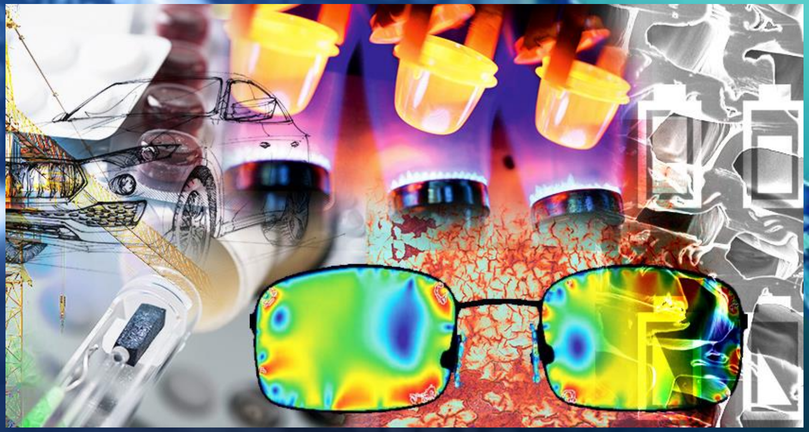
Materials Acceleration Platforms (MAPs)

Accelerating Materials Research and Development to Meet Urgent Societal Challenges

Simon Stier

Dec 6th 2024 – MRS Fall Meeting Boston



Background & Use case: Applied Material Science

Motivation

- Traditional slow approach

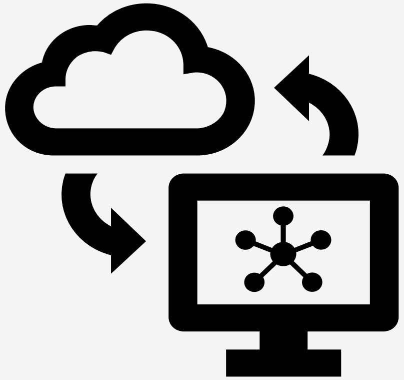
- Accelerated Research by multiplying the effort?

Motivation

Accelerated Research by reducing the human effort!

Automated sample production and testing

Automated data analysis, machine learning and AI



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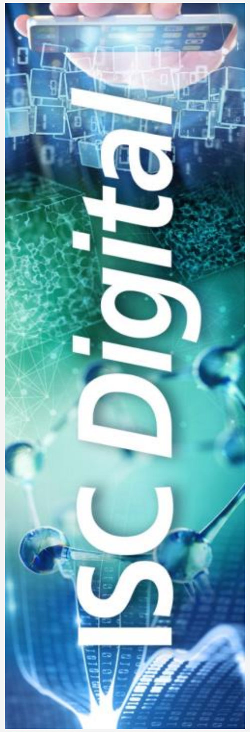
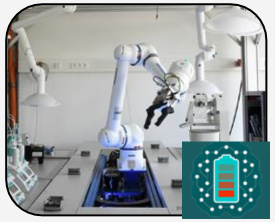


FAIR Data: eu-mace · Ontologies and semantic data spaces · EMMC

Hybrid information systems: Open Semantic Lab · Machine readable · AI, ML & Modeling · Human operable

Industry 4.0 (Lab & Fab): IoT / OPC UA · Automation & Robotics · Manual Tasks

Link: [ISC Digital/MAPs]



Battery material synthesis (BIG-MAP)

Nano particle synthesis

Tissue engineering / medical testing

Fully automatic Glas-Screening

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Head of Digital Transformation @ Fraunhofer ISC

MAPs: Accelerating materials research and development to meet urgent societal challenges

June 2022

EMIRI About us ⌄ Membership ⌄ EU Projects ⌄ News Events

Re-inventing Materials Research Workshop: in brief

After 2 days of IndTech Conference in Grenoble, EMIRI organised a workshop as a side event on June 30th focused on "**Re-inventing Materials Research: Towards accelerated development by closely orchestrating AI, data, robotics, and high-performance computing**"

The topic raised immediately a strong interest among the invited speakers and the audience and consequently, we were starting the session at 8.30AM with a very busy programme ahead of us. With more than 30 attendees physically and 20 connected online, the participants were able to engage in meaningful discussions that we expect to be the starting point of a future coordinated action for the materials community. A white paper on this topic was suggested as the first step of this coordinated action.

The workshop started showing the digital revolution underway in industrial labs, where we had the opportunity to see industrial case studies from BASF, DOW, SOLVAY and UMICORE. We continued with case studies from research centres such as HELMHOLTZ-INSTITUTE and FRAUNHOFER INSTITUT. We also had the case of the DTU illustrating the BIG-MAP project, in which EMIRI and many other organisations of the materials community are involved.

After a short coffee break, we came back to portray solutions to accelerate materials research already available on the market by CITRINE INFORMATICS, DASSAULT SYSTEMES, ATINARY TECHNOLOGIES, SCM SOFTWARE FOR CHEMISTRY AND MATERIALS and VSPARTICLE.

