

DOME 4.0 Showcases - User Guide

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1. Showcases List

Showcases



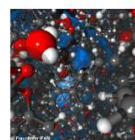
Marine emission dispersion simulator

Estimate dispersion of marine emission using ship data, weather data and chemistry knowledge



Enhanced data mining for improved lightweight solutions

Improve engineering prediction quality by recombination of available material data from different sources



Cheminformatics for polymeric additives

Estimate different properties of small molecules and combine them with public information



Fatigue life of structural adhesives

Integrating machine learning and physics-based modeling for enhanced prediction of structural adhesive joint fatigue life



Production equipment tools and service catalogues

MARKET4.0 marketplace equipment and services catalogue data



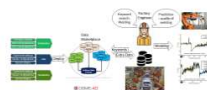
Automated and robust workflows for in-browser quantum mechanical calculations

Materials Cloud's AiIDalab offers in-browser quantum calculations on materials using OPTIMADE's extensive structure databases via DOME 4.0



Facets of substances: physico-chemical, trade and patent information

Simultaneously query multiple reliable information sources and integrate their answers



Quality monitoring of automated welding

Improving quality prediction of welding operations by discovering and embracing data via the DOME 4.0 platform



Virtual development of composite materials

Accelerating custom-tailored composite material design with materials informatics

Figure 1 - Showcases Page on the DOME 4.0 Platform

Figure 1 illustrates the Showcases Page on the DOME 4.0 platform, which features a mosaic of the nine B2B showcases that span various industry sectors, including marine, materials, and manufacturing. For a detailed overview, **Error! Not a valid bookmark self-reference.** lists the nine B2B showcases along with their respective industry sectors. The diversity of these showcases highlights the platform's versatility and its potential to drive innovation across multiple domains. Clicking on one of the tiles navigates to a page dedicated to that specific showcase, which is explained in the following section of this document.

Table 1 - DOME 4.0 B2B Showcases

| SC # | B2B SC | Sector | Owner(s) |
|------|---|--------------------------------------|--------------|
| SC 1 | Chemistry Knowledge Graph – marine, air quality and nanoparticles | MARINE, ENVIRONMENTAL, NANOPARTICLES | CMCL |
| SC 2 | Lightweight construction – fibre reinforced plastics | PLASTICS | FRAUN, BOSCH |
| SC 3 | Polymer additives for corrosion protection | POLYMERS | FRAUN, SISW |
| SC 4 | Structural adhesives: fatigue behaviour | ADHESIVES | FRAUN, SISW |
| SC 5 | Production equipment tools and service catalogues (metals, plastics, high-tech) – MARKET4.0 | MANUFACTURING | INTRA |
| SC 6 | Turnkey services & custom workflows integrating simulations and data | MATERIALS | EPFL |
| SC 7 | Formulated consumer products | CHEMICAL PROCESSES, MATERIALS | UKRI |
| SC 8 | Semantic analytics of manufacturing assets | SMART MANUFACTURING | BOSCH |
| SC 9 | Virtual development of composite materials | COMPOSITE MATERIALS | SISW |

2. Showcases Details

2.1 Showcase 1 – Chemistry Knowledge Graph – Marine, Air Quality and Nanoparticles

Showcase 1 features CMCL's Chemistry Knowledge Graph (KG), offering a robust framework to intelligently store, access, and interpret the rapidly expanding datasets on chemical information, marine emissions, location, and air quality. Utilising the DOME 4.0 ecosystem, it ensures semantic interoperability across diverse data sources, including ship location/positioning databases, marine nanoparticle emissions software, air quality dispersion modeling software, and data-based surrogate model generation software. This facilitates a comprehensive analysis of local air quality which can support informed decision-making in urban planning and manufacturing.

Showcase 1 benefits significantly from the DOME 4.0 platform in several ways. Firstly, the platform allows users to initiate new simulations by incorporating external data, such as ship locations, into the modeling workflow of Showcase 1. An example is shown below.

After logging in to the DOME 4.0 platform, users may search for ship location data by the keyword “AIS”. On the page of individual result compatible with the simulation tool of Showcase 1, a button allows user to pass the ship location data to Showcase 1, as shown in Figure 2.

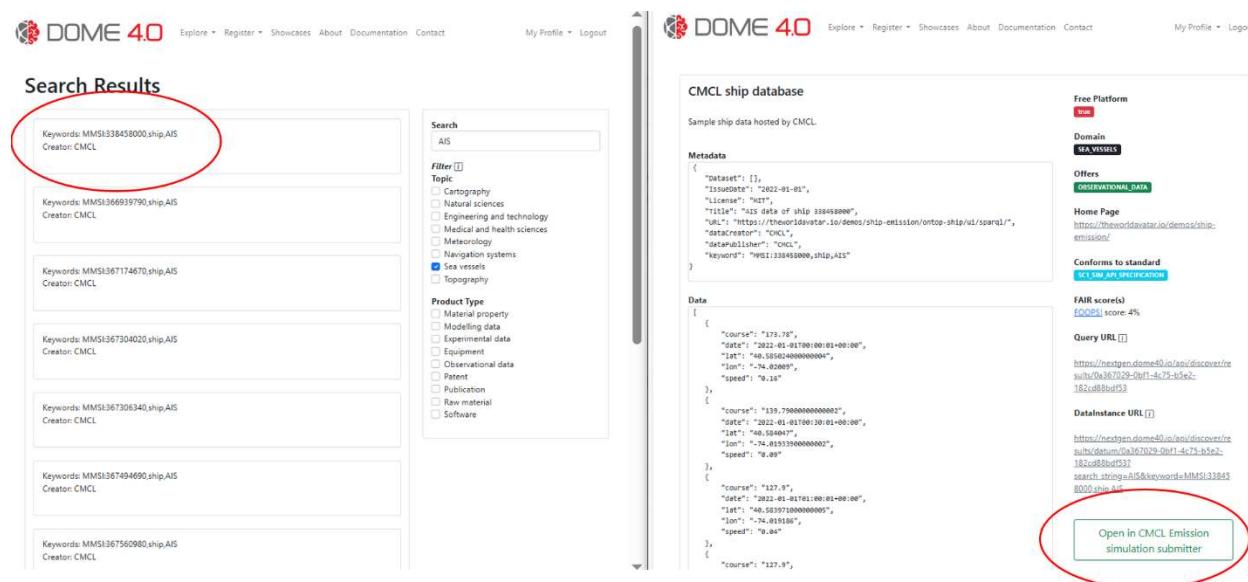


Figure 2 - Ship location data can be searched on the DOME 4.0 Platform

Users will be redirected to the simulation submitter interface as shown in Figure 3, where they can inspect the ship location data, configure the simulation and submit the simulation request to the remote server.

