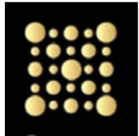




MaterialsCommons4EU

Federated Digital Infrastructure for European Advanced Materials Research and Development

Simon Stier | MaterialsCommons4EU Partners



Timeline of MaterialsCommons

MATERIALS 2030 MANIFESTO

Systemic Approach of Advanced Materials for Prosperity –
A 2030 Perspective

February 2022:

the European Commission, Member States, industry and research, and citizens to leverage collaboratively the interplay between advanced materials, digital technologies and circular strategies in order to accelerate the development, and reducing the cost and complexity of developing tomorrow's solutions for the twin green and digital transitions. It will avoid fragmentation amongst the different players in the Horizon EU programme, therefore enabling the EU to implement the green and digital transitions.



Strategic Materials Agenda, April 2023:

Common framework and organisational form

The initiative aims at providing a common framework (the so-called 'Materials Commons') for all stakeholders supporting their collaboration on advanced materials in a systemic approach across different innovation markets. An efficient organisational form is needed to facilitate multi-stakeholder engagement.



Strategic Research and Innovation Agenda (SRIA),
November 2024:

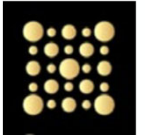
An integrated, trusted, and federated digital infrastructure is needed to support and engage all actors along the AMs value chain/life cycle to share, access and exchange data while retaining ownership rights and protecting confidential information. This infrastructure, called the **Materials Commons** in the EC communication on Advanced Materials for Industrial Leadership [2], encompasses a digital material ecosystem that involves the digitalisation of materials specifications, synthesis and processing, safety profiles, environmental and social sustainability, as well as circularity potential. The Materials Commons enables a new style of innovation processes: **collaborative innovation** including actors along value chains in single, repeatable innovation workflows, thus speeding up the overall innovation cycles. The governance model of the Materials Commons should **integrate international (European) and national initiatives** such as EOSC, PMD and DIADEM and should be guided by the **Technology Council for Advanced Materials**. To this end, **semantic data models** for the general material domain and for specific context-aware data representations in sub-domains of strategic innovation markets need to be established.





HORIZON-CL4-INDUSTRY-2025-01-MATERIALS-45




Initial Infrastructure elements of MaterialsCommons4.eu



Selection of initial consortia and repositories, that will be linked in MaterialsCommons



Welcome to the **DataPortal** for sharing material data sets provided by **Platform MaterialDigital**

Durchsuchen Sie unsere 


CAPeX
Pioneer Center for Accelerating P2X Materials Discovery

Accelerating Discovery for Sustainable Energy Solutions
Innovating Materials for **Power-to-X**



NFDI-MatWerk – National Research Data Infrastructure for MSE


We support researchers in **Materials Science and Engineering (MSE)** with **FAIR data solutions** that enable new discovery.



LEARN WORK DISCOVER EXPLORE ARCHIVE

MATERIALSCLOUD

Built for seamless sharing of resources in computational materials science.



NOMAD
Materials science data managed and shared

NOMAD lets you manage and share your materials science data in a way that makes it truly useful to you, your group, and the community. **Free and open source.**

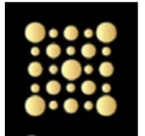


The PEPR DIADEM
Discovery Acceleration for the Deployment of Emerging Materials



... and many more!

MaterialsCommons - project partners



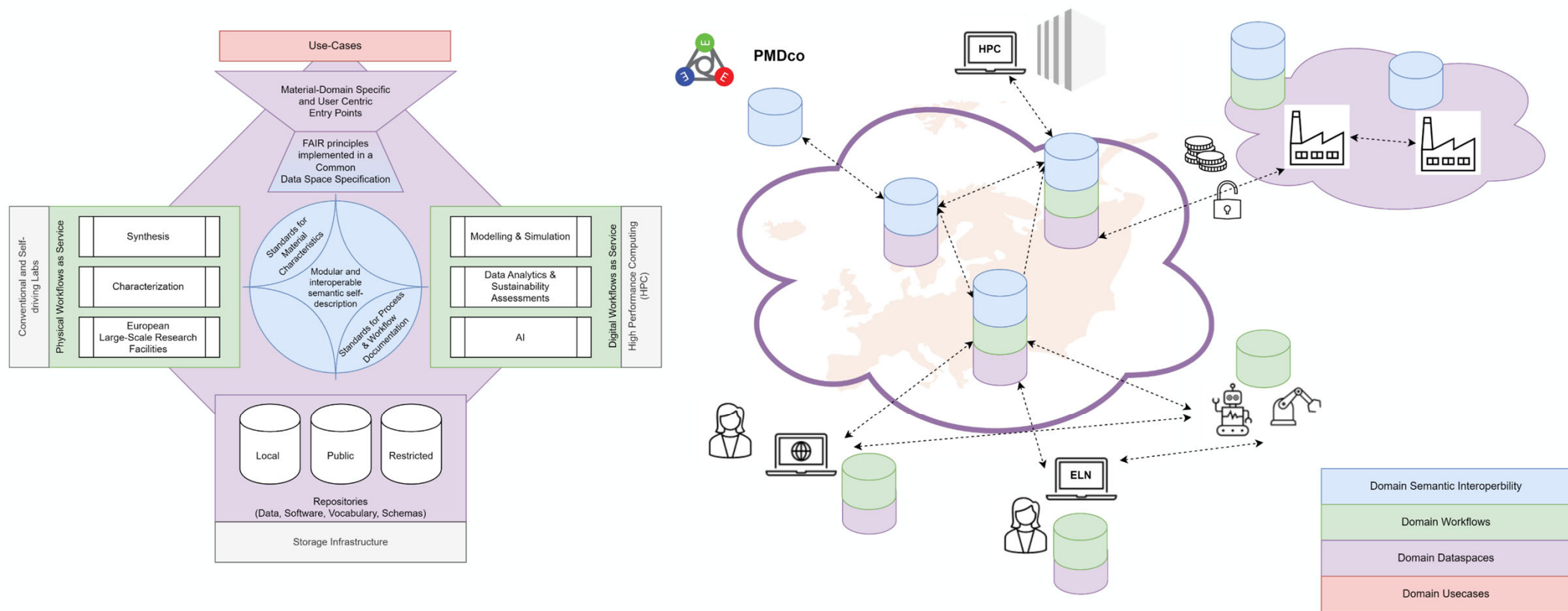
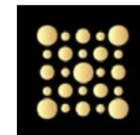
Associated Partners



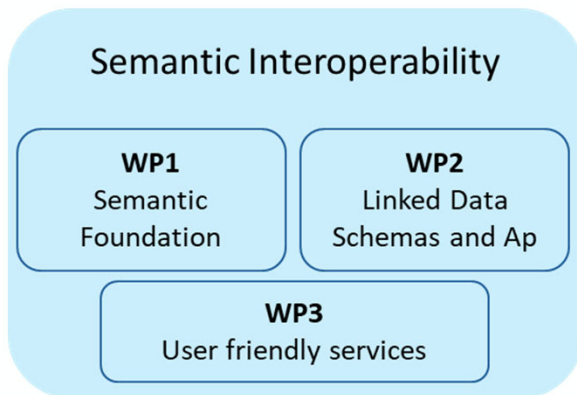
Associated Collaborators



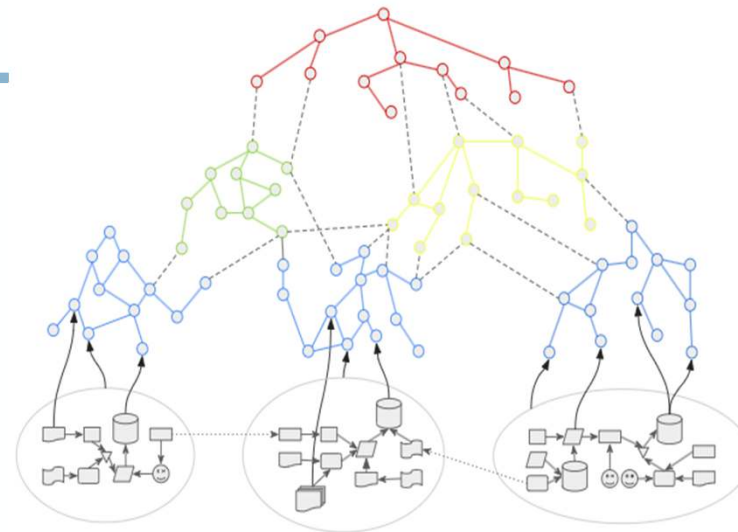
Architecture of MaterialsCommons



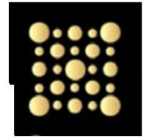
Structure of MaterialsCommons



Establish user-friendly services for semantic annotation of FAIR data by schemas actionable in application programming interfaces



