite		Cannot tell. R&D material, not for specific use		Yes		*Yes*
NiZnFe4O8 30 nm NRCWE-020	nickel-zinc ferrite		Cannot tell. R&D material, not for specific use		Yes		*Yes*
SWCNT (P2-SWNT)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
PAMAM dendrimer-NH2	poly(amido amine) dendrimer	Tunable responsiveness	Drug delivery	Copolymer is stimuli-responsive	No, single molecule	*yes*	*No* (single molecules are no NM)
PAMAM-NH2 (Dendritech Inc.)	poly(amido amine) dendrimer	Tunable responsiveness	Drug delivery	Copolymer is stimuli-responsive	No, single molecule	*yes*	*No* (single molecules are no NM)
PAMAM-OH (Dendritech Inc.)	poly(amido amine) dendrimer	Tunable responsiveness	Drug delivery	Copolymer is stimuli-responsive	No, single molecule	*yes*	*No* (single molecules are no NM)
SWCNT (?) - GSE83516	single-walled carbon nanotube?		*FIBRE-REINFORCED COMPOSITES?*				
SWCNT (?) - GSE83516	single-walled carbon nanotube?		*FIBRE-REINFORCED COMPOSITES?*				
SWCNT (Carbon Nanotechnology, CNI)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
SWCNT (SES research)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
SWCNT (Sigma-Aldrich)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
SWCNT (iron-enriched)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*

			COMPOSITES				
SWCNT (purified)	single-walled carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
SWCNT 2 nm NM-411	carbon nanotube	conductivity	*FIBRE-REINFORCED COMPOSITES*	Can achieve conductivity at lower loading than w/ CB.	yes	*yes*	*yes*
Silica (2D nanosilicates, a layered clay)	silicon dioxide nanoparticle	Barrier & adsorption properties	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
Silica NP (DMPC-coated magnetic mesoporous)	silicon dioxide nanoparticle	Filler		Cannot tell. R&D material, not for specific use	yes	*Yes (multicomponent)*	*yes*
Silica NP (PEG-coated magnetic mesoporous)	silicon dioxide nanoparticle	Filler		Cannot tell. R&D material, not for specific use	yes	*Yes (multicomponent)*	*yes*
Silica NP (pristine magnetic mesoporous)	silicon dioxide nanoparticle	Filler		Cannot tell. R&D material, not for specific use	yes	*Yes (multicomponent)*	*yes*
TiO2 nanobelts (Custom made)	titanium dioxide nanoparticle	Filler		Cannot tell. R&D material, not for specific use	yes	*Yes (targeted structure*	*yes*
TiO2 nanotubes (100nm, Custom made)	titanium dioxide nanoparticle	Filler	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*borderline*
TiO2 nanotubes (30nm, Custom made)	titanium dioxide nanoparticle		Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2NF_1.1_NF	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2NF_9,1_Sol_BM_15h	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_1.1_NF	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_11_Sil_Sol	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*Cannot tell by name*

TiO2_9.1_NF	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_9.1_NF_BM	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_9.1_sol_BM	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*Cannot tell by name*
TiO2_NF_BM_2h	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_NF_BM_4h	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_NF_BM_6h	titanium dioxide nanoparticle	pigment	Particle-reinforced composite	Paint, paper, plastics, …	yes	*no*	*yes*
TiO2_NF_BM_9h	titanium dioxide nanoparticle	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 (multicomponent)*	*yes*
phage mimetic nanorods (PMN)	nanorod						
rGO - Carbon NRCWE-059	graphene (via reduction of GO)	Barrier properties	*PARTICLE REINFORCED COMPOSITES*	Laminate structures, other 2D fillers	Yes	*Yes (graphene 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 (https://openai.com/api/). 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.

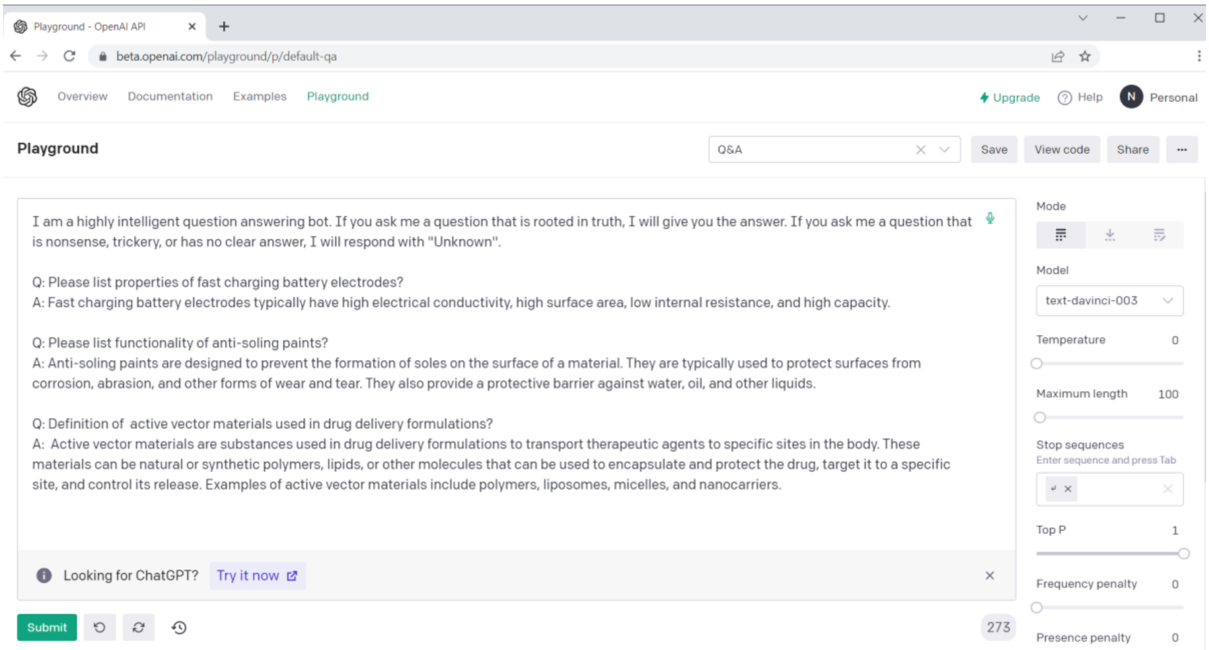


Figure 20. Screenshot of OpenAI playground for question answering. The user provides the question (Q:) and the OpenAI generates the answer. The same Q&A functionality can be requested programmatically.

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.