DOME Showcase 1: Chemistry Knowledge Graph - Marine, Air Quality And Nanoparticles

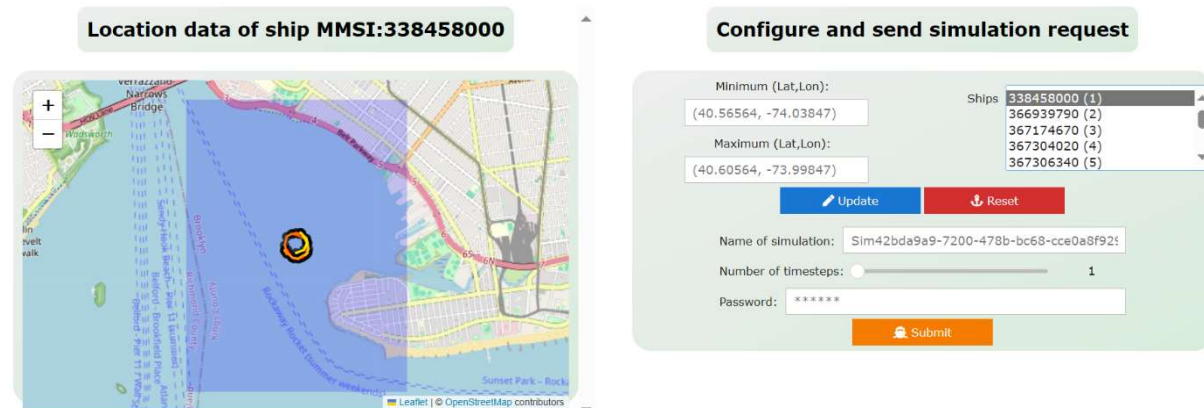


Figure 3 - Simulation submitter for SC1

Once the simulations are completed, the modeling results are made available through the DOME 4.0 platform. Users may search with the keyword "ship" for available simulation data, as shown in Figure 4. A button will appear to allow users to view the simulation data with the visualisation tool, which is also embedded on the showcase page as shown in Figure 5. This user-friendly access ensures that stakeholders can easily interpret and utilise the data for informed decision-making.

Additionally, the platform offers the potential for further processing of these results using other tools available within the DOME 4.0 ecosystem. This capability allows for more comprehensive analyses and the development of more sophisticated models, ultimately supporting better outcomes in urban planning, environmental monitoring, and other related fields.

Figure 4 - Simulation output of SC1 can be searched on the DOME 4.0 Platform

Showcase 1

Chemistry Knowledge Graph - Marine, Air Quality And Nanoparticles



This showcase entails CMCL's chemistry knowledge graph (KG) and provides a consistent framework to store, access and interpret vastly growing chemical data, marine emissions data, location data and air quality data, in an intelligent manner using the DOME 4.0 ecosystem. Semantic interoperability is established between a variety of data sources (ship location/positioning databases, marine nanoparticle emissions software, air quality - dispersion modelling software, data-based surrogate model generation software).

To achieve this interoperability across multiple domains, CMCL employs and extend its existing ontologies (Ontokin); its detailed (mesoscopic and continuum) emissions prediction software, kinetics; its data-based model development toolkit, MoDS.

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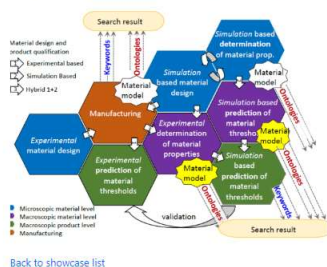
DISCLAIMER: The development platform has been created as part of the DOME 4.0 project, funded by Horizon 2020, the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement no 953163). The demonstrator is for research and innovation purposes at a low technology readiness level (~TRL 4). The project consortium is not responsible for any errors, accuracy or omissions of any information posted on the development platform and shall not be responsible for any decisions made based on such information.

Figure 5 - SC1 Page on the DOME 4.0 Platform

2.2 Showcase 2 – Lightweight Construction – Fiber Reinforced Plastics

Showcase 2 is related to the material data exchange for engineering simulations concerning fiber reinforced polymeric materials. Fiber reinforced polymeric materials especially of the short fiber reinforced type have several special features requiring a significant effort for material parameter determination, including a disordered, spatially varying microstructure, complex temperature dependence across the glass transition of the matrix, strong humidity effects as well as a strong tendency towards creep deformation, aging and other long-term effects.

Showcase 2 Enhanced data mining for improved lightweight solutions



Considering the creep response of short fiber reinforced polymers consisting of recycled material, this showcase employs the DOME 4.0 ecosystem to enhance the knowledge on the mechanical material response of composites by re-combining the data available in different sources. The data sources include material data directly available on data platforms, on the manufacturers data sheets, in research publications of all kinds as well as data determined to order in both, experimental characterizations and numerical multiscale simulations.

Due to the variety of data required for a complete creep material data card considering all essential aspects such as temperature and humidity dependence, rate and stress dependence, aging and other environmental effects etc., available data sources do not normally contain the complete information in a single record. Putting all the material data together, the design engineers are enabled to improve the quality of their simulations significantly.

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Figure 6 - SC2 Page on the DOME 4.0 Platform

In this showcase the DOME4.0 platform is employed to enrich the usually limited data available for the long-term response – here the creep response – of short fiber reinforced plastics by using pre-existing data from a variety of different sources. These may include experimental data sets for the same material or similar materials made readily available by different data providers on DOME4.0 or other data exchange platforms registered to the DOME4.0 platform, information from material manufacturers available on the

Web, numerical data from various multiscale studies or analyses made-to-order as well as material data and other information from the vast body of scientific literature in the field. Recombination of all these data helps to significantly improve the prognosis quality of engineering simulations, thereby reducing the required (own) experimental effort to a minimum, reducing unnecessary conservatisms, enhancing the utilization of the material, and not least reducing the time-to-market.