Top-Level Ontologies



Mid-Level Ontologies



Application Ontologies



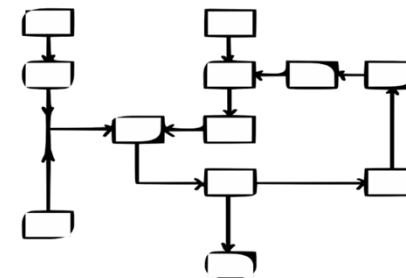
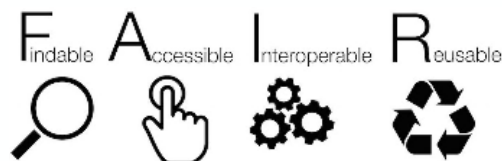
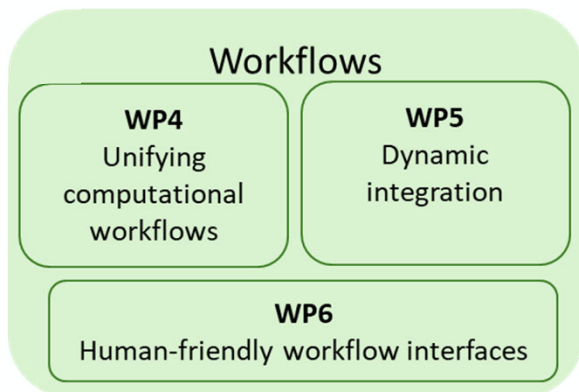
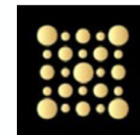
Domains

- Processes
- Raw Data
- Processed Data



- Building a FAIR-compliant semantic framework with specified quality requirements, governance rules, and publication workflows
- Creating a technical specification for human and machine actionable linked data schema language
- Providing user-friendly tools for documentation, search, and knowledge integration
- Foundation for interoperability between data, software, and communities

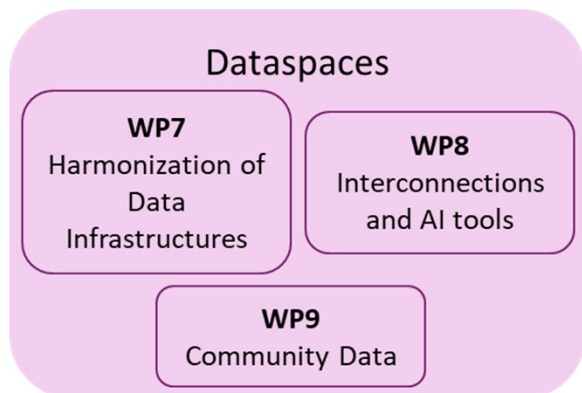
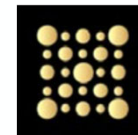
Structure of MaterialsCommons



- Interoperable workflow definition for simulation, experiment, and machine learning
- FAIR-compliant and machine-readable description of individual process steps
- Integration of self-driving labs, electronic lab notebooks, and AI-supported automation
- Support for closed, adaptive research and development cycles

Develop interoperable workflows able to create ML-actionable links between materials modelling and self-driving laboratories

Structure of MaterialsCommons



- Harmonization of European materials data infrastructures
- Federated access to distributed data via shared APIs and standards
- Secure data use, literature data acquisition, and federated learning
- Validation using real-world community data scenarios

Provide access to different dataspaces, databases, computing environments



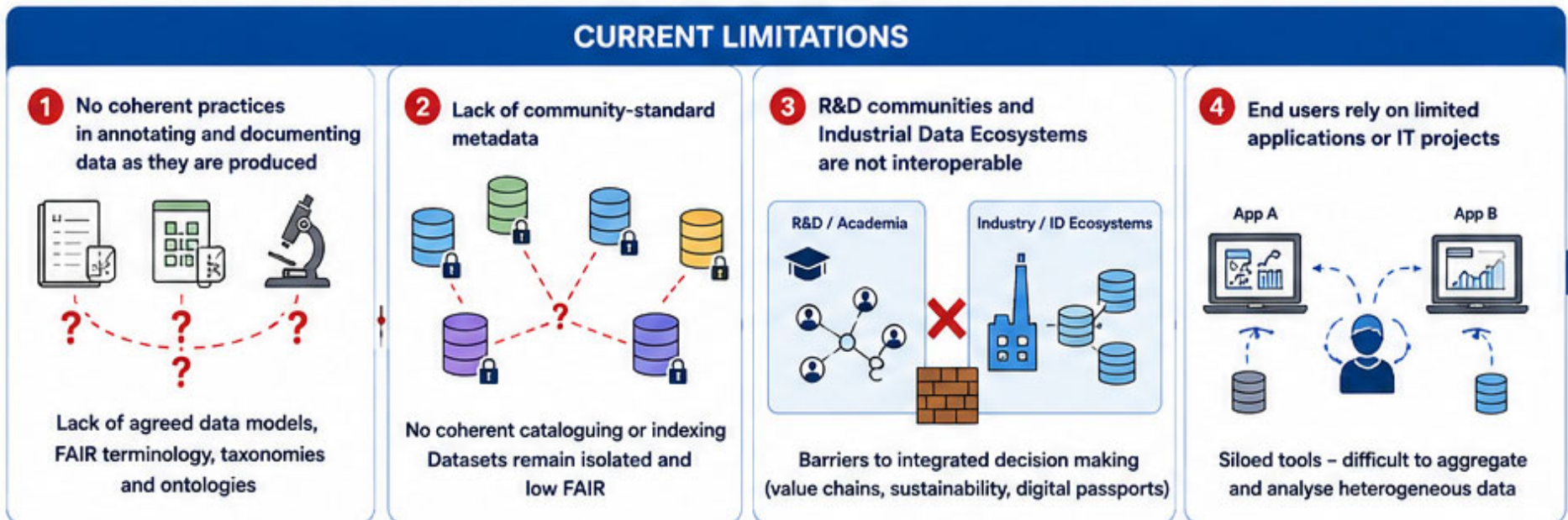
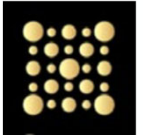
MATERIALSCLOUD



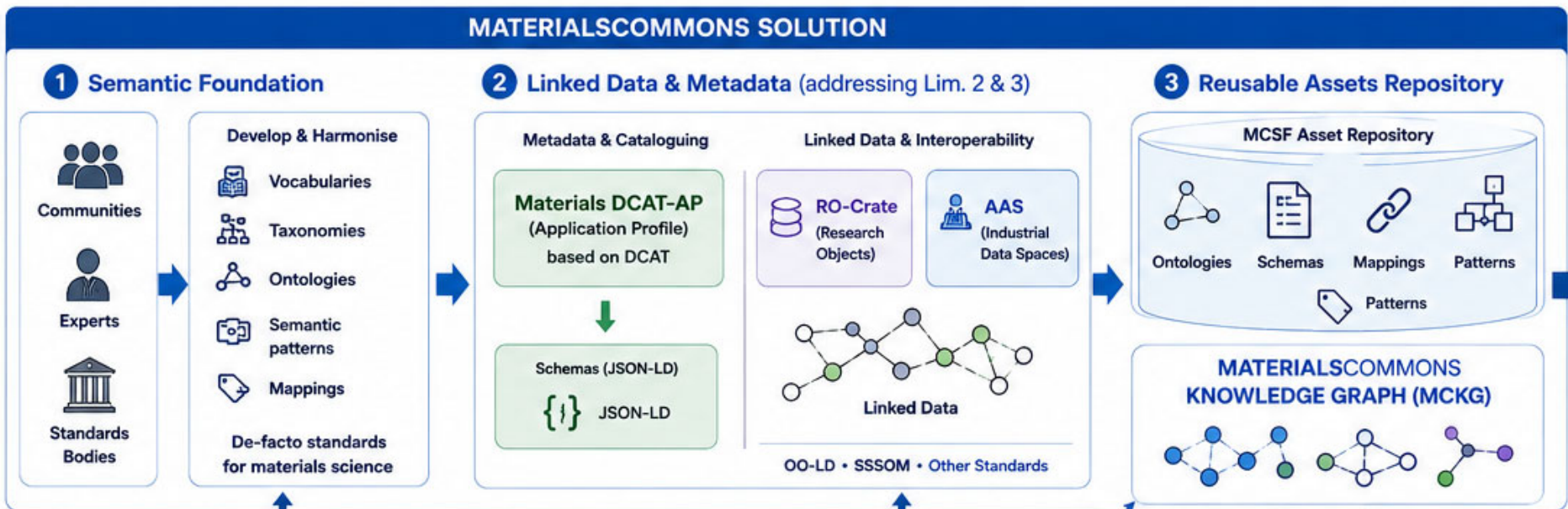
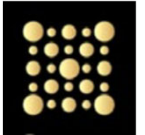
NOMAD