We believed that it was important to allocate some time also to review policy initiatives such as the Mission Innovation's Collaborative Platform: Materials for Energy (M4E) and the French imitative DIADEM – Discovery Acceleration for the Deployment of Emerging Materials.

https://emiri.eu/2022/07/04/digital-revolution-in-materials-discovery/

Oct 2023

Memorandum

THE SIGNIFICANCE OF ACCELERATED DISCOVERY OF ADVANCED MATERIALS TO ADDRESS SOCIETAL CHALLENGES

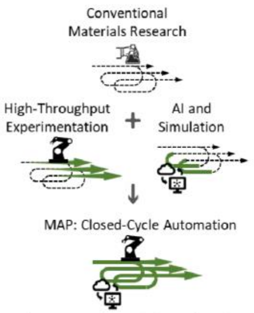
Preprint for Information/Recommendation

SUMMARY

Climate Change and **Materials Criticality** challenges are driving **urgent responses** from global governments. These global responses drive policy to achieve **sustainable, resilient, clean solutions** with **Advanced Materials (AdMats)** for industrial supply chains and economic prosperity.

The **research landscape comprising industry**, academe and government identified a critical path to **accelerate the Green Transition** far beyond slow conventional research through Digital Technologies that harness Artificial Intelligence, Smart Automation and High Performance Computing through **Materials Acceleration Platforms, MAPs.**

It is recommended that public European, national and regional institutions **collectively support** accelerated materials discovery and development as a foundational element in climate mitigation and resource sustainability through **Materials Acceleration Platform** technology.



The concept of Materials Acceleration Platforms (MAP)

THIS PROPOSITION IS SUPPORTED BY THE FOLLOWING INSTITUTIONS AND INDUSTRIES:

Fraunhofer, JÜLICH Forschungszentrum, DTU, cnrs, Aixelo Rethink Innovation, UKRI Science and Technology Facilities Council, SCM Software for Chemistry & Materials, CIC energiGUNE, VTT, SINTEF, KIT Karlsruher Institut für Technologie, cnr DIITET, 3DS BIOVIA, HZB Helmholtz Zentrum Berlin, Natural Resources Canada

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Sep 2024

PERSPECTIVE ADVANCED MATERIALS www.advmat.de

Materials Acceleration Platforms (MAPs): Accelerating Materials Research and Development to Meet Urgent Societal Challenges

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Climate Change and Materials Criticality challenges are driving urgent responses from global governments. These global responses drive policy to achieve sustainable, resilient, clean solutions with Advanced Materials (AdMats) for industrial supply chains and economic prosperity. The research landscape comprising industry, academe, and government identified a critical path to accelerate the Green Transition far beyond slow conventional research through Digital Technologies that harness Artificial Intelligence, Smart Automation and High Performance Computing through Materials Acceleration Platforms, MAPs. In this perspective, following the short paper, a broad overview about the challenges addressed, existing projects and building blocks of MAPs will be provided while concluding with a review of the remaining gaps and measures to overcome them.

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Materials Acceleration Platforms (MAPs)

Accelerating Materials Research and Development to meet Urgent Societal Challenges

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Motivation

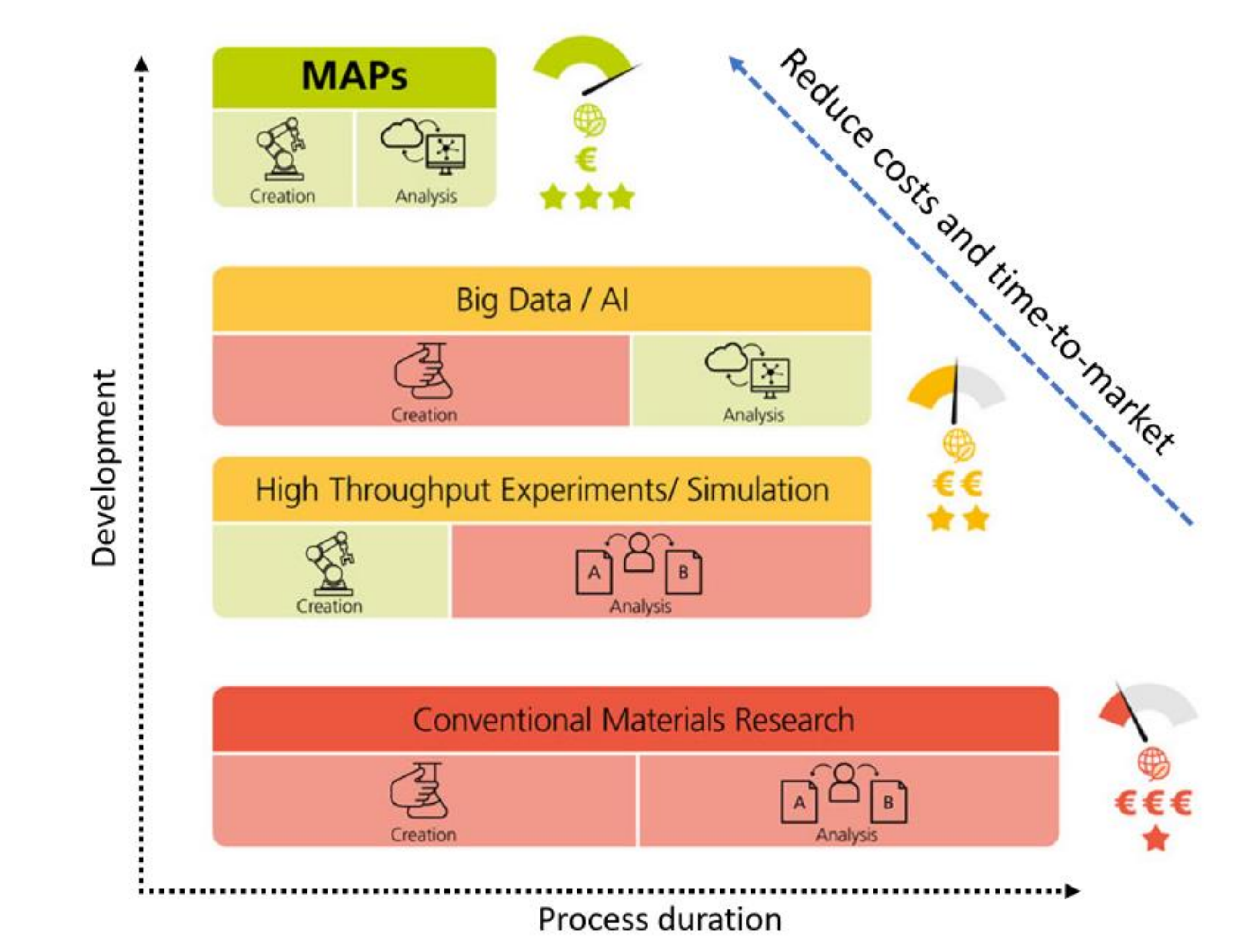
- Governments globally are addressing climate change and resource demand