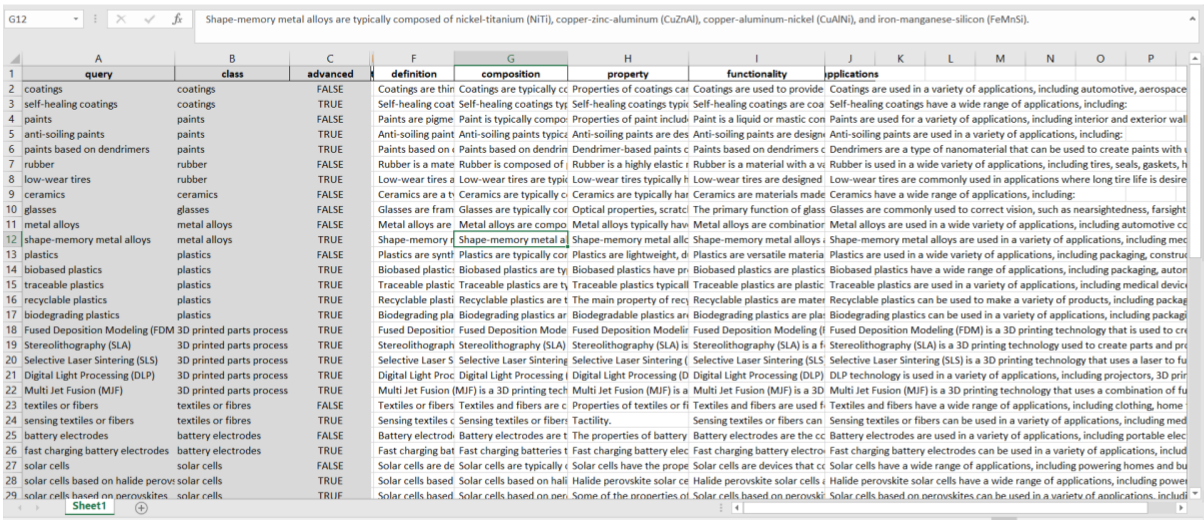


Figure 21. Screenshot of automatic augmentation of InnoMat.Life classification based on OpenAI (GPT-3) query answering.

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).

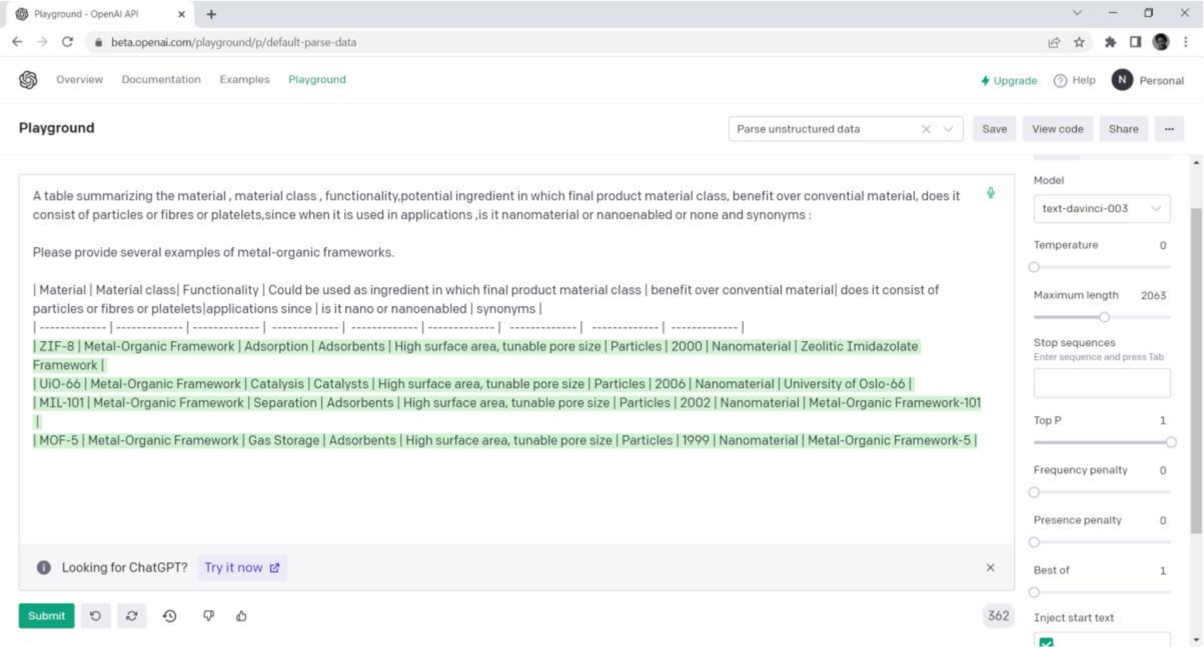
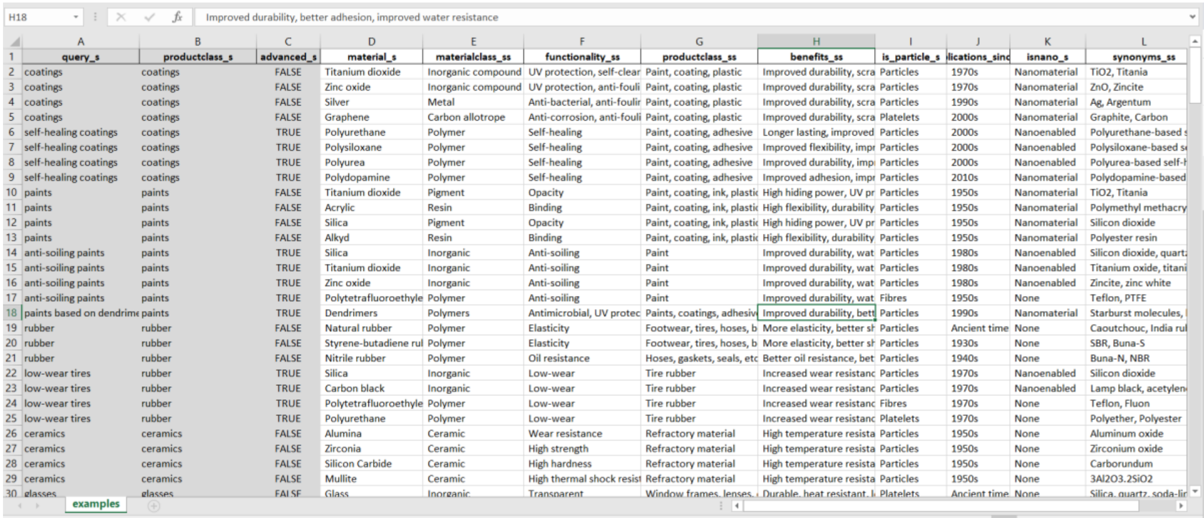


Figure 22. Screenshot of OpenAI playground for unstructured data parsing. The user provides the question and a table template and the OpenAI generates the answer, filling in the table. The same functionality can be requested programmatically.