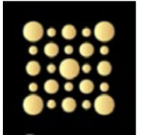
Challenges in Semantic Interoperability



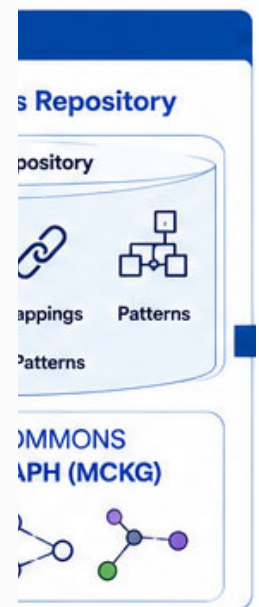
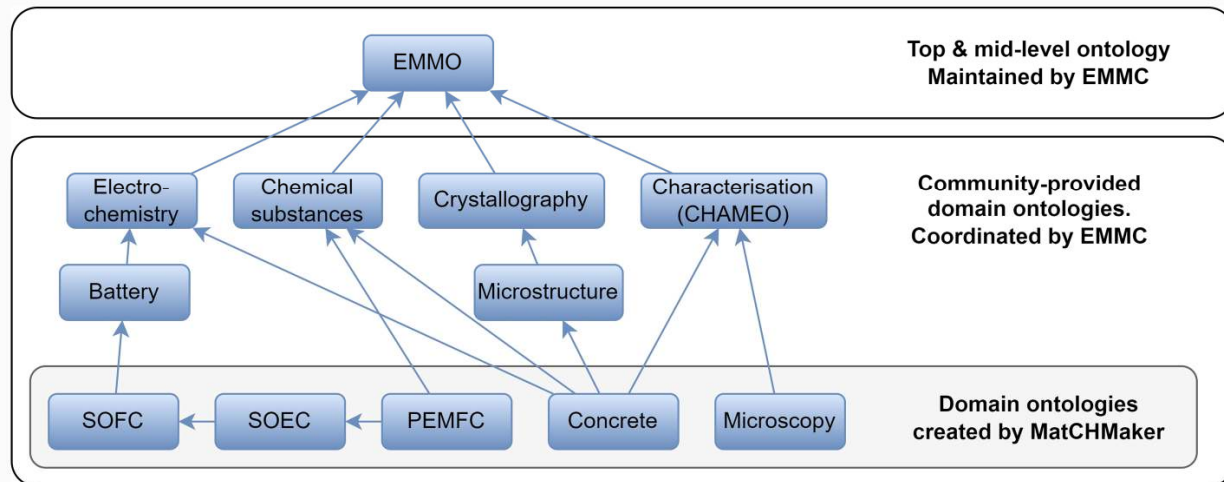
Proposed Solutions



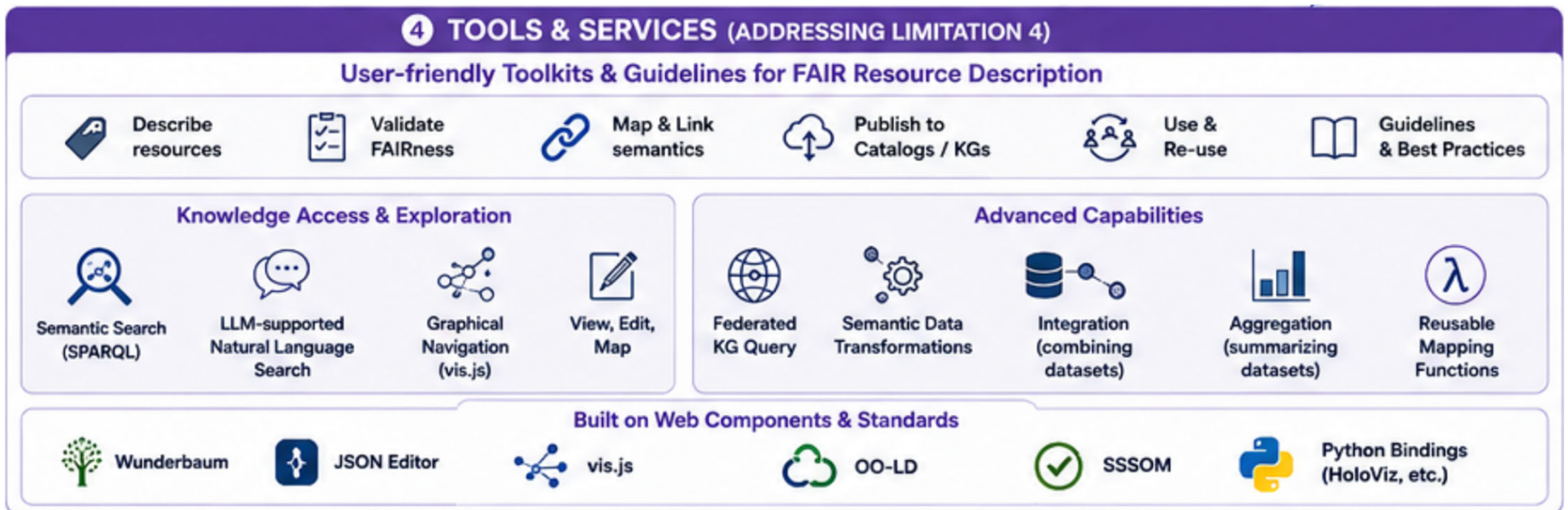
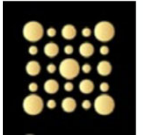
Proposed Solutions



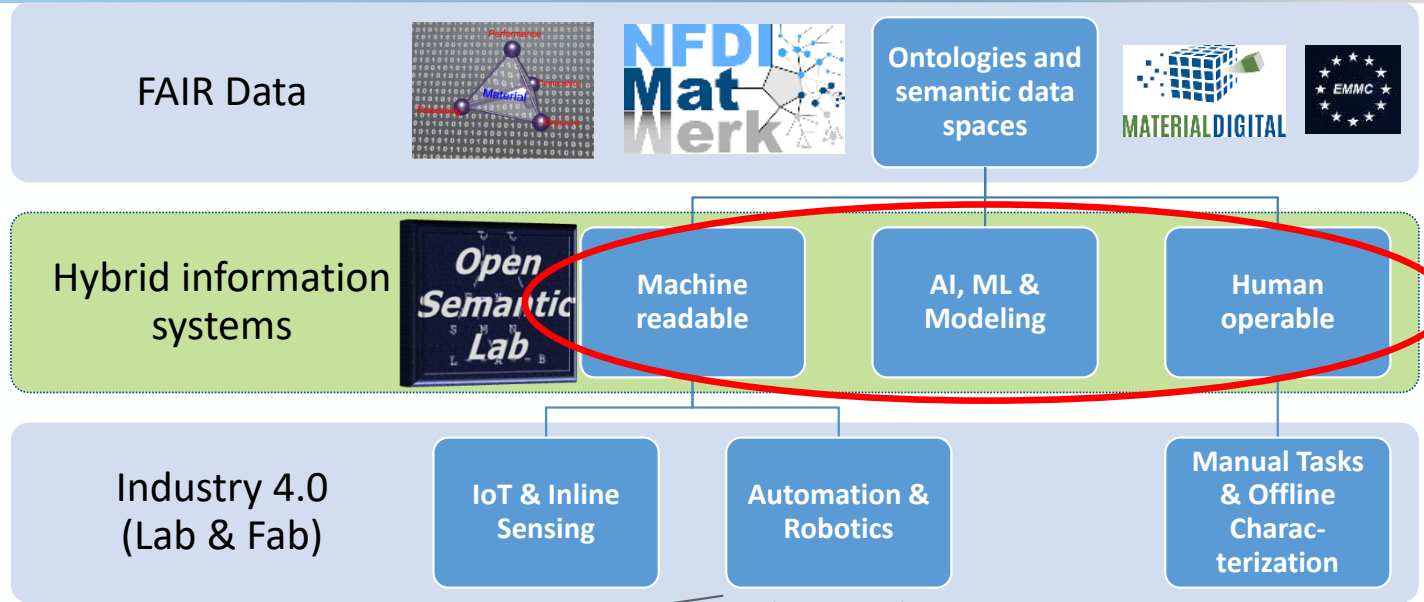
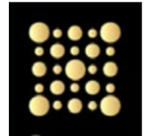
Dedicated domain ontologies to capture use case knowledge



Provided Service Building Blocks



Materials Acceleration @ Fraunhofer



Link: [ISC Digital/MAPs](https://isc-digital.com/MAPs)



Battery material synthesis (BIG-MAP)