- Rising global energy consumption and recent gas shortages highlight the urgent need for **sustainable energy solutions** to meet SDG 7 (clean and affordable energy) and SDG 13 (climate action).

- **Advanced Materials (AdMats)** are crucial for mitigating climate change impacts, energy resilience, and economic prosperity, with 20% of the industrial base and 70% of technical innovations relying on them.
- Materials research is essential for lower-cost, less toxic, and environmentally friendly AdMat solutions reducing reliance on **critical raw materials (CRMs)** and supporting circular economy practices

- The **European Green Deal** Industrial Plan supports climate neutrality and competitiveness, emphasizing the importance of a single EU market for resilience and global access, and is bolstered by the **Twin Transition** (green and digital transition).
- The **Materials 2030 Manifesto** calls for systemic collaboration across sectors to accelerate advanced materials development, aiming to **reduce development cycles and costs through digital technologies and high-throughput experimentation**.

About MAPs


MAPs
Creation
Analysis
€
Reduce costs and time-to-market
Big Data / AI
Creation
Analysis
€€
High Throughput Experiments/ Simulation
Creation
A
B
Analysis
Conventional Materials Research
Creation
A
B
Analysis
€€€
Development
Process duration

About MAPs - Why will it be superior?

Closed loop: MAPs use, optimizing materials and **advanced computational approaches to guide experiments and provide continuous feedback** devices across the entire parameter space.

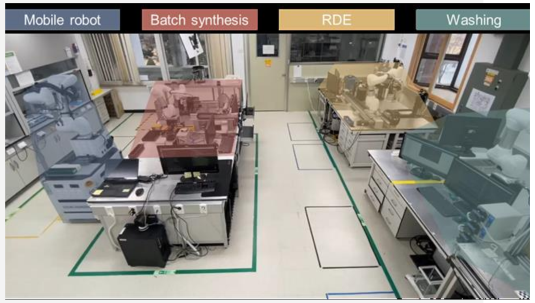
FAIR: MAPs produce **fully documented, meta-data rich, and structured data** sets that are Findable, Accessible, Interoperable, and Reusable (FAIR), ensuring comprehensive data management and stewardship.

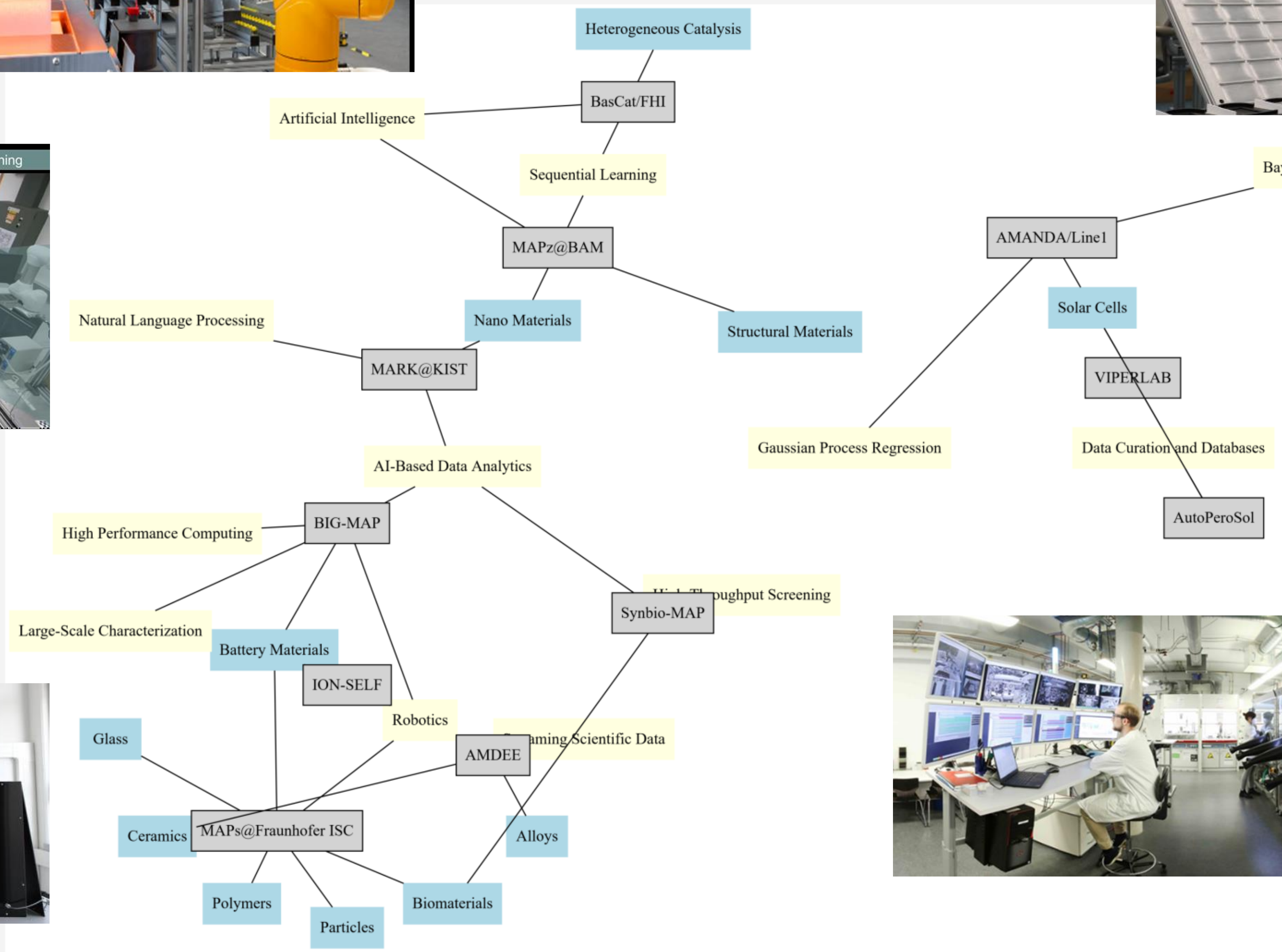
Holistic: MAPs accelerate materials development across various industrial sectors by optimizing **not just individual materials but entire devices** for their intended applications.