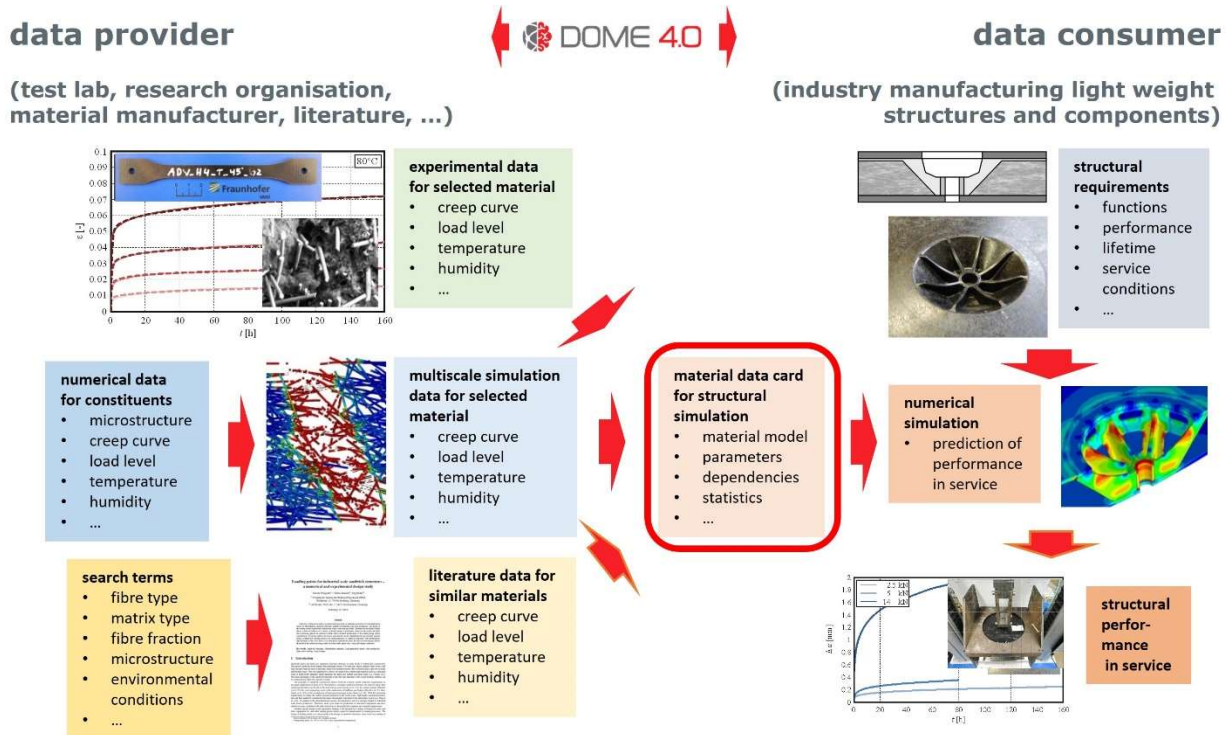


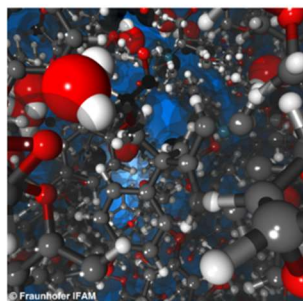
Figure 7: Data flow and re-combination in Showcase 2.

Using the DOME4.0 platform, the data providers can easily register their data sets using the “register catalog data” option of the platform by providing keywords and some related information on the data together with a URL through which the data is available. The data set itself remains on the data providers platform (or a third party data exchange/marketplace platform) with no need to transfer the data to the DOME4.0 platform. By this means, the data providers may also restrict the access to the provided data sets to specific users or users from specific regions using the password protection capabilities of their own platform. By this means business models to provide available data on a pay-per-view or pay-per-download basis are also possible. Although the data preferably is provided in interoperable formats like .json it may also be in other formats as well. In the same manner, articles from the scientific literature may be registered by their DOI leading the data consumer to the publisher’s repository together with the respective subscription requirements of their choice without violation of copyright requirements.

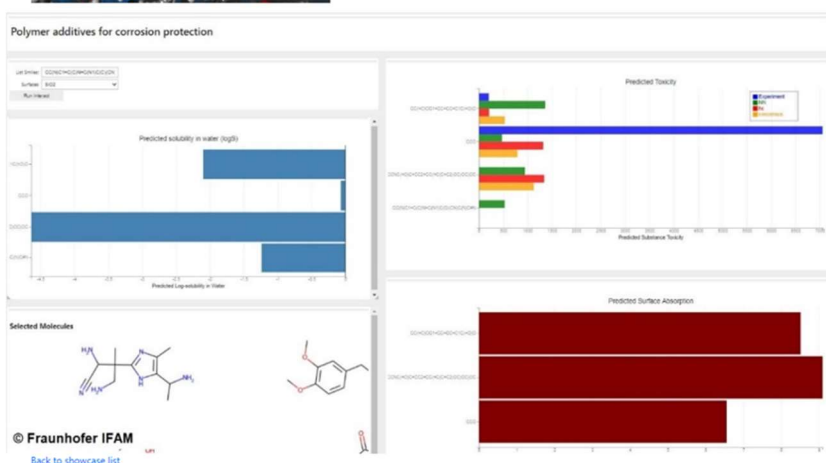
The data consumers can simply search the DOME4.0 platform for availability of material data for their specific materials. DOME4.0 then returns all relevant hits providing all information the data providers have provided when registering their catalog data.

2.3 Showcase 3 – Polymer additives for corrosion protection

Showcase 3 Cheminformatics for polymeric additives



This showcase is currently leveraging a Cheminformatics and data-driven approach to support the development of polymeric additives for example for corrosion protection. The showcase integrates data from multiple publicly available sources such as Pubchem for GHS data, and connects them with Cheminformatics methods to predict water solubility and surface adsorption to support the selection of suitable polymeric additives. DOME 4.0 provides an entry point to collect and combine the information.



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Figure 8 - SC3 Page on the DOME 4.0 Platform

In showcase 3 Cheminformatics and data-driven approaches are combined to expedite the development of polymeric additives for corrosion protection. The showcase integrates data from multiple publicly available sources, such as Pubchem, and connects them with Cheminformatics methods. Figure 8 shows a screenshot of the showcase 3 page and interactive application.

The information is presented as dashboard with individual cells for different types of information, e.g. hazard data, water solubility or toxicology. The individual cells are draggable and resizable.

The molecules that shall be analyzed are specified in the top, left cell (see Figure 9). The molecules are specified a list of SMILES (comma separated). The SMILES (Simplified Molecular Input Line Entry System)

is a specification for describing the structure of chemical species using short ASCII strings¹. The drop-down menu below allows to specify a surface used for the calculation of the surface adsorption. The button starts the analysis.

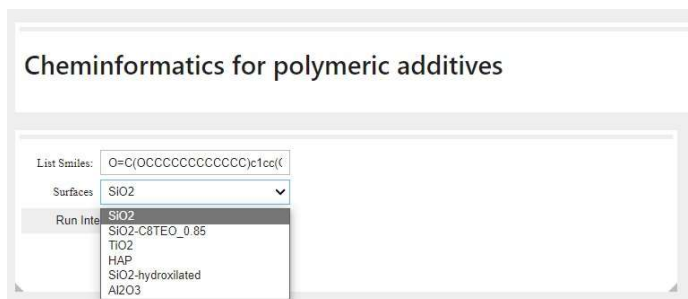


Figure 9 - Top left cell of the dashboard used for specification of molecules and surfaces.