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*).



H18 | Improved durability, better adhesion, improved water resistance

	A	B	C	D	E	F	G	H	I	J	K	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 s
7	self-healing coatings	coatings	TRUE	Polysiloxane	Polymer	Self-healing	Paint, coating, adhesive	Improved flexibility, impr	Particles	2000s	Nanoenabled	Polysiloxane-based se
8	self-healing coatings	coatings	TRUE	Polyurea	Polymer	Self-healing	Paint, coating, adhesive	Improved durability, impi	Particles	2000s	Nanoenabled	Polyurea-based self-h
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 methacry
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, quartz
15	anti-soiling paints	paints	TRUE	Titanium dioxide	Inorganic	Anti-soiling	Paint	Improved durability, wat	Particles	1980s	Nanoenabled	Titanium oxide, titani
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 dendrime	paints	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 rul
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 resistanc	Particles	1970s	Nanoenabled	Silicon dioxide
23	low-wear tires	rubber	TRUE	Carbon black	Inorganic	Low-wear	Tire rubber	Increased wear resistanc	Particles	1970s	Nanoenabled	Lamp black, acetylen
24	low-wear tires	rubber	TRUE	Polytetrafluoroethyle	Polymer	Low-wear	Tire rubber	Increased wear resistanc	Fibres	1970s	None	Teflon, Fluon
25	low-wear tires	rubber	TRUE	Polyurethane	Polymer	Low-wear	Tire rubber	Increased wear resistanc	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-lir

examples

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.

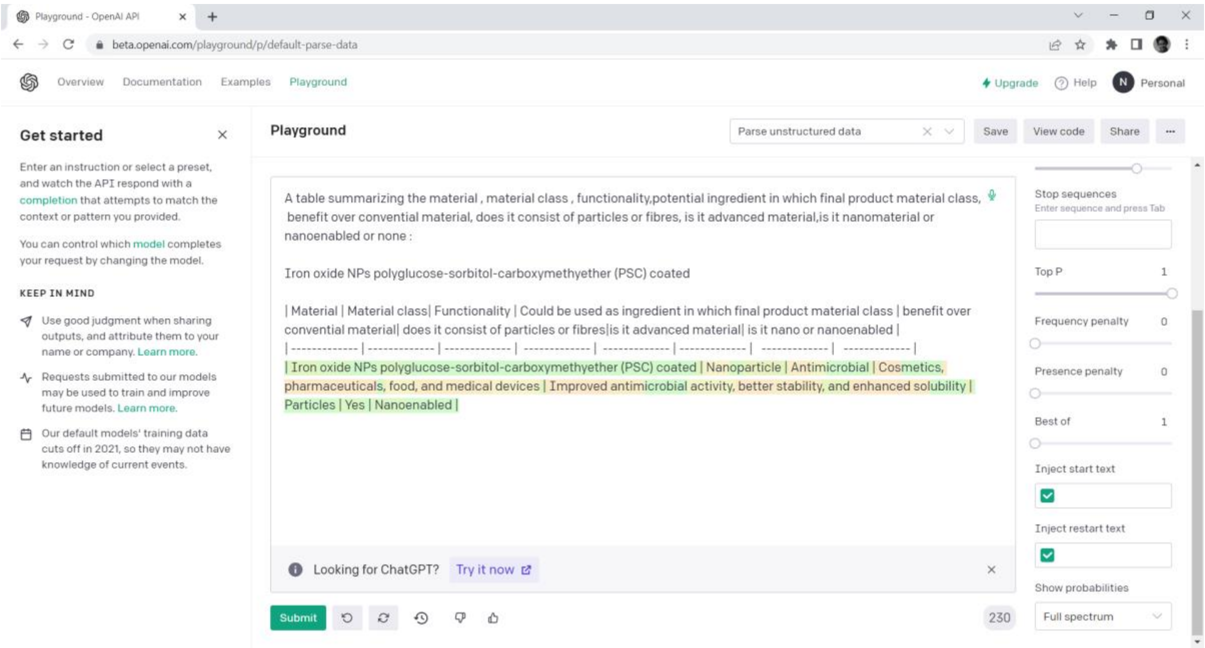
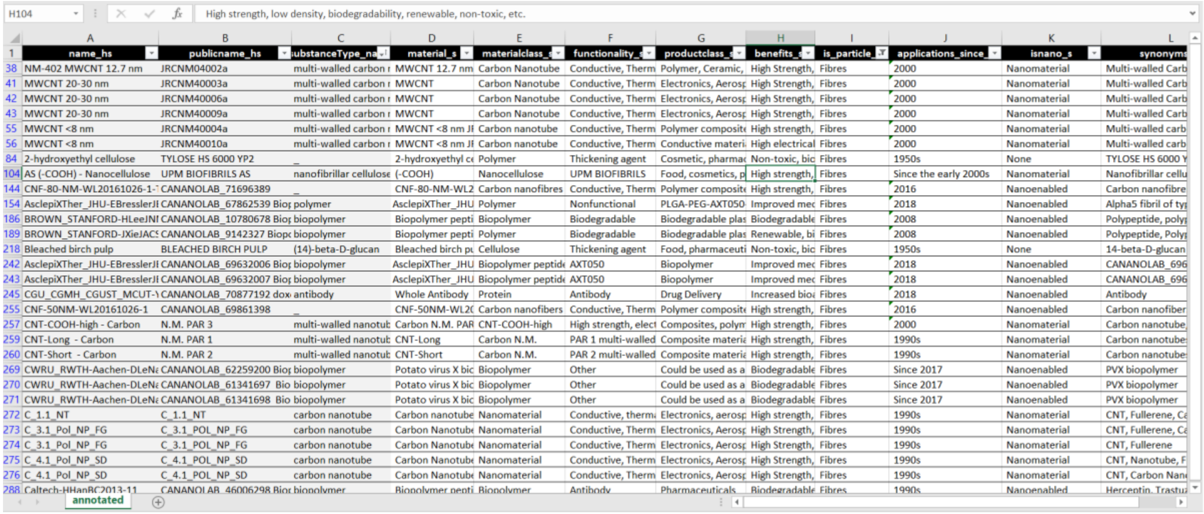


Figure 24. Screenshot of OpenAI playground for unstructured data parsing. The user provides the question and a table template and the OpenAI generates the answer, filling in the table. (The color code relates to the uncertainty of the prediction of particular letters – green – high confidence, red –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