Collaborative and cross-domain: MAPs enable **connectivity of material data across multiple sectors**, fostering collaboration and leveraging AI-driven transfer learning to bridge knowledge gaps and promote "**Safe and Sustainable by Design**" approaches.

Decentralized and modular: MAPs can integrate decentralized equipment through a centralized data repository, allowing global researchers to access, control, and utilize data, offering "**experiments as a service**" to regions with limited infrastructure.

Projects





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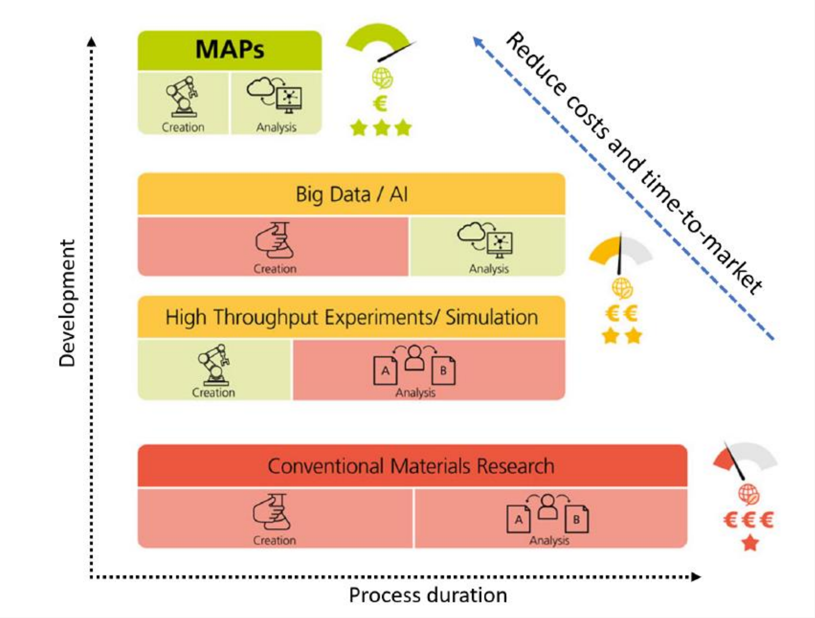
Early Impact

Particularly in the field of biological tissues engineering,[42] **significant increases in quality and throughput** have been achieved through laboratory automation while **human effort** for nanoparticle synthesis could be **reduced by approx. 44 %**[44].