After starting the analysis, the top, right cells will depict the molecules selected. The remaining cell will subsequently be populated when the results were calculated or collected from the public sources. The cells will show:

- calculated water solubility (logS), based on a model derived from experimental solubilities (Figure 10 top left),
- predicted surface adsorption, estimated as distance between the molecule and the surface in the Hansen Solubility Parameter space (Figure 10 top right),
- predicted toxicity, calculated by the WebTEST² service of the EPA. Shown are the oral rat LD₅₀ values calculated using different QSAR Methodologies, e.g. hierarchical clustering or group contribution (Figure 10 bottom),
- documented GHS data (Globally Harmonized System of Classification and Labeling of Chemicals) requested from Pubchem. For each molecule the tables will, if the data is available, show the H-Code and the respective source.

For all calculations the numerical data is also shown as a table in separate cells.

¹ For the generation of SMILES based on 2D structures see e.g. PubChem Sketcher <https://pubchem.ncbi.nlm.nih.gov/edit3/index.html>

² <https://www.epa.gov/comptox-tools/users-guide-webtest-version-10-web-services-toxicity-estimation-software-tool>

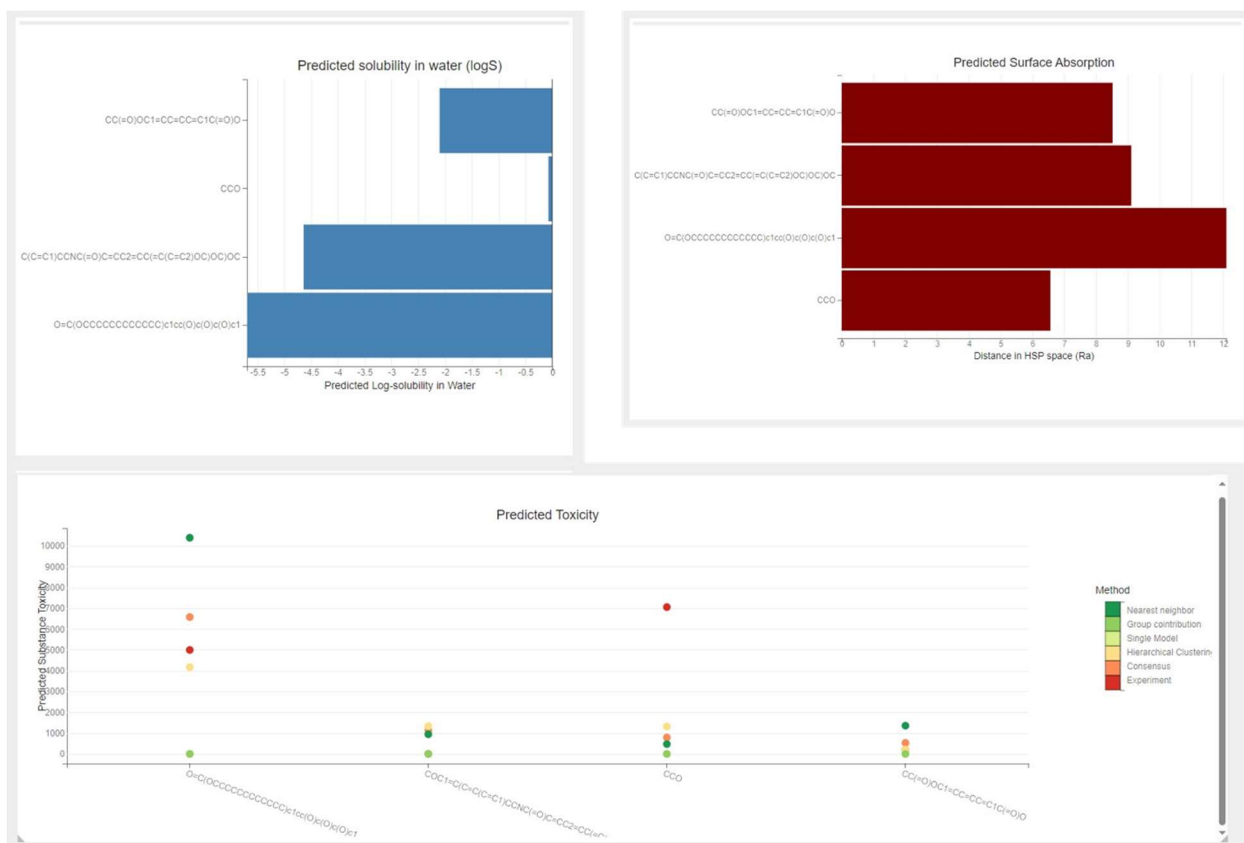


Figure 10 - Examples for the predicted results (water solubility, surface adsorption, toxicity)of showcase 3 APP.

2.4 Showcase 4 – Fatigue life of structural adhesives

Showcase 4 presents a workflow designed to streamline the fatigue life prediction of adhesives through the utilization of machine learning (ML) models. Its aim is to assist customers in the selection of the appropriate adhesive for adhesively bonded structures, considering specific geometrical and material attributes, as well as usage conditions. This objective is realized through a collaborative effort involving data-provider Fraunhofer and Citrine Informatics, which specializes in materials-aware AI for advancing next-generation materials and chemicals. The showcase caters to a range of industry sectors, including material manufacturers, product manufacturers, software and service providers, and data providers.

For a deeper dive into the industrial context of this showcase, please read our blog post titled [“Advancements in predicting the fatigue lifetime of structural adhesive joints”](#).

Showcase 4 Predicting the Fatigue Lifetime of Structural Adhesive Joints



This showcase addresses the challenge of accurately predicting the fatigue lifetime of structural adhesive joints, which are integral to various engineering applications. It explores the potential of combining Artificial Intelligence and Machine Learning with physics-based modeling to improve prediction efficiency. The hybrid models developed from this research aim to refine the understanding of adhesive behavior under cyclic loading conditions, contributing to more reliable material selection and design processes.

This showcase is the result of a research collaboration between Fraunhofer IFAM, Siemens Digital Industries Software, and Citrine Informatics.

Further details on this subject can be found [here](#).

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INFORMATICS

Adhesive

Adhesive:

Young Modulus (MPa):

Geometry

Specimen Width (mm):

Notch: Internally Externally

Notch Type:

Loading

Nominal Stress Amplitude (MPa):

↳ Predicted Fatigue Life

Bebel, V. C., & Schneider, B. (2020). Fatigue of structural adhesives under stress concentrations: Notch effect on fatigue strength, crack initiation and damage evolution. International Journal of Fatigue, 140, 105824. <https://doi.org/10.1016/j.ijfatigue.2020.105824>

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Figure 11 - SC4 Page on the DOME 4.0 Platform

Figure 11 depicts the showcase page for SC4, featuring a brief description of the showcase along with an embedded iframe containing the interactive tool at its core.