Nano particle synthesis



Tissue engineering / medical testing

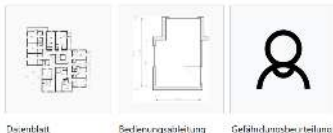


Fully automatic Glas-Screening

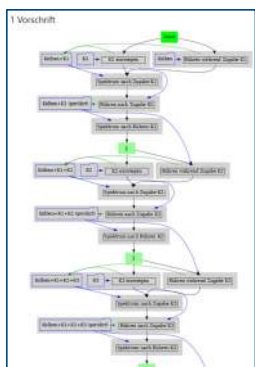
- *Strong cooperation with lab automation and materials domain experts*

OpenSemanticLab Concept

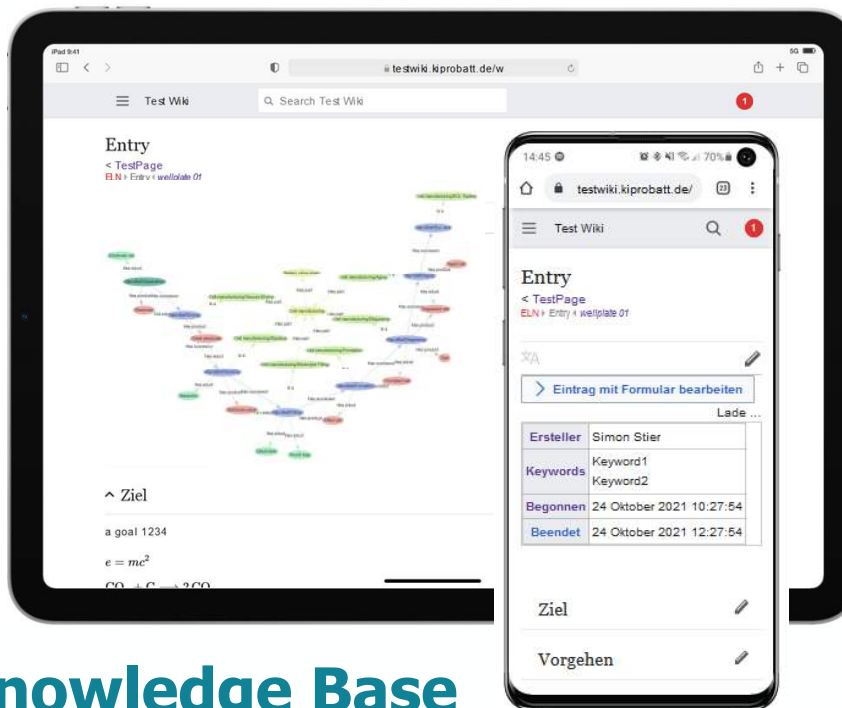
G1	
Anzeigenname	G1
Vollständiger Name	Gerat131452
Gerätetyp	Gerätetyp1
Berichtsnummer	12345678
Verantwortung	
Geräteverantwortlicher	Esehet, Test Person, Mex Muster
Standort	H.1.1
Gerätetyp1	
Anzeigenname	GT1
Vollständiger Name	Gerätetyp1
Hersteller	Bosch
Typenbezeichnung	Buogerat
Geräteklasse	Kategorie:KatGerat; Kategorie:TestGerat



Inventory Management



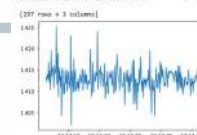
Standardized Processes



Knowledge Base & (Lab) Notebook

```

TimeStep: 2022-01-12 14:22:13.240000-00:00; Sensor: ID: 1; Value: 1.412378
command: readTime
cursor: 0
client: 00000000000000000000
    0 2022-01-12 14:22:13.240000-00:00 1 1.412378
    1 2022-01-12 14:22:13.240000-00:00 1 1.412380
    2 2022-01-12 14:22:13.240000-00:00 1 1.412367
    3 2022-01-12 14:22:13.240000-00:00 1 1.412364
    4 2022-01-12 14:22:13.240000-00:00 1 1.412351
    5 2022-01-12 14:22:09.412000-00:00 1 1.412378
    6 2022-01-12 14:22:09.412000-00:00 1 1.412374
    7 2022-01-12 14:22:09.412000-00:00 1 1.412374
    8 2022-01-12 14:22:12.412000-00:00 1 1.412388
    9 2022-01-12 14:22:12.412000-00:00 1 1.412362
    10 2022-01-12 14:22:12.412000-00:00 1 1.412378
    
```



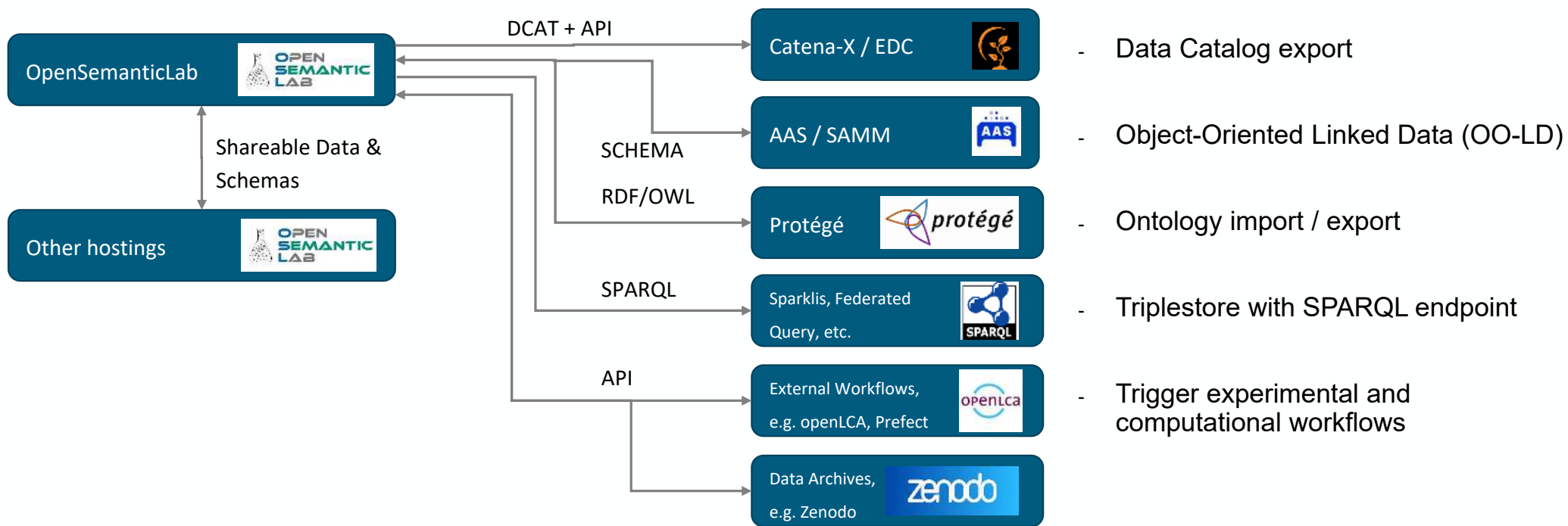
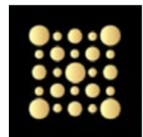
Machine Interfaces