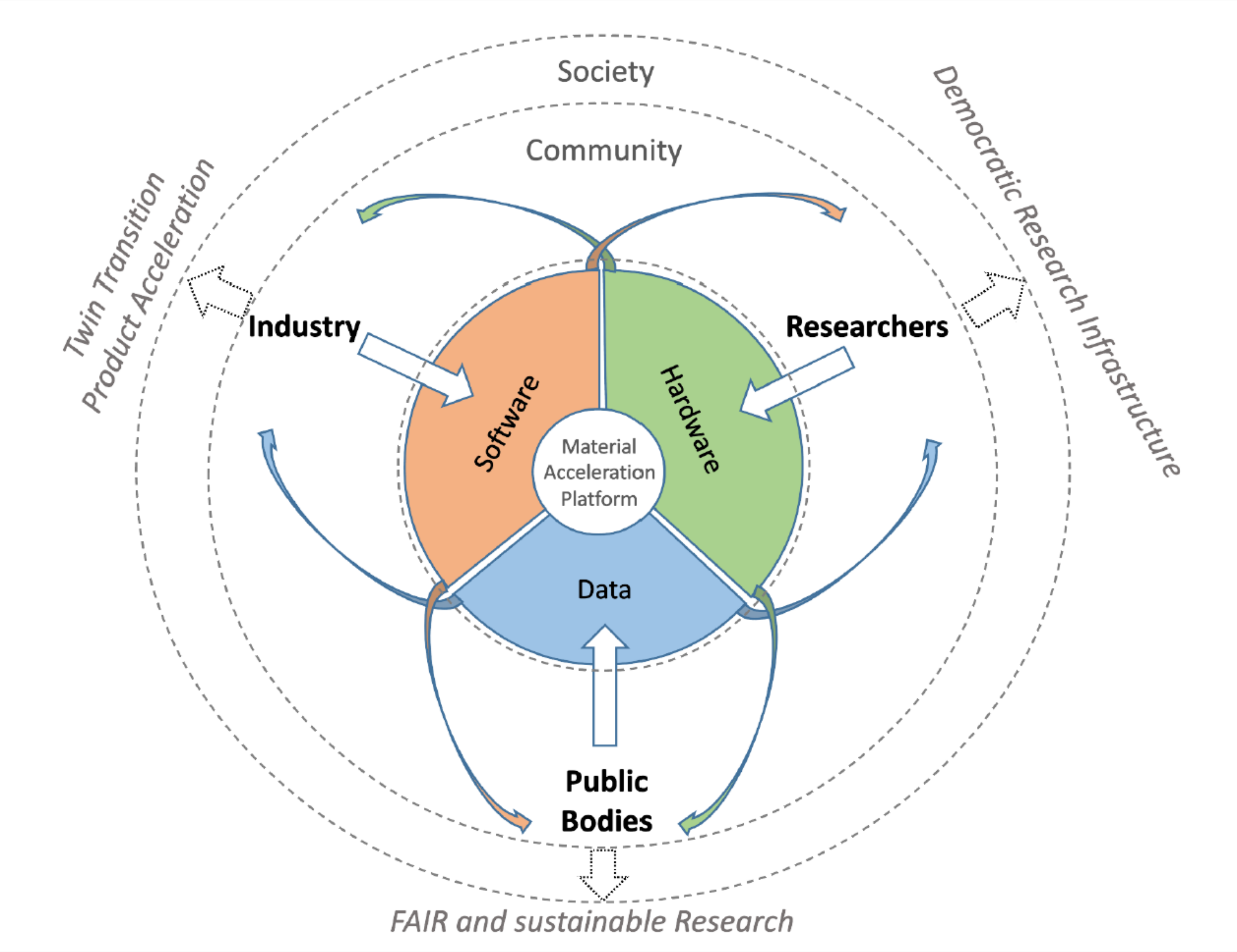


AMANDA has, with reference to edisonian high-throughput experimentation, achieved an acceleration starting at **30-fold**[49] reaching recently over **100-fold**[50, 51].
Among others this has lead to the **identification of ultrastable perovskite** compositions in the multidimensional parameter space. [52]

Within **less than 100 catalysts** created and tested (**requiring less than 3 months**), a new promoter combination was found that is **competitive** to the one presently used by BASF in their commercial Oleflex process. [58]

For instance, recently published success stories claim a **reduction of experimental workloads in general by up to 90 %**[113] and an **acceleration** of the development of new rare earth-free permanent magnets by a **factor of 200**[114]

Building Blocks



Building Blocks

Hardware

- Integrated **automation of lab experiments with synthesis and characterization** equipment.
- **Robots** for automating and accelerating **sample handling**.
- **Specialized lab equipment** for synthesis and analysis.
- **Custom design** and in-house built modules for flexibility.
- **Safety requirements** - equipment must handle hazardous substances.

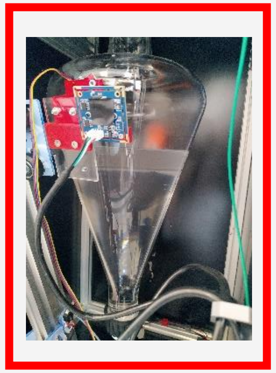
Communication Protocols and Interfaces

- Interfaces connect hardware components to IT infrastructure.
- Need for **remotely controlled lab equipment**.
- **Well-documented APIs** are essential.
- **Ethernet and IP-based** protocols recommended.
- **Industry-grade OPC-UA and OpenAPI conform HTTP REST protocols** for communication.