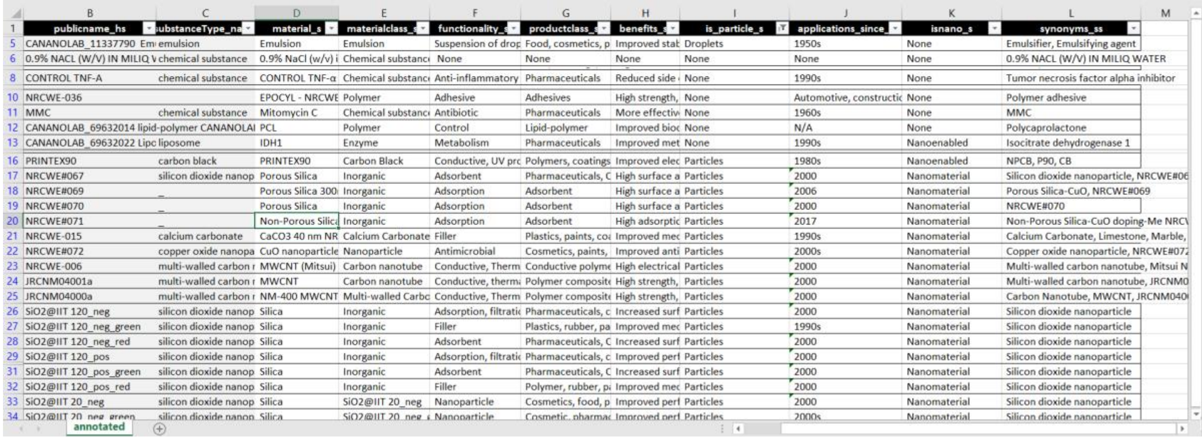
Similarly, we can ask for structured data of specific material (Figure 24) and performed this programmatically for over 2000 materials in eNanoMapper HARMLESS database (this number includes caNanoLab) , resulting in a table of 2269 rows. Excerpts of the annotation are shown in Figure 25, the annotation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



H104 | High strength, low density, biodegradability, renewable, non-toxic, etc.

1	name_hs	publicname_hs	substanceType_na	material_s	materialclass_s	functionality_s	productclass_s	benefits_s	is_particle	applications_since	isnano_s	synonyms
38	NM-402 MWCNT 12.7 nm	JRCNM04002a	multi-walled carbon r	MWCNT 12.7 nm	Carbon Nanotube	Conductive, Therm	Polymer, Ceramic,	High Strength,	Fibres	2000	Nanomaterial	Multi-walled Carb
41	MWCNT 20-30 nm	JRCNM40003a	multi-walled carbon r	MWCNT	Carbon Nanotube	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	2000	Nanomaterial	Multi-walled Carb
42	MWCNT 20-30 nm	JRCNM40006a	multi-walled carbon r	MWCNT	Carbon Nanotube	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	2000	Nanomaterial	Multi-walled Carb
43	MWCNT 20-30 nm	JRCNM40009a	multi-walled carbon r	MWCNT	Carbon Nanotube	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	2000	Nanomaterial	Multi-walled Carb
55	MWCNT <8 nm	JRCNM40004a	multi-walled carbon r	MWCNT <8 nm JI	Carbon nanotube	Conductive, Therm	Polymer composite	High strength,	Fibres	2000	Nanomaterial	Multi-walled carb
56	MWCNT <8 nm	JRCNM40010a	multi-walled carbon r	MWCNT <8 nm JI	Carbon nanotube	Conductive, Therm	Conductive materi	High electrical	Fibres	2000	Nanomaterial	Multi-walled carb
84	2-hydroxyethyl cellulose	TYLOSE HS 6000 YP2	_	2-hydroxyethyl ce	Polymer	Thickening agent	Cosmetic, pharmac	Non-toxic, bic	Fibres	1950s	None	TYLOSE HS 6000 Y
104	AS (-COOH) - Nanocellulose	UPM BIOFIBRILS AS	nanofibrillar cellulose	(-COOH)	Nanocellulose	UPM BIOFIBRILS	Food, cosmetics, p	High strength,	Fibres	Since the early 2000s	Nanomaterial	Nanofibrillar cellu
144	CNF-80-NM-WL20161026-1-1	CANANOLAB_71696389	_	CNF-80-NM-WL2	Carbon nanofibres	Conductive, Therm	Polymer composite	High strength,	Fibres	2016	Nanoenabled	Carbon nanofibre
154	AsclepiXTher_JHU-EBresslerJI	CANANOLAB_67862539 Bioj	polymer	AsclepiXTher_JHU	Polymer	Nonfunctional	PLGA-PEG-AXT050	Improved mec	Fibres	2018	Nanoenabled	Alpha5 fibril of typ
186	BROWN_STANFORD-HLeeJNI	CANANOLAB_10780678 Bioj	biopolymer	Biopolymer pepti	Biopolymer	Biodegradable	Biodegradable plas	Biodegradable	Fibres	2008	Nanoenabled	Polypeptide, polyp
189	BROWN_STANFORD-JXieJACS	CANANOLAB_9142327 Biopc	biopolymer	Biopolymer pepti	Polymer	Biodegradable	Biodegradable plas	Renewable, bi	Fibres	2008	Nanoenabled	Polypeptide, Polyp
218	Bleached birch pulp	BLEACHED BIRCH PULP	(14)-beta-D-glucan	Bleached birch pu	Cellulose	Thickening agent	Food, pharmaceuti	Non-toxic, bic	Fibres	1950s	None	14-beta-D-glucan
242	AsclepiXTher_JHU-EBresslerJI	CANANOLAB_69632006 Bioj	biopolymer	AsclepiXTher_JHU	Biopolymer peptide	AXT050	Biopolymer	Improved mec	Fibres	2018	Nanoenabled	CANANOLAB_696
243	AsclepiXTher_JHU-EBresslerJI	CANANOLAB_69632007 Bioj	biopolymer	AsclepiXTher_JHU	Biopolymer peptide	AXT050	Biopolymer	Improved mec	Fibres	2018	Nanoenabled	CANANOLAB_696
245	CGU_CGMH_CGUST_MCUT-\	CANANOLAB_70877192 dox	antibody	Whole Antibody	Protein	Antibody	Drug Delivery	Increased bioa	Fibres	2018	Nanoenabled	Antibody
255	CNF-50NM-WL20161026-1	CANANOLAB_69861398	_	CNF-50NM-WL2(	Carbon nanofibers	Conductive, Therm	Polymer composite	High strength,	Fibres	2016	Nanoenabled	Carbon nanofiber
257	CNT-COOH-high - Carbon	N.M. PAR 3	multi-walled nanotub	Carbon N.M. PAR	CNT-COOH-high	High strength, elect	Composites, polym	High strength,	Fibres	2000	Nanomaterial	Carbon nanotube,
259	CNT-Long - Carbon	N.M. PAR 1	multi-walled nanotub	CNT-Long	Carbon N.M.	PAR 1 multi-walled	Composite materia	High strength,	Fibres	1990s	Nanomaterial	Carbon nanotube
260	CNT-Short - Carbon	N.M. PAR 2	multi-walled nanotub	CNT-Short	Carbon N.M.	PAR 2 multi-walled	Composite materia	High strength,	Fibres	1990s	Nanomaterial	Carbon nanotube
269	CWRU_RWTH-Aachen-DLeNa	CANANOLAB_62259200 Bioj	biopolymer	Potato virus X bic	Biopolymer	Other	Could be used as a	Biodegradable	Fibres	Since 2017	Nanoenabled	PVX biopolymer
270	CWRU_RWTH-Aachen-DLeNa	CANANOLAB_61341697 Bio	biopolymer	Potato virus X bic	Biopolymer	Other	Could be used as a	Biodegradable	Fibres	Since 2017	Nanoenabled	PVX biopolymer
271	CWRU_RWTH-Aachen-DLeNa	CANANOLAB_61341698 Bio	biopolymer	Potato virus X bic	Biopolymer	Other	Could be used as a	Biodegradable	Fibres	Since 2017	Nanoenabled	PVX biopolymer
272	C_1.1_NT	C_1.1_NT	carbon nanotube	Carbon nanotube	Nanomaterial	Conductive, therm	Electronics, aerosp	High strength,	Fibres	1990s	Nanomaterial	CNT, Fullerene, Ca
273	C_3.1_Pol_NP_FG	C_3.1_POL_NP_FG	carbon nanotube	Carbon Nanotube	Nanomaterial	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	1990s	Nanomaterial	CNT, Fullerene, Ca
274	C_3.1_Pol_NP_FG	C_3.1_POL_NP_FG	carbon nanotube	Carbon Nanotube	Nanomaterial	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	1990s	Nanomaterial	CNT, Fullerene
275	C_4.1_Pol_NP_SD	C_4.1_POL_NP_SD	carbon nanotube	Carbon Nanotube	Nanomaterial	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	1990s	Nanomaterial	CNT, Nanotube, F
276	C_4.1_Pol_NP_SD	C_4.1_POL_NP_SD	carbon nanotube	Carbon Nanotube	Nanomaterial	Conductive, Therm	Electronics, Aerosp	High Strength,	Fibres	1990s	Nanomaterial	CNT, Carbon Nan
288	Caltech-HHanBC2013-11	CANANOLAB_46006298 Bioj	biopolymer	Biopolymer pepti	Biopolymer	Antibody	Pharmaceuticals	Biodegradable	Fibres	1990s	Nanoenabled	Herceptin, Trastu