A detailed view of the interactive tool is presented in Figure 12. Here, users can select the type of adhesive they are interested in, with the corresponding Young's modulus updating automatically. Additionally, users can input geometric details related to specimen and notch sizes, as well as the nominal stress amplitude applied. By clicking the "Predict" button, the input data is sent to the trained Machine Learning (ML) model on the Citrine platform, which then returns the expected fatigue life of the selected adhesive under the specified conditions, expressed in both the number of cycles until failure and its logarithmic value. The tool also provides the auxiliary quantity, Length of Highly Stressed Region, for additional context.

For further technical details about the quantities and the fatigue dataset used to train the ML model that powers this tool, please refer to the scientific publication: Beber, V. C., & Schneider, B. (2020). Fatigue of structural adhesives under stress concentrations: Notch effect on fatigue strength, crack initiation and damage evolution. *International Journal of Fatigue*, 140, 105824. <https://doi.org/10.1016/j.ijfatigue.2020.105824>.

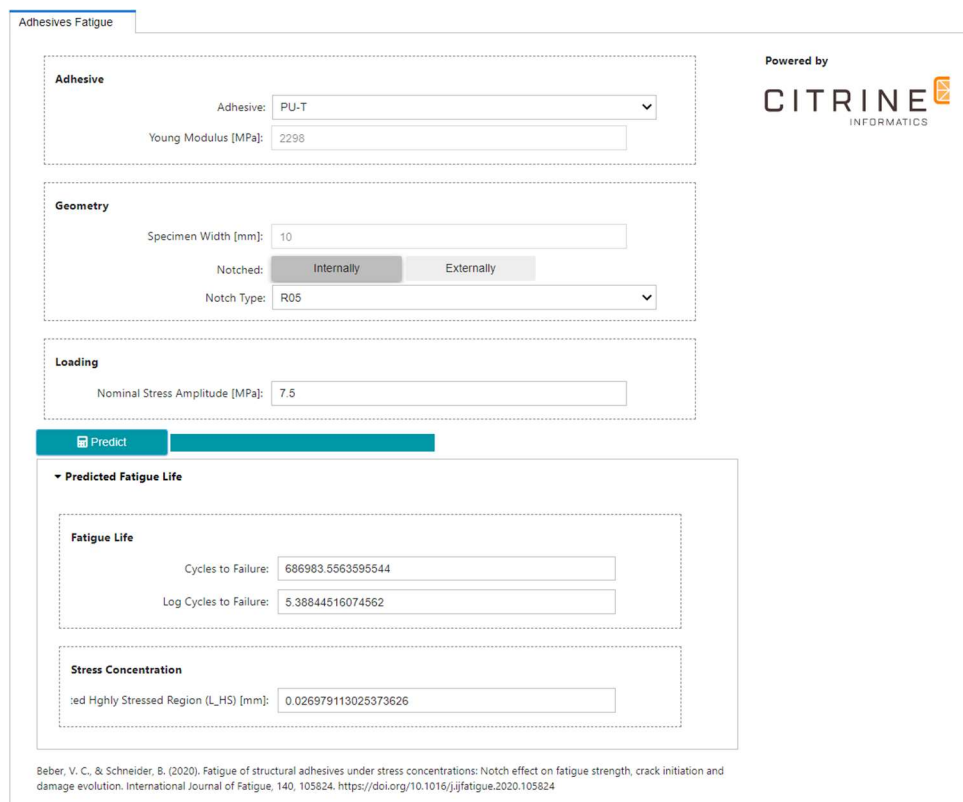


Figure 12 - SC4 Prediction Tool

In addition to the described showcase page and interactive tool, datasets related to the fatigue life of structural adhesives and adhesive joints have been registered on the DOME 4.0 platform, complete with detailed metadata and keywords to facilitate search and retrieval. Users are notified that these datasets are related to SC4 through the "SC4 API Specification," which indicates an associated tool by displaying a green button in the right panel. This button directs users to the SC4 showcase page. An example demonstrating the association between a dataset and the tool can be seen in Figure 13.

Structural Adhesives Fatigue Data

Structural Adhesives Fatigue Data

Metadata

```

{
  "dataset": [],
  "issueDate": "2024-06-20",
  "license": "Public",
  "title": "Structural Adhesives Fatigue Data ",
  "url": "https://sintef.sharepoint.com/:x:/r/teams/DOME4.0/DeltaS200dokumenter/WPA/Datasets/SC4_data_fat",
  "dataCreator": "Fraunhofer_IFAM",
  "dataPublisher": "Fraunhofer_IFAM",
  "keyword": "structural adhesive, fatigue life, structural bonding, stress concentration, lifetime"
}
                    
```

Domain
ENGINEERING_AND_TECHNOLOGY

Conforms to standard
[SC4 API SPECIFICATION](#)

DataInstance URL

[https://nextgen.dome40.io/api/discover/results/datum/?search_string=structural adhesive&keyword=structural adhesive fatigue life structural bonding stress concentration lifetime prediction fatigue design SN curve notch](https://nextgen.dome40.io/api/discover/results/datum/?search_string=structural%20adhesive&keyword=structural%20adhesive%20fatigue%20life%20structural%20bonding%20stress%20concentration%20lifetime%20prediction%20fatigue%20design%20SN%20curve%20notch)