Components

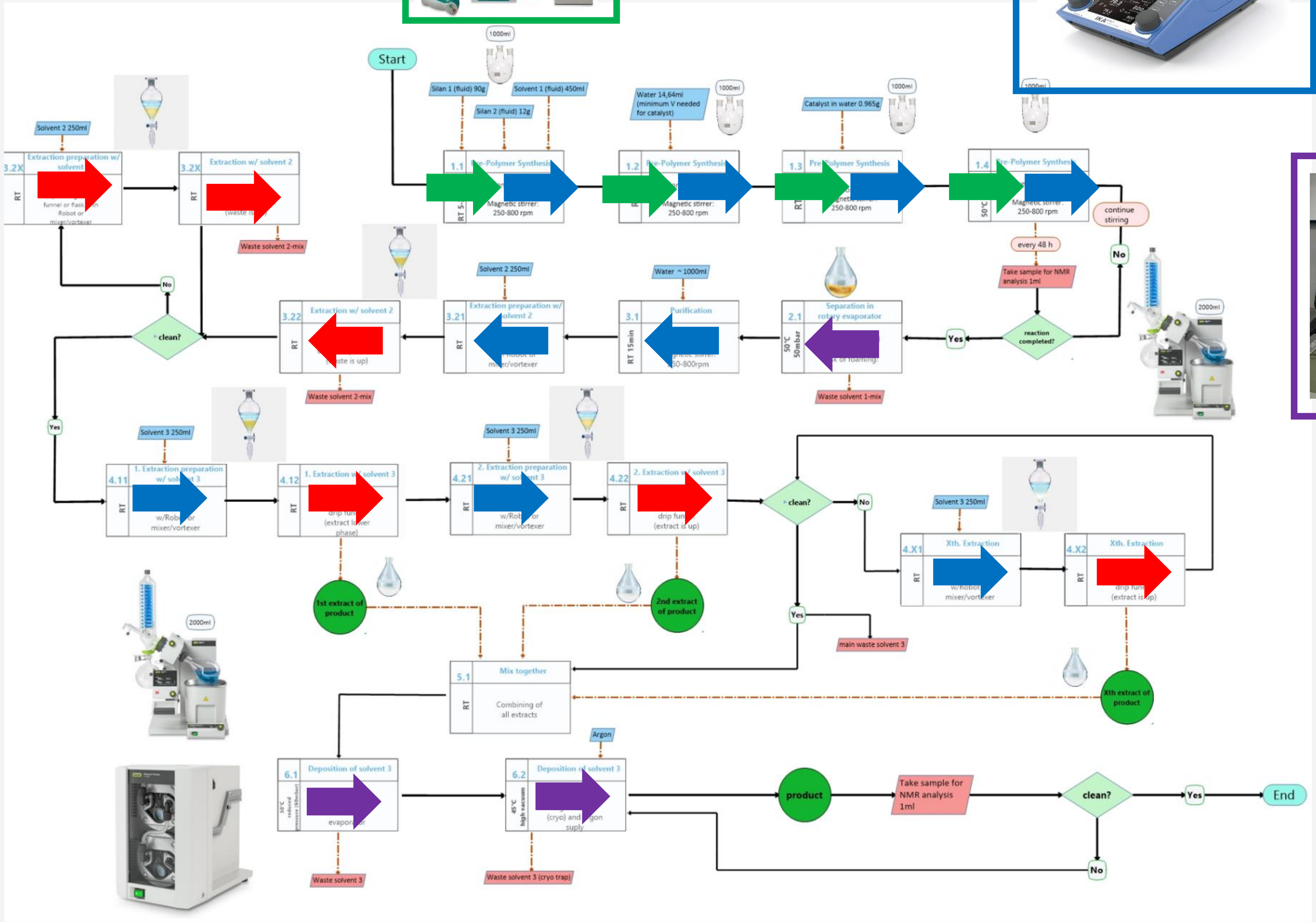
Dosing Units

Mixer-Weight-Heater



Liquid-liquid extraction (LLE)

Rotary Evaporator



Physical Platform Integration

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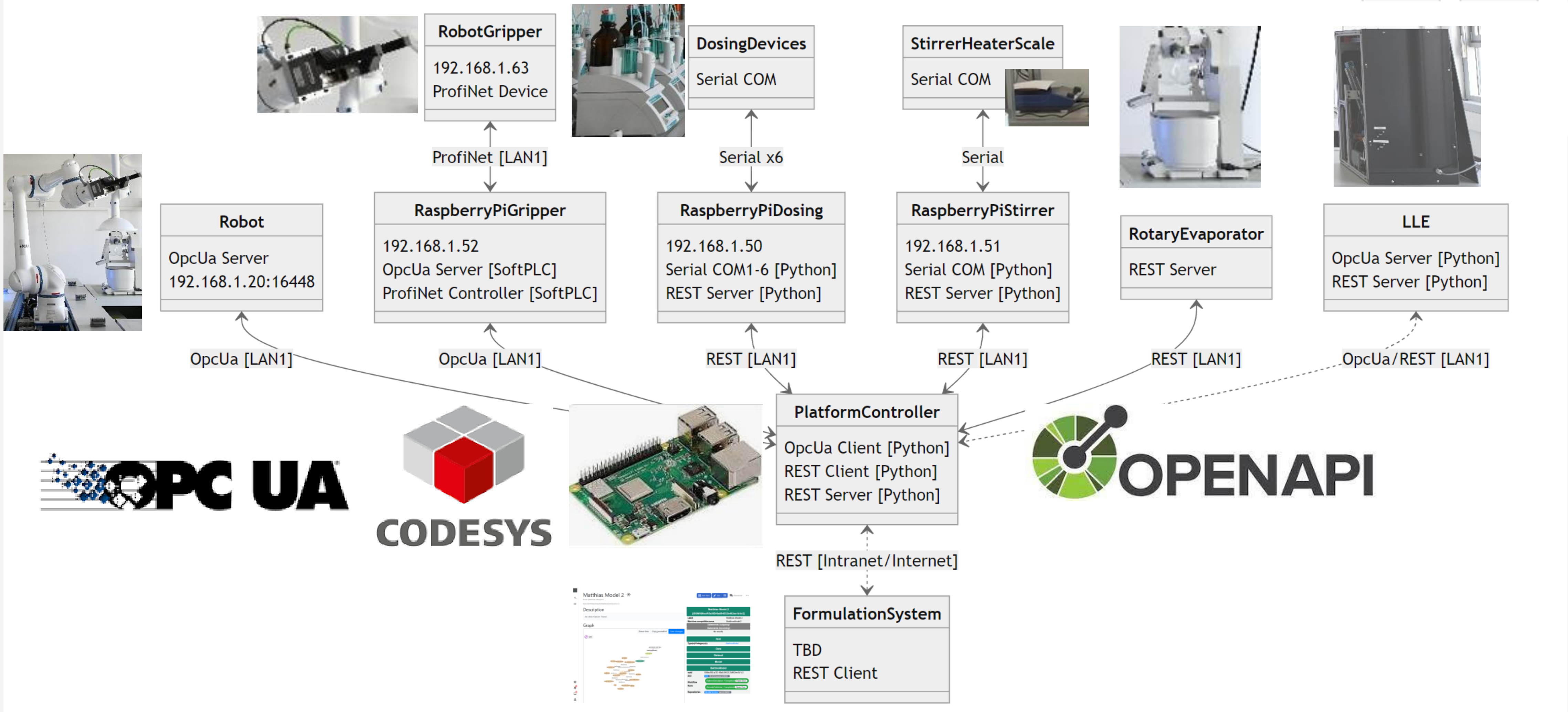
Technical Integration