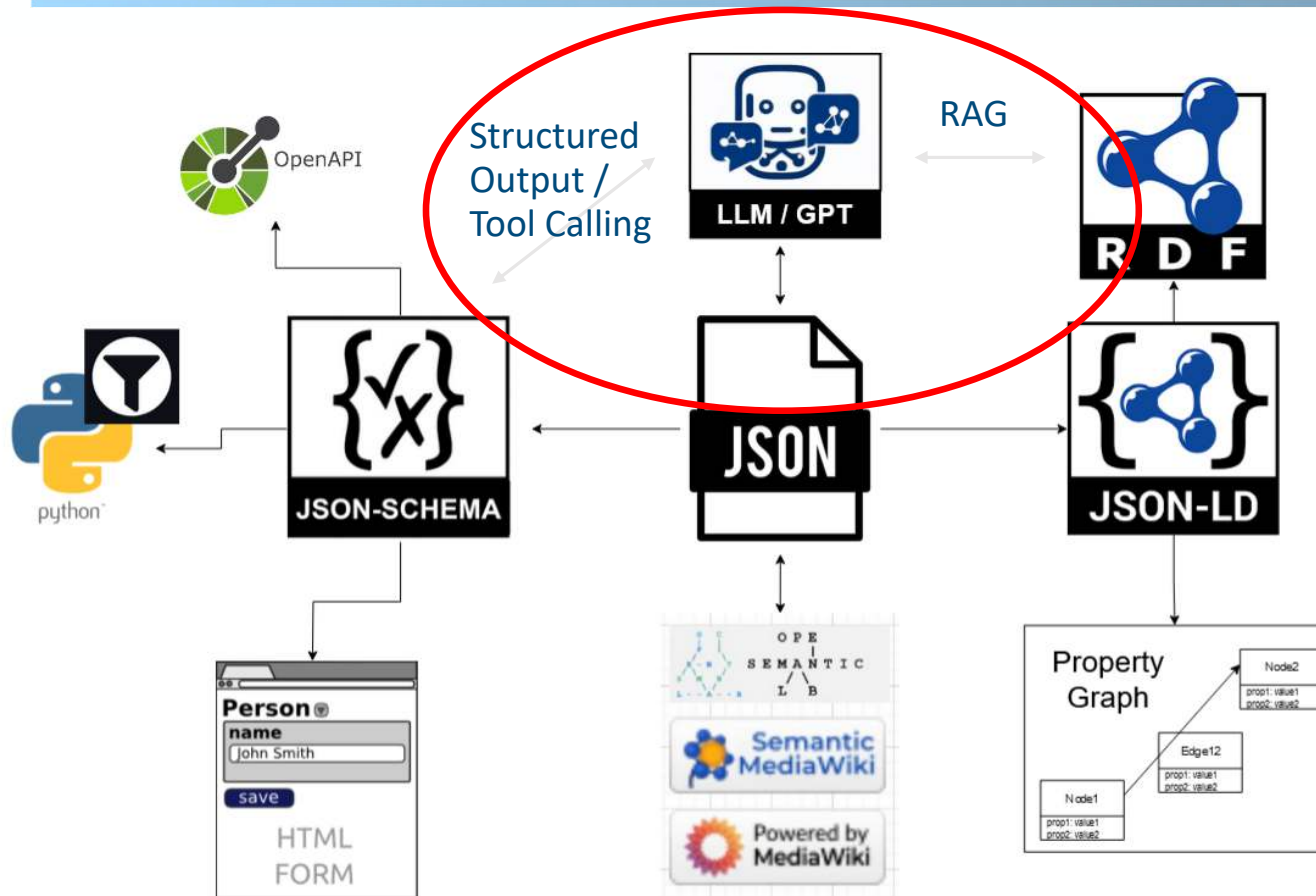
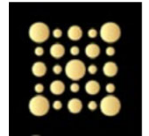
Computational science



(Generative) AI



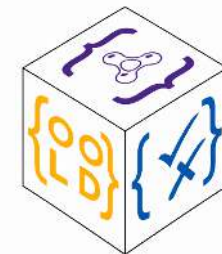
Technology overview of semantic interoperability



- OpenSemanticLab is based on object oriented linked data schemas (OO-LD) as meta-industry standard

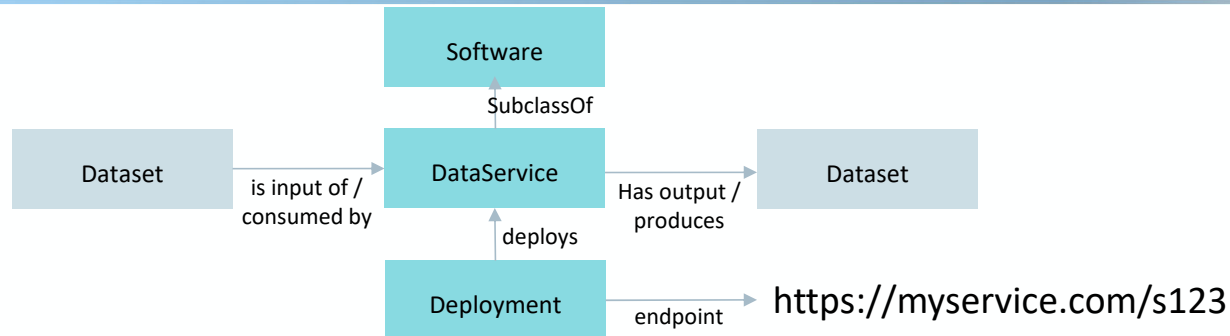
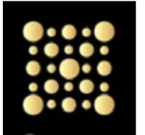
- On the one hand, those schemas **auto-generate both human (UI) and machine interfaces (API)**

- On the other hand, those schemas can be **annotation with arbitrary ontologies in order to auto-create RDF graphs in the background**

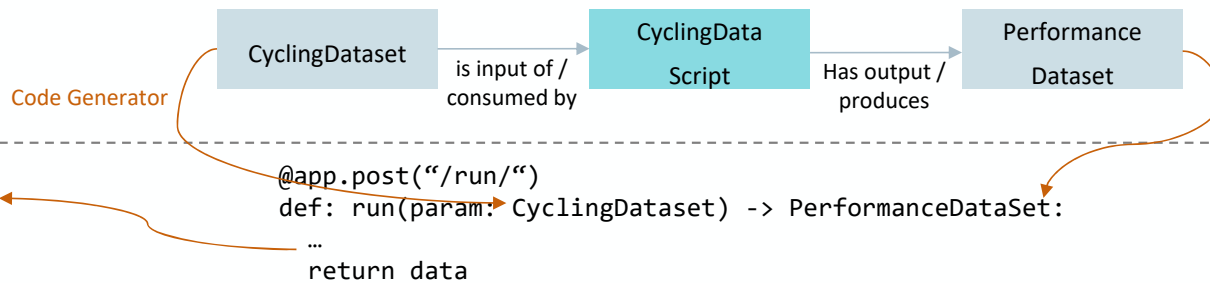


<https://github.com/OO-LD/schema>

Technology overview of semantic interoperability



Schema



Instance

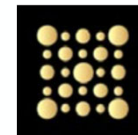
Server Code

Deployment (e.g. Prefect, Pyiron)

```
data = CyclingDataset()
res: PerformanceDataSet = PerformanceDataSet(
  **requests.post("https://myservice.com/s123/run/", json=data.json() ).json()
)
```

Client Code

In the area of LLMs, how much integration is still required?



Navigation in knowledge platform

Mat-O-Lab OSL

Welcome to *OpenSemanticLab* for [Mat-O-Lab](#)

OpenSemanticLab is a hybrid, human and machine-readable database for domain knowledge and data, including a [SPARQL-Endpoint](#)

Tutorial: [Working with SPARQL and LocalAI](#)

^ Common Features

- Article**
A generic entry that can contain both text and media content
CREATE
- Tutorial**
Instruction in written or cinematic form
CREATE
- Funding Call**
Announcement of a funding opportunity with details of the funding conditions
CREATE
- ELN Entry**
Contains notes and data about experiments

^ Inventory maintenance

EVE Chat Assistant

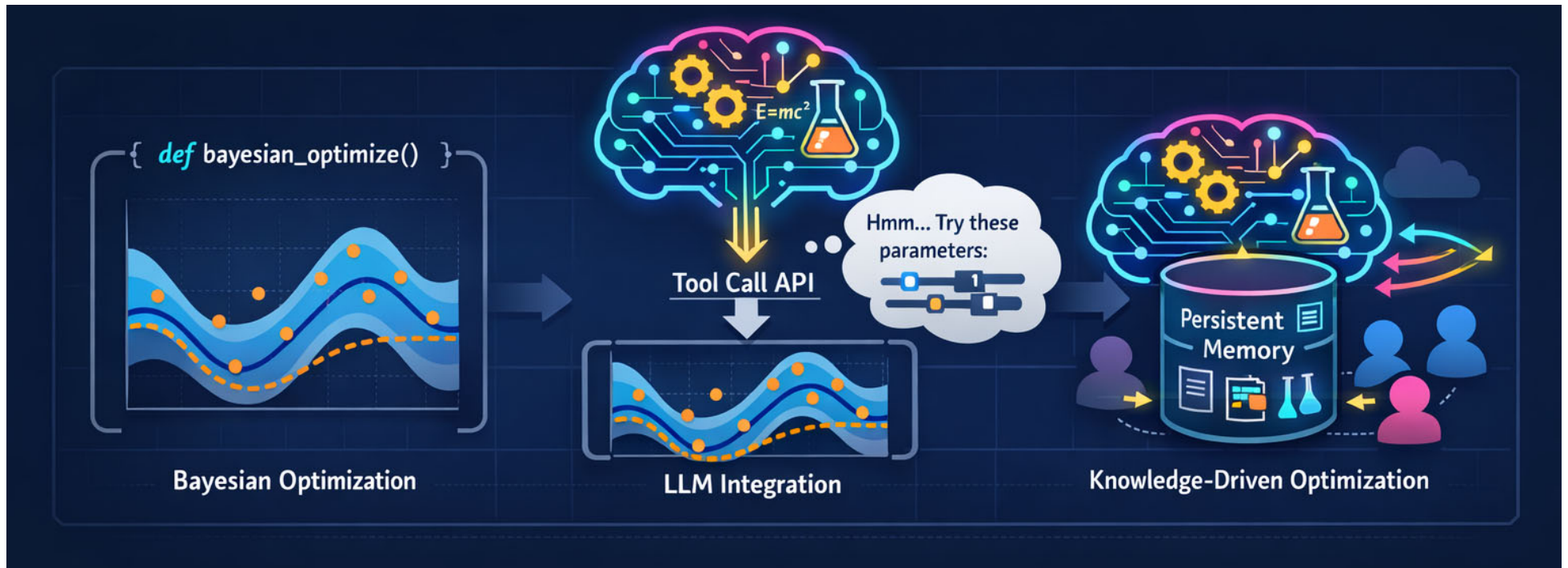
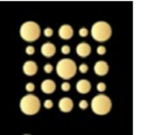
Assistant

How can I help you?