annotated



1	publicname_hs	substanceType_na	material_s	materialclass_s	functionality_s	productclass_s	benefits_s	is_particle_s	applications_since	isnano_s	synonyms_ss
5	CANANOLAB_11337790 Em	emulsion	Emulsion	Emulsion	Suspension of drop	Food, cosmetics, p	Improved stat	Droplets	1950s	None	Emulsifier, Emulsifying agent
6	0.9% NACL (W/V) IN MILIQ V	chemical substance	0.9% NaCl (w/v) i	Chemical substance	None	None	None	None	None	None	0.9% NACL (W/V) IN MILIQ WATER
8	CONTROL TNF-A	chemical substance	CONTROL TNF-α	Chemical substance	Anti-inflammatory	Pharmaceuticals	Reduced side	None	1990s	None	Tumor necrosis factor alpha inhibitor
10	NRCWE-036		EPOCYL - NRCWE	Polymer	Adhesive	Adhesives	High strength,	None	Automotive, constructic	None	Polymer adhesive
11	MMC	chemical substance	Mitomycin C	Chemical substance	Antibiotic	Pharmaceuticals	More effectiv	None	1960s	None	MMC
12	CANANOLAB_69632014 lipid-polymer	CANANOLAI	PCL	Polymer	Control	Lipid-polymer	Improved bioc	None	N/A	None	Polycaprolactone
13	CANANOLAB_69632022 Lipc	liposome	IDH1	Enzyme	Metabolism	Pharmaceuticals	Improved met	None	1990s	Nanoenabled	Isocitrate dehydrogenase 1
16	PRINTEX90	carbon black	PRINTEX90	Carbon Black	Conductive, UV prc	Polymers, coatings	Improved elec	Particles	1980s	Nanoenabled	NPCB, P90, CB
17	NRCWE#067	silicon dioxide nanop	Porous Silica	Inorganic	Adsorbent	Pharmaceuticals, C	High surface a	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle, NRCWE#06
18	NRCWE#069	_	Porous Silica 300	Inorganic	Adsorption	Adsorbent	High surface a	Particles	2006	Nanomaterial	Porous Silica-CuO, NRCWE#069
19	NRCWE#070	_	Porous Silica	Inorganic	Adsorption	Adsorbent	High surface a	Particles	2000	Nanomaterial	NRCWE#070
20	NRCWE#071	_	Non-Porous Silica	Inorganic	Adsorption	Adsorbent	High adsorptic	Particles	2017	Nanomaterial	Non-Porous Silica-CuO doping-Me NRC\
21	NRCWE-015	calcium carbonate	CaCO3 40 nm NR	Calcium Carbonate	Filler	Plastics, paints, co	Improved mec	Particles	1990s	Nanomaterial	Calcium Carbonate, Limestone, Marble,
22	NRCWE#072	copper oxide nanopa	CuO nanoparticle	Nanoparticle	Antimicrobial	Cosmetics, paints,	Improved anti	Particles	2000s	Nanomaterial	Copper oxide nanoparticle, NRCWE#07
23	NRCWE-006	multi-walled carbon r	MWCNT (Mitsui)	Carbon nanotube	Conductive, Therm	Conductive polyme	High electrical	Particles	2000	Nanomaterial	Multi-walled carbon nanotube, Mitsui N
24	JRCNM04001a	multi-walled carbon r	MWCNT	Carbon nanotube	Conductive, therm	Polymer composite	High strength,	Particles	2000	Nanomaterial	Multi-walled carbon nanotube, JRCNM0
25	JRCNM04000a	multi-walled carbon r	NM-400 MWCNT	Multi-walled Carbo	Conductive, Therm	Polymer composite	High strength,	Particles	2000	Nanomaterial	Carbon Nanotube, MWCNT, JRCNM040
26	SiO2@IIT 120_neg	silicon dioxide nanop	Silica	Inorganic	Adsorption, filtratic	Pharmaceuticals, c	Increased surf	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
27	SiO2@IIT 120_neg_green	silicon dioxide nanop	Silica	Inorganic	Filler	Plastics, rubber, pa	Improved mec	Particles	1990s	Nanomaterial	Silicon dioxide nanoparticle
28	SiO2@IIT 120_neg_red	silicon dioxide nanop	Silica	Inorganic	Adsorbent	Pharmaceuticals, C	Increased surf	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
29	SiO2@IIT 120_pos	silicon dioxide nanop	Silica	Inorganic	Adsorption, filtratic	Pharmaceuticals, c	Improved perf	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
31	SiO2@IIT 120_pos_green	silicon dioxide nanop	Silica	Inorganic	Adsorbent	Pharmaceuticals, C	Increased surf	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
32	SiO2@IIT 120_pos_red	silicon dioxide nanop	Silica	Inorganic	Filler	Polymer, rubber, pa	Improved mec	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
33	SiO2@IIT 20_neg	silicon dioxide nanop	Silica	SiO2@IIT 20_neg	Nanoparticle	Cosmetics, food, p	Improved perf	Particles	2000	Nanomaterial	Silicon dioxide nanoparticle
34	SiO2@IIT 20_neg_green	silicon dioxide nanop	Silica	SiO2@IIT 20_neg	Nanoparticle	Cosmetic, pharmac	Improved perf	Particles	2000s	Nanomaterial	Silicon dioxide nanoparticle