Building Blocks

Software Infrastructure

- Supports multiple hardware systems, network infrastructure, and cloud platforms.
- Provides flexibility to **scale**, adapt and add functionality.
- Ensures **multi-user access via web interfaces**.
- Emphasizes **security** for data and software hosting.
- **Microservice-based architectures** for workflow orchestration and automation.

Software

- **Planning and Optimization**: AI-driven research process for efficient resource use.
- **Experimental Execution**: Interface between planning modules, lab equipment, and backend system.
- **Predictive Material Modeling and Digital Twins**: Virtual experiments and simulations.
- **Documentation**: Standardized data acquisition and storage.
- **Data Analytics and Insights**: data processing and visualization.

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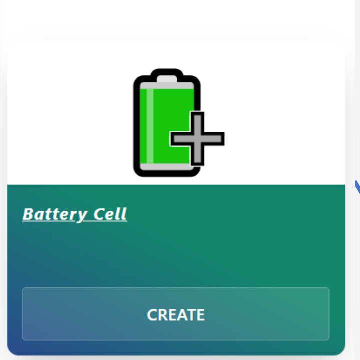
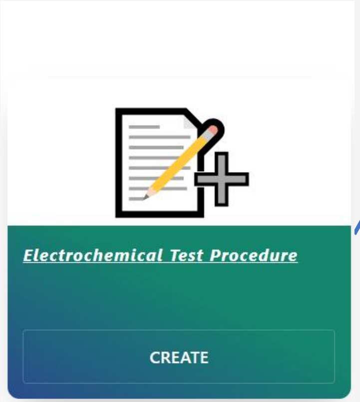
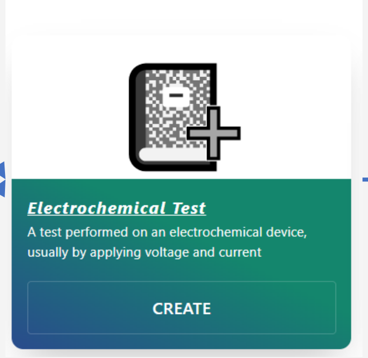
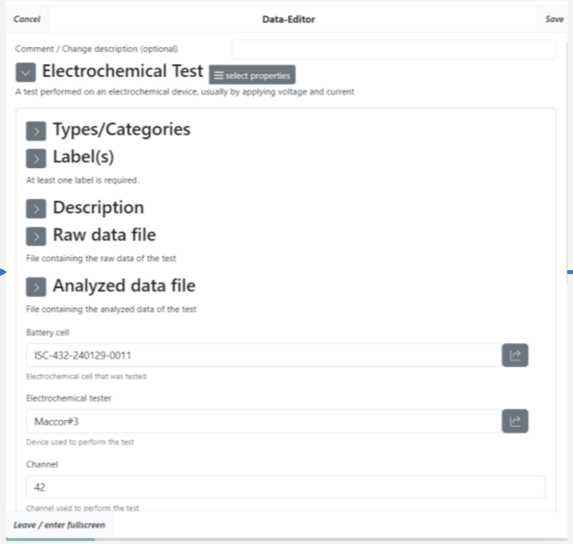
Linked Data Schemas