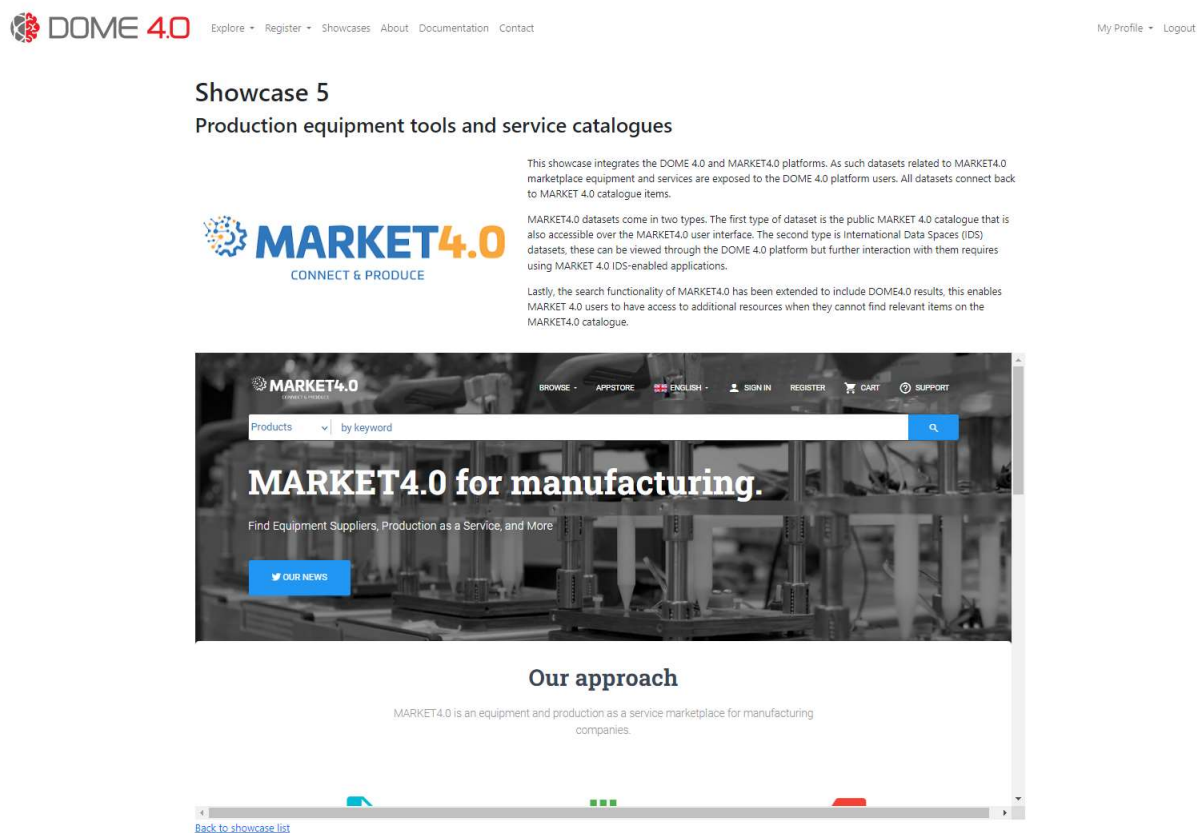
Open in Structural Adhesives Fatigue Life Prediction

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Figure 13 - Example of a dataset associated to SC4

2.5 Showcase 5 – Production equipment tools and service catalogues (metals, plastics, high-tech) – MARKET4.0

Showcase 5 deals with the integration of the MARKET4.0 marketplace with the DOME 4.0 platform. Showcase 5 has enriched the DOME 4.0 platform with data coming from the production equipment procurement domain.



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Figure 14 - SC5 Page on the DOME 4.0 Platform

Due to the nature of the MARKET4.0 platform two kinds of data sources were integrated in the DOME 4.0 platform. The public catalogue data that are available over a typical HTTP API and private supplier data that are available over IDS. Both types are seamlessly integrated and are available for querying over the platform's search functionality. In Figure 15 one dataset is presented for using the keyword 'copper'. This dataset will lead back to the MARKET4.0 platform where the users may further interact with the supplier of the equipment.

MARKET4.0 IDS data of metal processing equipment

Metadata

```

{
  "dataset": [
    ],
    "license": "CC-BY",
    "license": "Market 4.0 license",
    "title": "Platine Fiber 1536-VL5600",
    "url": "https://platform.market4.eu/index.html/search/products?search=Platine Fiber 1536-VL5600",
    "datacreator": "Primo Power",
    "datapublisher": "Innoportpower.com",
    "keyword": "Machine data"
  ]
}
          
```

Data

```

{
  "description": "FLEXIBILITY AND HIGH QUALITY IN ALL THICKNESSES",
  "externalid": null,
  "isp": 44,
  "machinefiles": [
    {
      "isp": 71,
      "machine": null,
      "name": "Wlastnotber.flw",
      "type": false
    },
    {
      "isp": 72,
      "machine": null,
      "name": "Wlastnotber.flw",
      "type": true
    }
  ],
  "manufacturer": {
    "address": "11, sales@primopower.com",
    "contact": "info@primopower.com",
    "externalid": null,
    "isp": 4424,
    "latitude": "7.60390",
    "longitude": "45.09264",
    "name": "Primo Power",
    "phone": "+33 01 41811",
    "phone2": "+33 01 41811"
  },
  "manufacturer2": {
    "name": "Primo Power",
    "externalid": "124",
    "manufacturer": "150",
    "name": "Platine Fiber 1536-VL5600"
  }
}
          
```

Domain
BUSINESS AND TECHNOLOGY

Offers
COOPER

Conforms to standard
[ISO 15926-2](#)

FAIR score(s)
LOQPS score: 4%

Query URL [?]
https://testopen.dome4.eu/api/discover/result/34f97852-b6d0-4343-8b61-34e0566c78b?search_string=copper&keyword=Machine data

Datainstance URL [?]
https://testopen.dome4.eu/api/discover/result/34f97852-b6d0-4343-8b61-34e0566c78b?search_string=copper&keyword=Machine data

[Open in MARKET4.0 website](#)

Figure 15 MARKET4.0 dataset for keyword 'copper'

However, when searching for data in DOME4.0 different sectors results will appear which provides an opportunity to the users to explore combinations of different information. For example, equipment supplier information in combination with material information. Lastly, DOME4.0 data are also accessible over the MARKET4.0 platform. For example, see Figure 16 results for keyword 'Digitoxin'. Showcase 5 acts as two-way gateway between the DOME4.0 and MARKET4.0 platforms enabling both platforms to take advantage of the other user base.

The screenshot shows the MARKET4.0 website interface. At the top, there is a navigation bar with 'MARKET4.0' logo, 'BROWSE', 'APPSTORE', 'ENGLISH', 'TEST USER', 'CART', and 'SUPPORT'. Below this is a search bar with 'Products' and 'digitoxin' entered. The main content area displays 'DOME4.0 platform results' and a table with two columns: 'dataset' and 'Digitoxin (EC: 200-760-5)'. The 'dataset' column lists 'Title: Title', 'License: Chemeo EULA', 'Data creator: Chemeo', and 'URL: url'. The 'Digitoxin (EC: 200-760-5)' column lists 'Title: Digitoxin (EC: 200-760-5)', 'License: Use of the information, documents and data from the ECHA website is subject to the terms and condi...', 'Data creator: PubChem', and 'URL: https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/?q=digitoxin'. At the bottom, there is a footer with 'ABOUT US', social media icons, and '© 2024, Market4.0'.

| dataset | Digitoxin (EC: 200-760-5) |
|----------------------|--|
| Title: Title | Title: Digitoxin (EC: 200-760-5) |
| License: Chemeo EULA | License: Use of the information, documents and data from the ECHA website is subject to the terms and condi... |
| Data creator: Chemeo | Data creator: PubChem |
| URL: url | URL: https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/?q=digitoxin |

Figure 16 DOME 4.0 dataset for keyword 'digitoxin'

2.6 Showcase 6 – TITLE

Showcase 6

Automated and robust workflows for in-browser quantum mechanical calculations using AiiDALab



Quantum ESPRESSO is the most used open-source package in the world for quantum mechanical simulations of materials - with more than 4,000 papers published every year.