annotated

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	Functionality	Could be used as ingredient in which final product material class	benefit over convential material	does it consist of particles or fibres	industrial usage since	is it nano or nanoenabled
NRCWE-006 MWCNT (Mitsui)	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Conductive polymers, composites, coatings, etc.	Higher conductivity, thermal and mechanical properties	Particles	2000	Nanomaterial
AgNP (7−10 nm, stabilized with	silver nanoparticle	Antimicrobial	Textiles, plastics, paints, coatings, etc.	Higher antimicrobial activity,	Particles	2000s	Nanomaterial

polyethylenimine)				improved durability, and better color retention			
AuNP (Alkanethiol/lipid, Custom made)	gold nanoparticle	Antimicrobial, catalytic, optical, and electrical properties	Cosmetics, pharmaceuticals, food, and medical devices	Improved performance, enhanced properties, and cost savings	Particles	2000s	Nanomaterial
AuNP (Citrate, Custom made)	gold nanoparticle	Antimicrobial, catalytic, optical, and electrical properties	Cosmetics, pharmaceuticals, food, and medical devices	Improved performance, enhanced properties, and cost savings	Particles	2000s	Nanomaterial
AuNP (Poly(allylamine hydrochloride), Custom made)	gold nanoparticle	Antimicrobial	Cosmetics, pharmaceuticals, food, etc.	Increased antimicrobial activity, improved solubility, and enhanced stability	Particles	Since 2000s	Nanomaterial
AuNP (Poly(allylamine hydrochloride)/lipid, Custom made)	gold nanoparticle	Antimicrobial	Cosmetics, pharmaceuticals, food, etc.	Increased antimicrobial activity, improved solubility, and enhanced stability	Particles	2000s	Nanomaterial
AuNP oligonucleotide complexes	gold nanoparticle	Antibacterial	Pharmaceuticals, cosmetics, food, and other consumer products	Increased stability, improved solubility, and enhanced bioavailability	Particles	2000	Nanomaterial
Bentonite - Nano-clay	BENTONITE	Adsorption, Absorption, Cation Exchange	Cosmetics, Pharmaceuticals, Paints, Drilling Fluids	High adsorption capacity, Low cost, Non-toxic	Particles	1950s	Nanoenabled
CNTSmall, CNT - Carbon NRCWE-026	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, rubbers, coatings, composites, etc.	High strength, high thermal conductivity, low weight	Particles	2000	Nanomaterial
ENP (S-nitrosoglutathione (GSNO)-loaded Eudragit RL nanoparticles)	Polymer nanoparticle	Drug delivery	Pharmaceuticals	Improved drug delivery	Particles	Since 2000s	Nanomaterial

ENP (empty Eudragit RL nanoparticles)	Polymer nanoparticle	Drug delivery	Pharmaceuticals	Improved drug solubility, increased bioavailability, improved stability	Particles	2000	Nanomaterial
EPOCYL - NRCWE-036	multi-walled nanotube suspended in liquid epoxy precursor	Reinforcement	composite materials	improved mechanical properties, increased thermal conductivity, improved electrical conductivity	particles	since 2000	nanomaterial
EPOXY-CNT - NRCWE-035	multi-walled nanotube in epoxy	Reinforcement	Epoxy resin	Increased strength and stiffness, improved thermal and electrical conductivity	Particles	Since 2000	Nanomaterial
GO - Carbon NRCWE-058	graphene oxide	Conductive, barrier, adsorptive	Polymers, composites, coatings, films, etc.	High electrical conductivity, high thermal conductivity, high mechanical strength, high chemical stability, low cost	Platelets	Since 2010	Nanoenabled
Graphene oxide (NH2-functionalized)	graphene oxide	Adsorption, filtration, catalysis, etc.	Polymers, composites, coatings, etc.	High surface area, high electrical conductivity, etc.	Particles	Since 2010	Nanomaterial
Graphene oxide (pristine?) - GSE83516	graphene oxide	Conductive, strong, lightweight	Electronics, batteries, composites, coatings, etc.	Higher conductivity, strength, and flexibility than conventional materials	Platelets	Unknown	Nanoenabled
Graphene oxide (pristine?) - GSE99929	graphene oxide	Conductive, barrier, adsorptive, etc.	Electronics, batteries, coatings, etc.	High electrical conductivity, high strength, low weight, etc.	Particles	Since 2010	Nanoenabled
Graphene quantum dots (hyrdoxyl-modified)	Carbon particle	Conductive, luminescent, and catalytic	Electronics, batteries, coatings, paints, etc.	High conductivity, high surface area, and low cost	Particles	2018	Nanoenabled