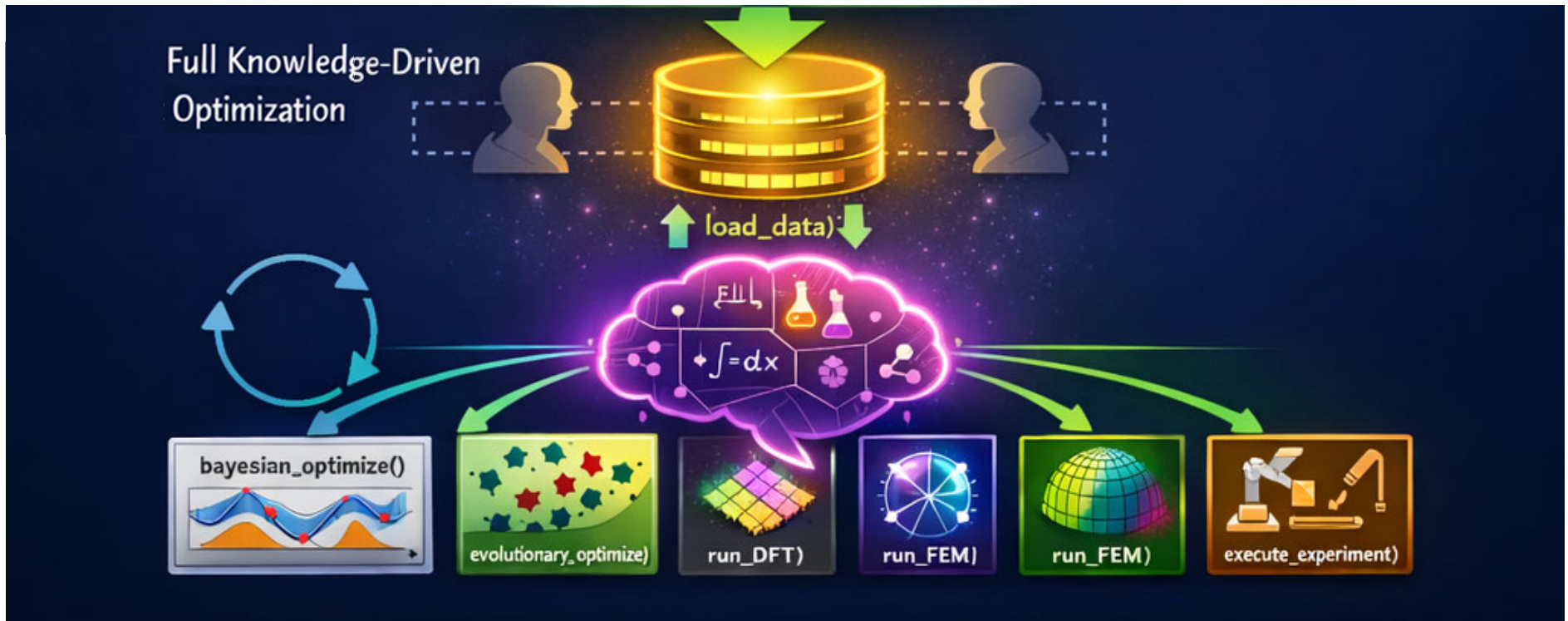
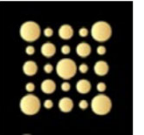
se

<https://www.youtube.com/watch?v=8XypKdFaxpM>

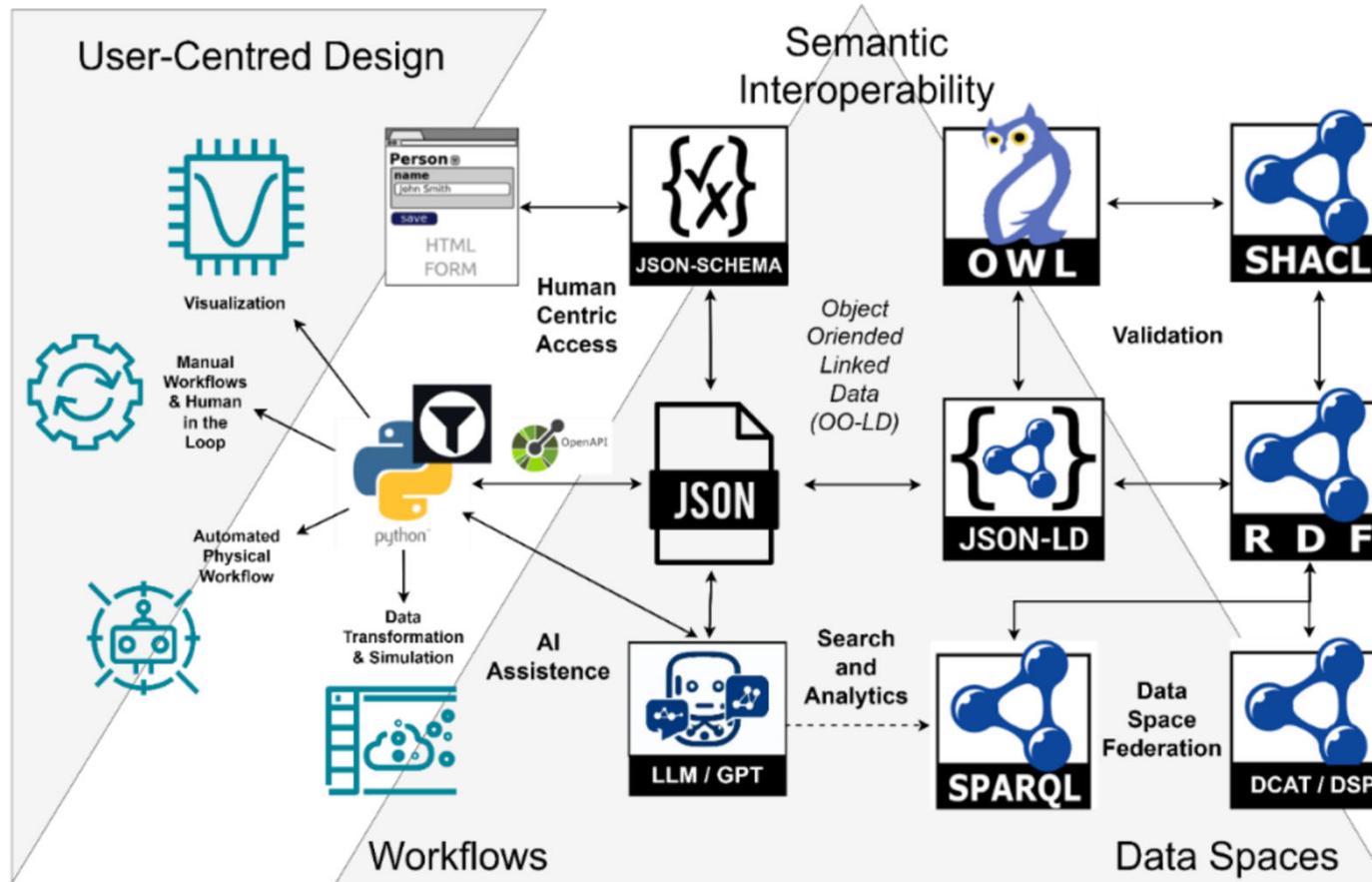
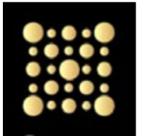
In the area of LLMs, how much integration is still required?