In this showcase, the Materials Cloud introduces a jupyter-like modeling tool known as AiiDALab, designed for in-browser quantum mechanical calculations, ready to be freely and openly used by non-experts to calculate materials properties. DOME 4.0 facilitates the seamless transfer of atomic structures adhering to the OPTIMADE standard to AiiDALab, offering considerable flexibility due to the extensive network of OPTIMADE providers, encompassing millions of structures. This integration mutually enhances AiiDALab by providing a substantial data source for quantum mechanical calculations and benefits OPTIMADE by incorporating a simulation tool capable of processing its served data.

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Figure 17 - SC6 Page on the DOME 4.0 Platform

2.7 Showcase 7 – Consumer-formulated products. Facets of substances: physico-chemical, trade and patent information

Showcase 7

Facets of substances: physico-chemical, trade and patent information



This showcase originates in relation to formulated goods, in other words fluid complex mixtures (involving solvents, salts, surfactants, etc.), that, for example, are commonly used to produce personal care, food, and cleaning products. Therefore, broadly speaking, this use-case involves data on material properties (chemical and physical properties from either simulations or experiments), information about purchasing raw materials, and relevant existing patents.

All this information comes from various web-based sources, which display heterogeneity at multiple levels. In fact, in general, different sources might use different data formats, different terms for the same entities and even different perspectives to describe the same domain (corresponding to syntactic, terminological, and conceptual heterogeneity, respectively, following Euzenat & Shvaiko). DOME 4.0 provides an entry point that enables a simultaneous query across the various data sources and combines, and where possible harmonizes, their answers.

DOME 4.0 Showcase 7

Search by freetext (DOME):

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Figure 18 - SC7 Page on the DOME 4.0 Platform

Context

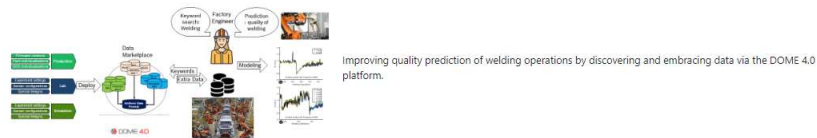
Showcase #7 is about *formulated goods*, in other words fluid complex mixtures (involving solvents, salts, surfactants, etc.), that, for example, are commonly used to produce personal care, food, and cleaning products. Broadly speaking, this use-case involves data on chemical and physical *material properties*, information about purchasing *raw materials*, and relevant existing *patents*. All this information comes from various web-based sources, which display heterogeneity at multiple levels. DOME 4.0 showcase #7 allows to simultaneously query these reliable information sources and combine their answers, providing a unified view of information (see Figure 19).

Conclusion

All the information to create a subgraph of the Knowledge Graph related to the searched string is available. The emphasis here is on the usability and accessibility afforded by the web UI.

2.8 Showcase 8 – TITLE

Showcase 8 Quality monitoring of automated welding



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Figure 20 - SC8 Page on the DOME 4.0 Platform

2.9 Showcase 9 – Virtual development of composite materials

Showcase 9 presents a comprehensive workflow for virtual composite material development, leveraging a machine learning (ML) framework integrated with the DOME 4.0 environment. The primary commercial objective is to empower material manufacturing companies to assist their customers in identifying optimal mixing ratios for open-compound material systems based on specific requirements. This objective is realized through collaborative efforts involving data-provider SABIC, a chemical company, and Citrine Informatics, a specialist in materials-aware AI for advancing next-generation materials and chemicals. The showcase caters to various industry sectors, including material manufacturers/chemical companies, product manufacturers, software and service providers, and data providers.

For a deeper dive into the industrial context of this showcase, please read our blog post titled “[Materials informatics accelerates customer tailored composite material design](#)”.

Showcase 9 Virtual Development of Composite Materials using Materials informatics



This showcase highlights the use of materials informatics to accelerate the design of custom polymer blends for automotive applications, where thermoplastics play a crucial role in improving efficiency and performance. By applying machine learning models to historical data, product developers can rapidly identify optimal masterbatch and polymer combinations, reducing the need for extensive experimentation. The result is a more efficient development process that offers accurate recommendations for customized solutions, improving customer experience and potentially saving time, materials, and costs.

This showcase is the result of a research collaboration between Siemens Digital Industries Software, SABIC, and Citrine Informatics.

Further details on this subject can be found [here](#).

Mixing Ratios Query | Mixing Ratios Search

Compounds System: Compound A + Compound B

Compound A: 0.25
Compound B: 0.75

Powered by CITRINE INFORMATICS

Get Properties

Properties

| | | | | |
|---|---------|-------------|--------|---|
| Mold Shrinkage after annealing [ISO 224-4] (%) | 1.08 | Deviation ± | 0.08 | ● |
| Mold Shrinkage [ISO 224-4] (%) | 0.98 | Deviation ± | 0.07 | ● |
| Melt Flow Index [ISO 1133] (g) | 10.50 | Deviation ± | 7.00 | ● |
| Ash Content [ISO 3481] (%) | 8.80 | Deviation ± | 1.10 | ● |
| Tensile Modulus (at 23°C) [ISO 527] (MPa) | 1553.02 | Deviation ± | 148.41 | ● |
| Flexural Modulus (at 23°C) [ISO 178] (MPa) | 1537.90 | Deviation ± | 88.07 | ● |
| Izod Impact (at 23°C) [ISO 180/1A] (kJ/m ²) | 32.07 | Deviation ± | 0.83 | ● |
| Charpy Impact (at 23°C) [ISO 179] (kJ/m ²) | 31.12 | Deviation ± | 12.94 | ● |

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Figure 21 - SC9 Page on the DOME 4.0 Platform

Figure 21 depicts the showcase page for SC9, featuring a brief description of the showcase along with an embedded iframe containing the interactive tool at its core.

This tool offers two distinct functionalities: (i) Mixing Ratio Query, detailed in Figure 22, and (ii) Mixing Ratio Search, illustrated in Figure 23.

Mixing Ratio Query: Users can specify a pair of open compounds (commercial names redacted) and the intended mixing ratio. By clicking the "Predict" button, this data is sent to the trained Machine Learning (ML) model on the Citrine platform, which then forecasts the resulting mechanical properties. Within a few seconds, the results are displayed in the lower box.

Mixing Ratio Search: Users can specify the desired mechanical properties, such as Mold Shrinkage, for a chosen pair of open compound systems. The inputs are sent to the Citrine platform, and after a few minutes, the suggested mixing ratios and the predicted mechanical properties are returned to the user.