Graphite (?) - GSE92899	graphite	Conductive	Electronics	Higher conductivity, lower cost	Particles	Unknown	None
Graphite (nanofibers, Sigma-Aldrich)	graphite	Conductive, thermal insulation	Battery electrodes, fuel cells, sensors	Higher conductivity, higher thermal insulation	Fibres	Since 2000s	Nanoenabled
Iron oxide NPs (Custom made, polyglucose-sorbitol-carboxymethyether (PSC) coated)	iron oxide nanoparticle	Magnetic	Magnetic fluids, paints, coatings, lubricants, etc.	Higher magnetic properties, better stability, and improved biocompatibility	Particles	Since 2000s	Nanomaterial
MWCNT (?) - E-TABM-679	multi-walled carbon nanotube	Conductive, thermal, and mechanical properties	Conductive polymers, composites, and coatings	Higher electrical conductivity, thermal conductivity, and mechanical strength	Particles	2000	Nanomaterial
MWCNT (?) - GSE43515	multi-walled carbon nanotube	Conductive, heat resistant, strong	Conductive materials, plastics, rubbers, coatings, etc.	Higher conductivity, heat resistance, and strength than conventional materials	Particles	2000s	Nanomaterial
MWCNT (Bayer material science)	multi-walled carbon nanotube	Conductive, thermal, mechanical, optical	Plastics, rubbers, coatings, composites, etc.	High strength, light weight, high electrical conductivity, high thermal conductivity	Particles	2000	Nanoenabled
MWCNT (Baytubes)	multi-walled carbon nanotube	Conductive, thermal, and mechanical properties	Plastics, rubbers, composites, coatings, etc.	Higher strength, lighter weight, better electrical and thermal conductivity	Particles	2000	Nanomaterial
MWCNT (SES research)	multi-walled carbon nanotube	Conductive, thermally conductive, and electrically conductive	Plastics, rubbers, coatings, and composites	Higher strength, lighter weight, and improved electrical and thermal conductivity	Particles	2000	Nanomaterial

MWCNT (Sigma-Aldrich)	multi-walled carbon nanotube	Conductive, thermal, mechanical, optical	Plastics, rubbers, coatings, composites, etc.	High strength, light weight, high electrical conductivity, high thermal conductivity	Particles	2000	Nanomaterial
MWCNT (carpet)	multi-walled carbon nanotube	Conductive, thermal, and mechanical properties	Conductive materials, plastics, rubbers, coatings, etc.	Higher conductivity, thermal stability, and mechanical strength	Particles	2000s	Nanomaterial
MWCNT 74 nm NRCWE-007	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Conductive polymers, composites, coatings, etc.	Higher conductivity, thermal stability, mechanical strength	Particles	2000	Nanomaterial
MWCNT Cheap Tubes 74 nm NRCWE-007	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	plastics, rubbers, coatings, composites, etc.	Increased strength, durability, and flexibility	Particles	2000	Nanomaterial
NM-411 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NN - Aluminosilicate clay	alluminosilicate	Adsorption, Absorption, Filtration	Polymers, Plastics, Coatings, Paints, Adhesives	Improved mechanical properties, Increased thermal stability, Improved barrier properties	Particles	1990s	Nanoenabled
NN-etched - Aluminosilicate clay	alluminosilicate	Adsorption, filtration, catalysis	Polymer, ceramic, composite	High surface area, high adsorption capacity, high thermal stability	Particles	Since 2000s	Nanoenabled
NP-ERL (Eudragit RL PO polymeric nanoparticles)	Polymer nanoparticle	Controlled release	Pharmaceuticals, food, cosmetics, agrochemicals	Improved drug delivery, improved stability, improved solubility	Particles	2000	Nanomaterial
NRCWE#065, Porous Silica 300 nm - Silica	silicon dioxide nanoparticle	Adsorption, filtration, catalysis	Pharmaceuticals, cosmetics, food, paints, coatings, adhesives, sealants, etc.	Increased surface area, improved adsorption, improved filtration,	Particles	Since 2000	Nanomaterial

				improved catalysis			
NRCWE#067, Porous Silica 100 nm - Silica	silicon dioxide nanoparticle	Adsorption, filtration, catalysis	Pharmaceuticals, cosmetics, food, paints, coatings, adhesives, sealants, etc.	Increased surface area, improved adsorption, improved filtration, improved catalysis	Particles	Since 2000	Nanomaterial
NRCWE#069, Porous Silica 300 nm-CuO - Silica	silicon dioxide nanoparticle	Adsorption, Catalysis, Separation	Pharmaceuticals, Cosmetics, Food, Agriculture, Environmental	High surface area, high porosity, high reactivity, low cost	Particles	2000	Nanomaterial
NRCWE#070, Porous Silica 100 nm-CuO - Silica	silicon dioxide nanoparticle	Adsorption, Catalysis, Separation	Pharmaceuticals, Cosmetics, Food, Agriculture	High surface area, High porosity, High reactivity	Particles	2000	Nanomaterial
NRCWE-020 NiZnFe4O8 30 nm	nickel-zinc ferrite	Magnetic	Magnetic materials	High coercivity and saturation magnetization	Particles	2000	Nanomaterial
NRCWE-021 ZnFe2O4 30 nm	zinc ferrite	Magnetic	Magnetic materials	High coercivity and saturation magnetization	Particles	Since 2000	Nanomaterial
NRCWE-022 NiFe2O4 30 nm	nickel ferrite	Magnetic	Magnetic materials	Higher coercivity and saturation magnetization	Particles	Since 2000s	Nanomaterial
NRCWE-040 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, elastomers, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-041 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-042 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-043 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial

NRCWE-044 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-045 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-046 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-047 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, rubbers, coatings, composites, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-048 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-049 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-051 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high electrical conductivity, high thermal conductivity	Particles	2000	Nanomaterial
NRCWE-052 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-053 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-054 - Carbon	multi-walled carbon nanotube	Conductive, Thermal,	Plastics, composites, coatings, elastomers, etc.	High strength, high thermal conductivity, high electrical	Particles	2000	Nanomaterial

		Mechanical		conductivity, low weight			
NRCWE-055 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-056 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high electrical conductivity, high thermal conductivity	Particles	2000	Nanomaterial
NRCWE-057 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Polymer composites, coatings, adhesives, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-061 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high electrical conductivity, high thermal conductivity	Particles	2000	Nanomaterial
NRCWE-062 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
NRCWE-063 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high electrical conductivity, high thermal conductivity	Particles	2000	Nanomaterial
NRCWE-064 - Carbon	multi-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, composites, coatings, etc.	High strength, high thermal conductivity, high electrical conductivity	Particles	2000	Nanomaterial
$NiFe_2O_4$ 30 nm NRCWE-022	nickel ferrite	Magnetic	Magnetic materials, such as magnets, motors, and generators	Higher coercivity and saturation magnetization	Particles	Since 2000s	Nanomaterial
$NiZnFe_4O_8$ 30 nm NRCWE-020	nickel-zinc ferrite	Magnetic	Magnetic materials	High coercivity and high saturation magnetization	Particles	Since 2018	Nanomaterial
SWCNT (P2-SWNT)	single-walled carbon nanotube	Conductive, thermally conductive,	Plastics, rubbers, coatings, composites, etc.	Higher strength, lighter weight, better electrical and thermal	Fibres	2000	Nanomaterial