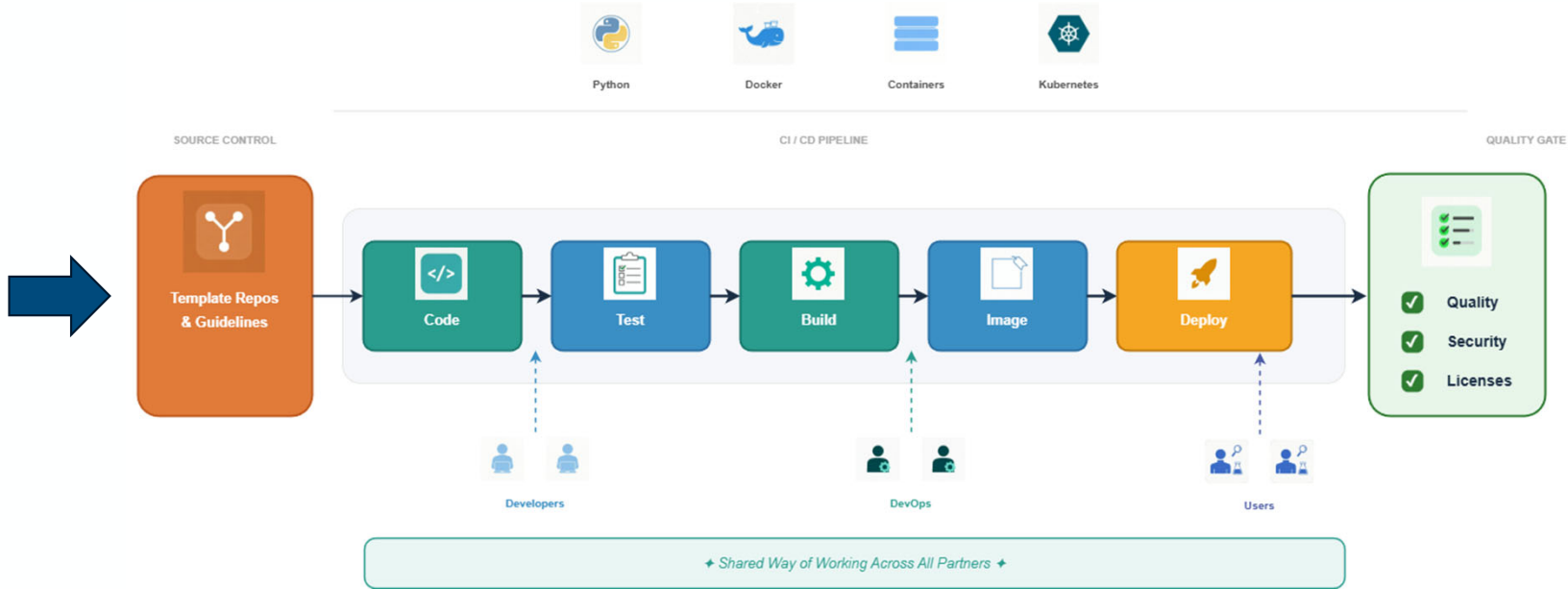
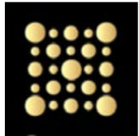
In the area of LLMs, how much integration is still required?



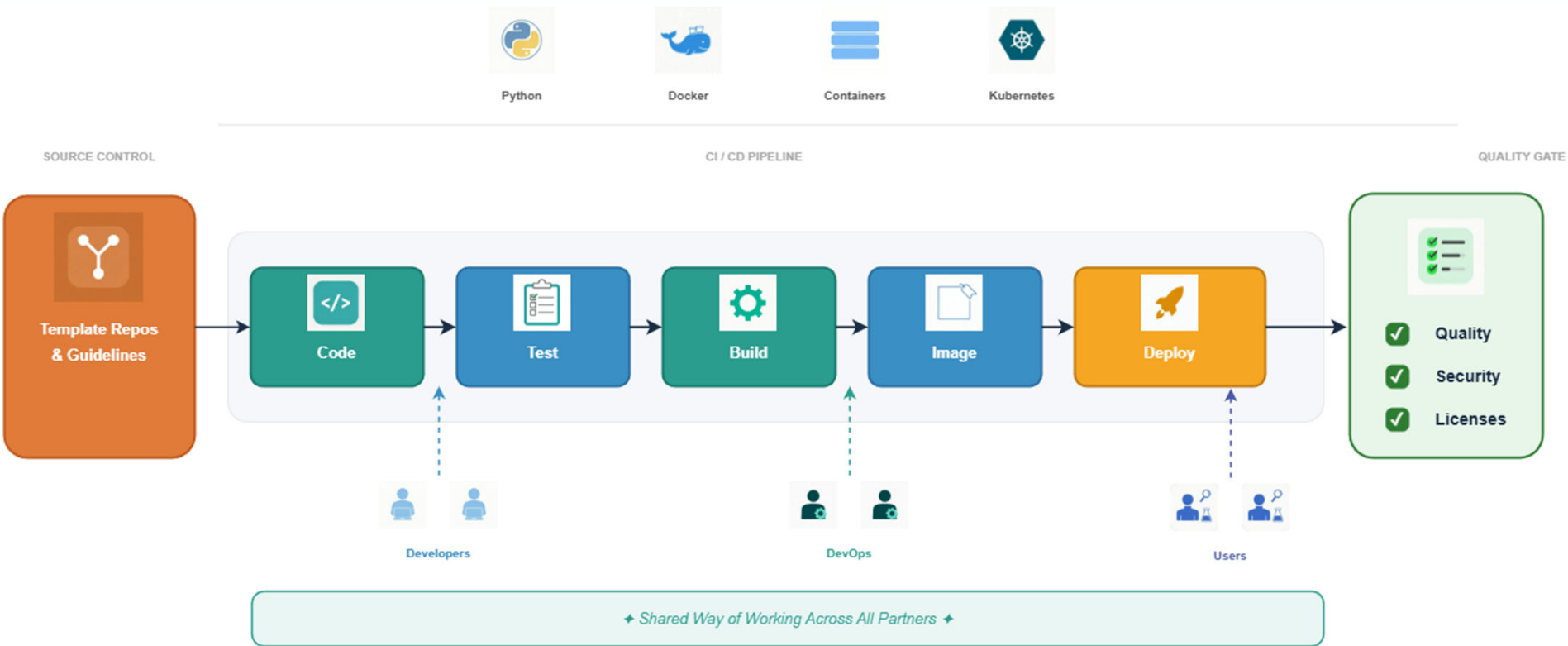
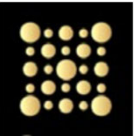
Technology overview of semantic interoperability



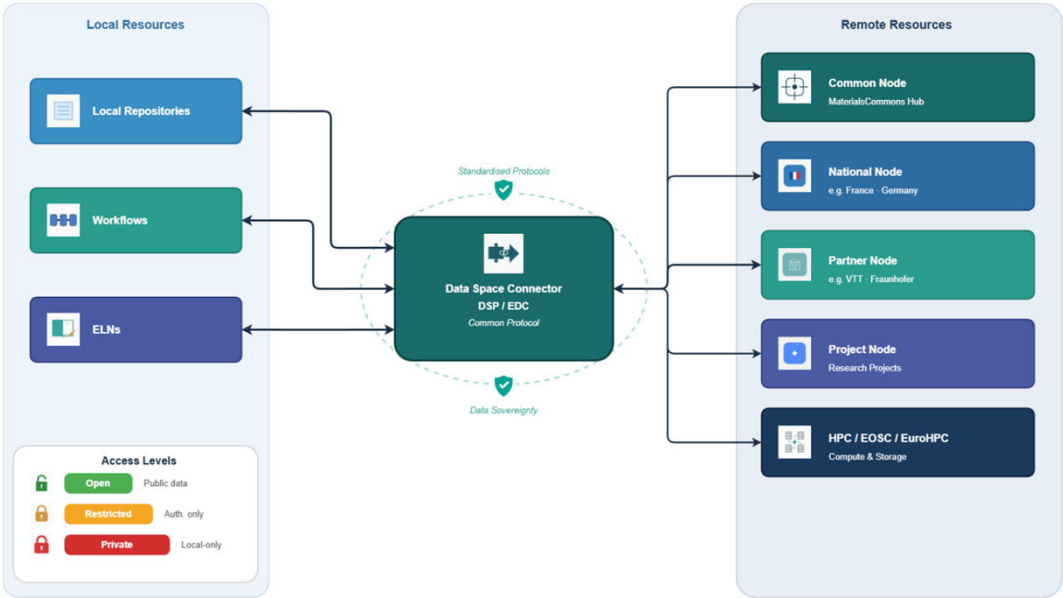
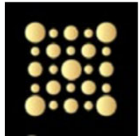
Coherent Software Development