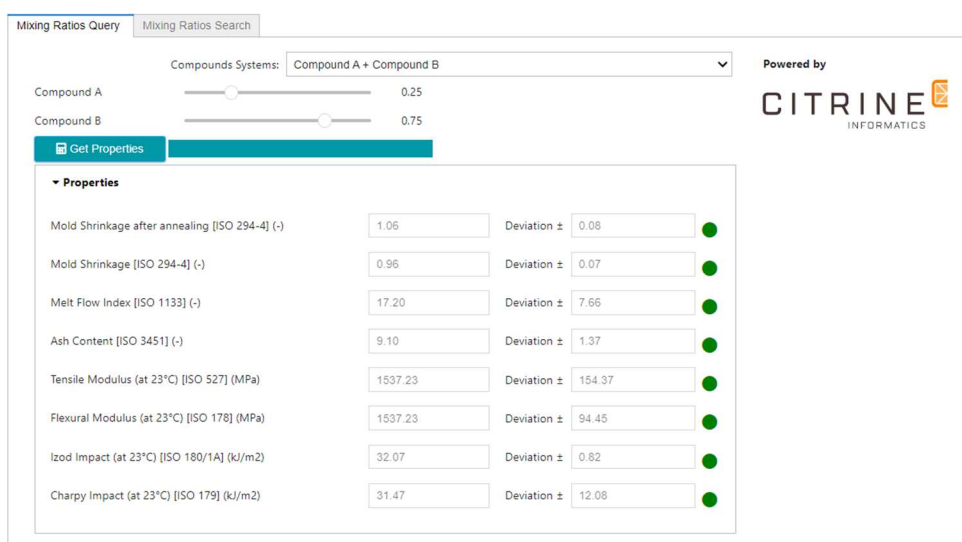


Figure 22 - SC9 Prediction Tool – Query

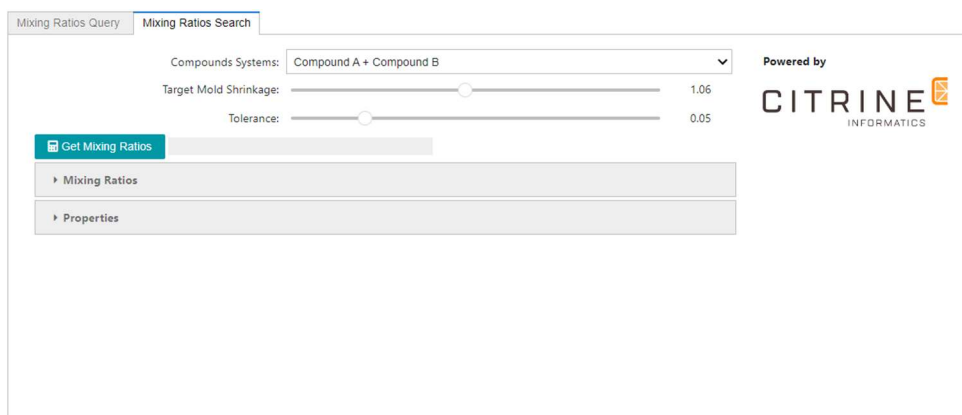
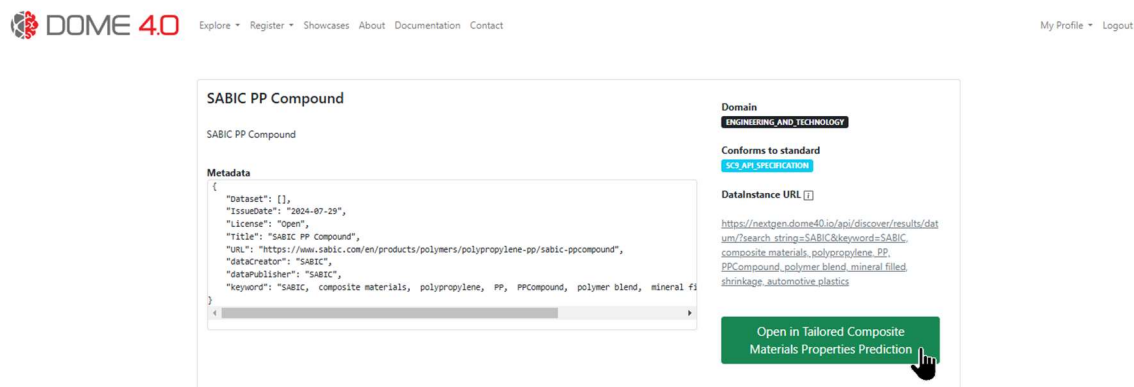


Figure 23 - SC9 Prediction Tool – Search

In addition to the described showcase page and interactive tool, datasets pertinent to this showcase, such as the list of open compounds, have been registered on the DOME 4.0 platform. These datasets come with detailed metadata and keywords to facilitate search and retrieval. Users are informed that these datasets are related to SC9 through the "SC9 API Specification," which highlights an associated tool by displaying a green button in the right panel. This button directs users to the SC9 showcase page. An example demonstrating the association between a dataset and the tool can be seen in Figure 24.



The screenshot shows the DOME 4.0 interface for a dataset titled "SABIC PP Compound". The page includes a navigation bar with "Explore", "Register", "Showcases", "About", "Documentation", and "Contact". On the right, there are links for "My Profile" and "Logout".

The dataset entry includes the following metadata:

```

{
  "dataset": [],
  "issueDate": "2024-07-29",
  "license": "Open",
  "title": "SABIC PP Compound",
  "url": "https://www.sabic.com/en/products/polymers/polypropylene-pp/sabic-ppcompound",
  "dataCreator": "SABIC",
  "dataPublisher": "SABIC",
  "keyword": "SABIC, composite materials, polypropylene, PP, PPCompound, polymer blend, mineral fi"
}

```

On the right side, the domain is listed as "ENGINEERING_AND_TECHNOLOGY". It also states "Conforms to standard" with a link to "SC9 API SPECIFICATION". A "DataInstance URL" is provided: [https://nextgen.dome40.io/api/discover/results/datum/?search_string=SABIC&keyword=SABIC composite materials polypropylene PP Compound polymer blend mineral filled shrinkage automotive plastics](https://nextgen.dome40.io/api/discover/results/datum/?search_string=SABIC&keyword=SABIC%20composite%20materials%20polypropylene%20PP%20Compound%20polymer%20blend%20mineral%20filled%20shrinkage%20automotive%20plastics). A prominent green button labeled "Open in Tailored Composite Materials Properties Prediction" is visible, with a mouse cursor pointing to it.

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Figure 24 - Example of a dataset associated to SC9