		optically active		conductivity, higher chemical stability			
PAMAM dendrimer-NH2	poly(amidoamine) dendrimer	Adsorption, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, biocompatibility, and solubility	Particles	1990s	Nanoenabled
PAMAM-NH2 (Dendritech Inc.)	poly(amidoamine) dendrimer	Adsorption, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, high solubility, biocompatibility, etc.	Particles	2000	Nanoenabled
PAMAM-OH (Dendritech Inc.)	poly(amidoamine) dendrimer	Adsorption, drug delivery, gene delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	High surface area, high solubility, biocompatibility, etc.	Particles	2000	Nanoenabled
SWCNT (?) - GSE83516	single-walled carbon nanotube	Conductive, thermally conductive, optically active	Conductive polymers, composites, coatings	Higher conductivity, thermal conductivity, optical activity	Particles	2000	Nanomaterial
SWCNT (?) - GSE83516	single-walled carbon nanotube	Conductive, thermally conductive, optically active	Conductive polymers, composites, coatings	Higher conductivity, thermal conductivity, optical activity	Particles	2000	Nanomaterial
SWCNT (Carbon Nanotechnology, CNI)	single-walled carbon nanotube	Conductive, thermally conductive, optically active	Electronics, batteries, composites, coatings, etc.	High strength, light weight, high electrical and thermal conductivity, high surface area	Particles	2000	Nanomaterial
SWCNT (SES research)	single-walled carbon nanotube	Conductive, thermally conductive, optically active	Plastics, rubbers, coatings, composites	High strength, light weight, high electrical and thermal conductivity, high surface area	Particles	2000	Nanomaterial

SWCNT (Sigma-Aldrich)	single-walled carbon nanotube	Conductive, Thermal, Mechanical	Plastics, Composites, Coatings	High strength, High electrical conductivity, High thermal conductivity	Particles	2000	Nanomaterial
SWCNT (iron-enriched)	single-walled carbon nanotube	Conductive, thermally and electrically	Conductive polymers, composites, coatings, etc.	High electrical and thermal conductivity, high strength, lightweight	Particles	2000	Nanomaterial
SWCNT (purified)	single-walled carbon nanotube	Conductive, thermally conductive, optically active	Conductive plastics, composites, coatings, etc.	Higher conductivity, thermal conductivity, and optical activity than conventional materials	Fibres	2000s	Nanomaterial
SWCNT 2 nm NM-411	carbon nanotube	Conductive, thermal, mechanical, optical	Electronics, aerospace, automotive, energy, medical, etc.	High strength, high electrical conductivity, high thermal conductivity, low weight	Particles	2000	Nanomaterial
Silica (2D nanosilicates, a layered clay)	silicon dioxide nanoparticle	Adsorption, Filtration, Catalysis	Cosmetics, paints, coatings, adhesives, sealants, etc.	Improved performance, enhanced properties, improved durability, etc.	Particles	Since 2000s	Nanomaterial
Silica NP (DMPC-coated magnetic mesoporous)	silicon dioxide nanoparticle	Adsorption, catalysis, drug delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	Higher surface area, improved reactivity, etc.	Particles	2000s	Nanomaterial
Silica NP (PEG-coated magnetic mesoporous)	silicon dioxide nanoparticle	Adsorption, catalysis, drug delivery, etc.	Pharmaceuticals, cosmetics, food, etc.	Increased surface area, improved solubility, etc.	Particles	2000s	Nanomaterial
Silica NP (pristine magnetic mesoporous)	silicon dioxide nanoparticle	Magnetic mesoporous	Pharmaceuticals, cosmetics, food, paints, coatings, adhesives, sealants, etc.	Improved solubility, stability, and bioavailability	Particles	2000s	Nanomaterial
TiO2 nanobelts (Custom made)	titanium dioxide nanoparticle	Photocatalyst	Paint, coating, plastics, paper, etc.	Higher photocatalytic activity, better UV protection, better	Particles	Since 2010	Nanomaterial

TiO2 nanotubes (100nm, Custom made)	titanium dioxide nanoparticle	photocatalyst	paints, coatings, plastics, textiles, etc.	thermal stability improved UV protection, increased durability, improved optical properties	particles	since 2000s	nanomaterial
TiO2 nanotubes (30nm, Custom made)	titanium dioxide nanoparticle	UV protection, photocatalysis, antibacterial, antifouling	Cosmetics, paints, coatings, plastics, textiles, etc.	Improved UV protection, photocatalysis, antibacterial, antifouling properties	Particles	2000s	Nanomaterial
TiO2NF_1.1_NF	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties	Particles	2000	Nanomaterial
TiO2NF_9,1_Sol_BM_15h	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_1.1_NF	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_11_Sil_Sol	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	Since 2000s	Nanomaterial
TiO2_9.1_NF	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, pharmaceuticals	Improved UV protection, whitening, anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_9.1_NF_BM	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_9.1_sol_BM	titanium dioxide nanoparticle	UV protection, whitening,	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-	Particles	2000s	Nanomaterial

		anti-bacterial		bacterial properties			
TiO2_NF_BM_2h	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	2000	Nanomaterial
TiO2_NF_BM_4h	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_NF_BM_6h	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	2000s	Nanomaterial
TiO2_NF_BM_9h	titanium dioxide nanoparticle	UV protection, whitening, anti-bacterial	Cosmetics, paints, coatings, plastics, paper, food, etc.	Improved UV protection, whitening, and anti-bacterial properties	Particles	2000s	Nanomaterial
ZnFe2O4 30 nm NRCWE-021	zinc ferrite	Magnetic properties	Magnetic materials	High coercivity and saturation magnetization	Particles	Since 2018	Nanomaterial
phage mimetic nanorods (PMN)	nanorod	Antimicrobial	Pharmaceuticals, cosmetics, food, and medical devices	High antimicrobial activity, low toxicity, and low cost	Particles	Since 2018	Nanomaterial
rGO - Carbon NRCWE-059	graphene (via reduction of GO)	Conductive, strong, lightweight	Electronics, composites, coatings, batteries, etc.	Higher conductivity, strength, and flexibility than conventional materials	Platelets	Since 2010	Nanomaterial

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 HDF5[1] 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] https://www.hdfgroup.org/solutions/hdf5/

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

innomat_annotated.xlsx

innomat_examples.xlsx

enm_annotated_parsed.xlsx

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