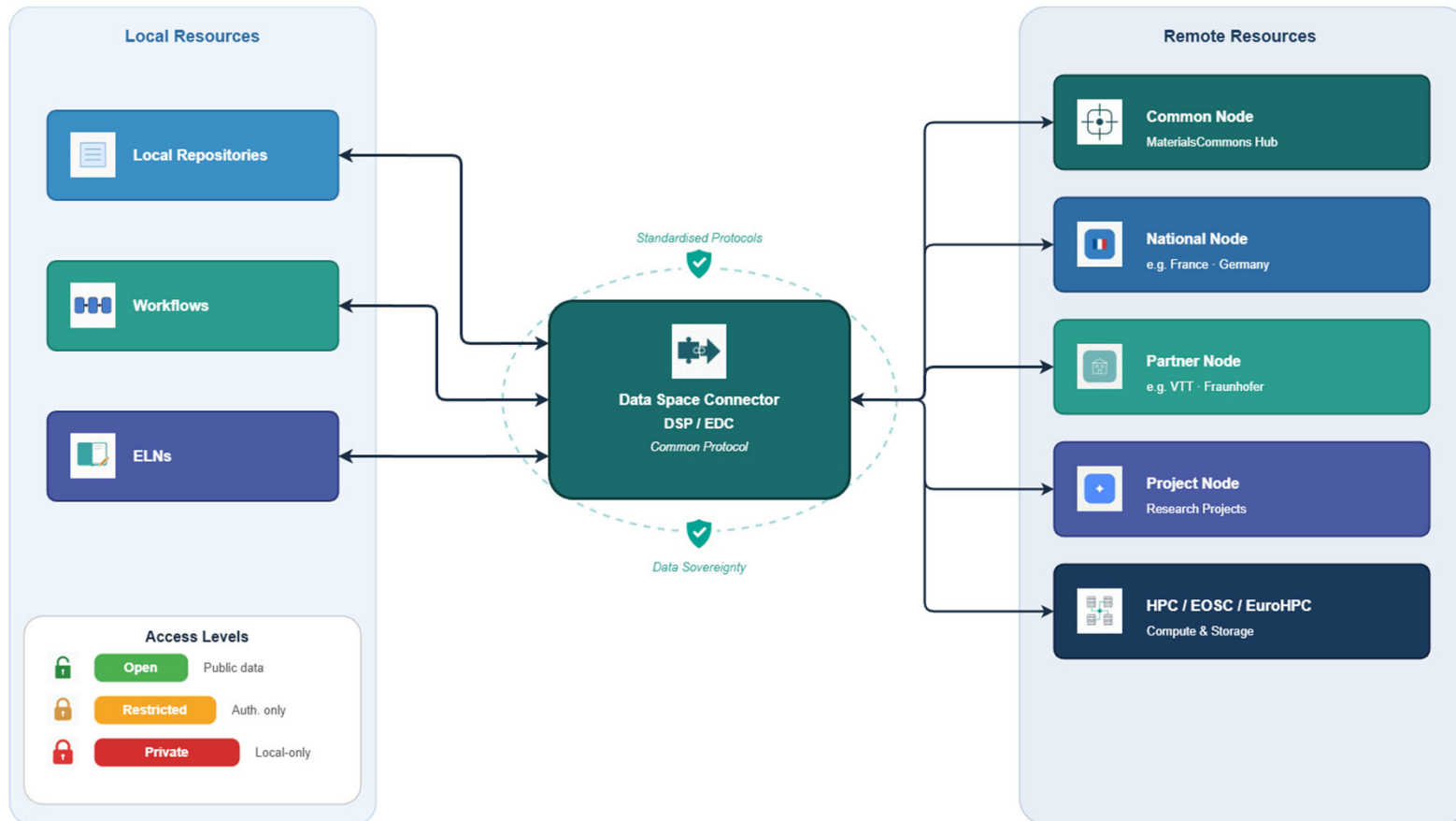
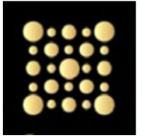
Coherent Software Development



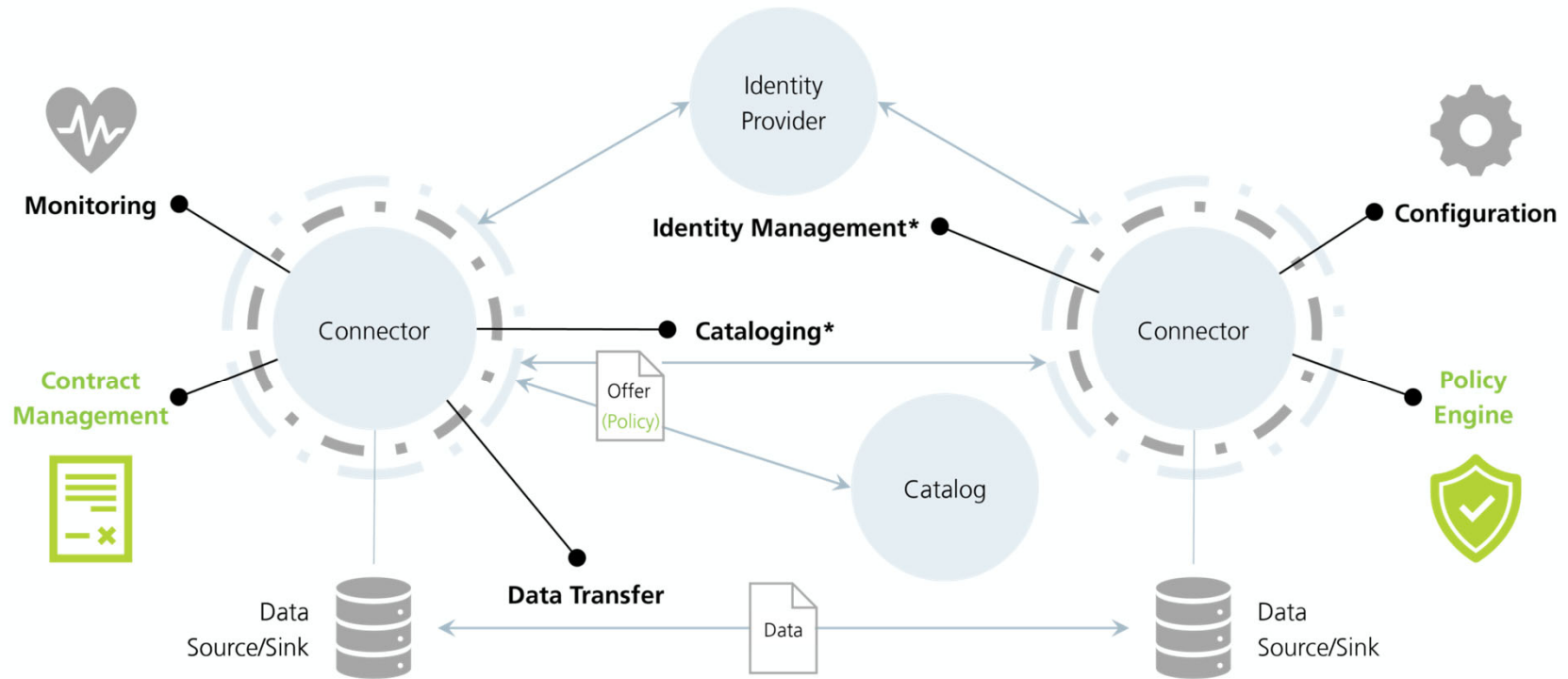
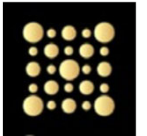
Federated AND User Centered



Federated...

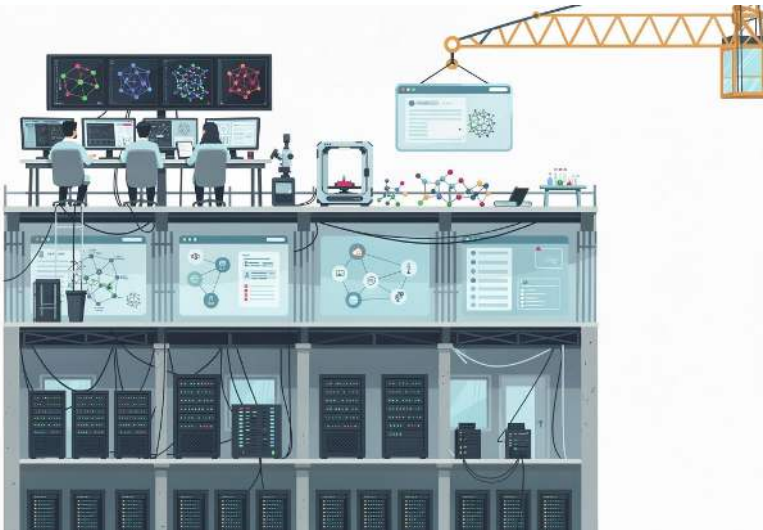
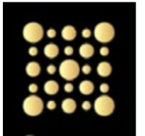


Federated...

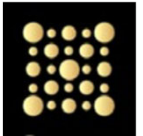


<https://eclipse-dataspace-protocol-base.github.io/DataspaceProtocol>

Federated ... AND User Centered



Federated ... AND User Centered



Contact

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Head of Digital Transformation

simon.stier@isc.fraunhofer.de

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97082 Würzburg

Germany