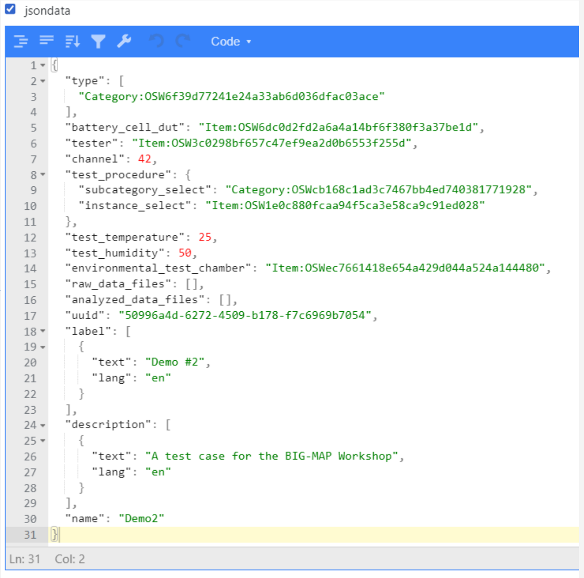
Common Repositories









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    }
  ],
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}
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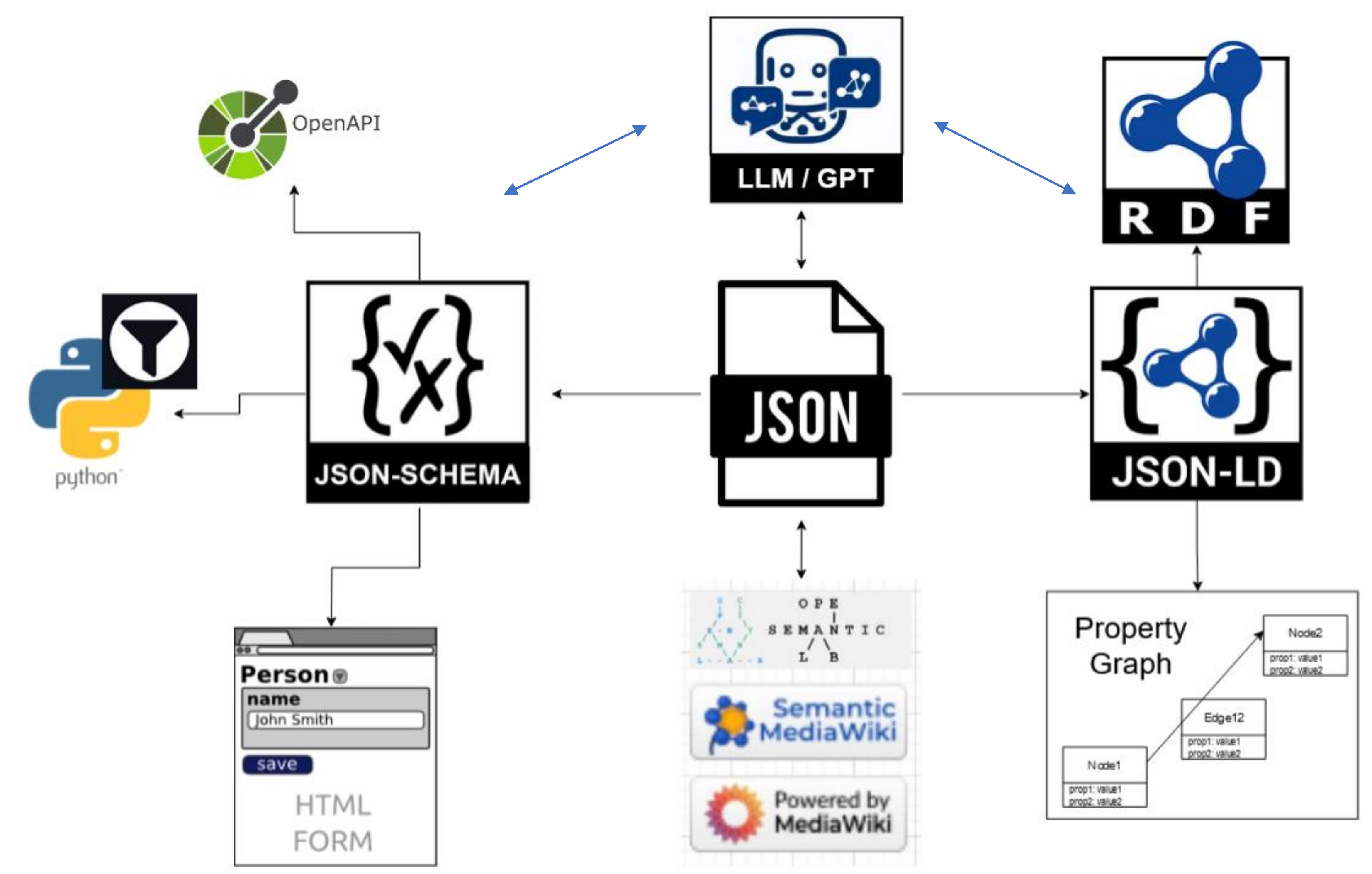
- *… and send to digital workflows*

- independent schemas …
- … Combined to application specific structures
- What you see
- What you create in the background

https://github.com/OO-LD/schema https://oo-ld.github.io/playground-yaml/

The OpenSemanticLab Stack



https://github.com/OpenSemanticLab

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Extract Metadata with AI


```
Time;Crosshead separation;Load;Extensometer elongation
(sec);(mm);(kN);(%)
0;0;0,25459;0,05855
0,1;0,00104;0,2551;0,05854
0,2;0,00284;0,25807;0,0586
0,3;0,00544;0,26516;0,05864
0,4;0,00888;0,28904;0,05871
0,5;0,0136;0,36803;0,0591
0,596;0,01936;0,46857;0,05952
0,678;0,02512;0,56985;0,06006
0,754;0,03116;0,66987;0,06058
0,828;0,03768;0,77193;0,06105
0,926;0,04748;0,87257;0,0614
1,026;0,05908;0,94973;0,06157
1,126;0,07236;1,01332;0,06174
1,226;0,08716;1,0828;0,06216
1,326;0,10336;1,17029;0,06253
1,412;0,11848;1,27039;0,06294
1,49;0,13296;1,37123;0,06332
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1,7;0,176;1,6772;0,06463
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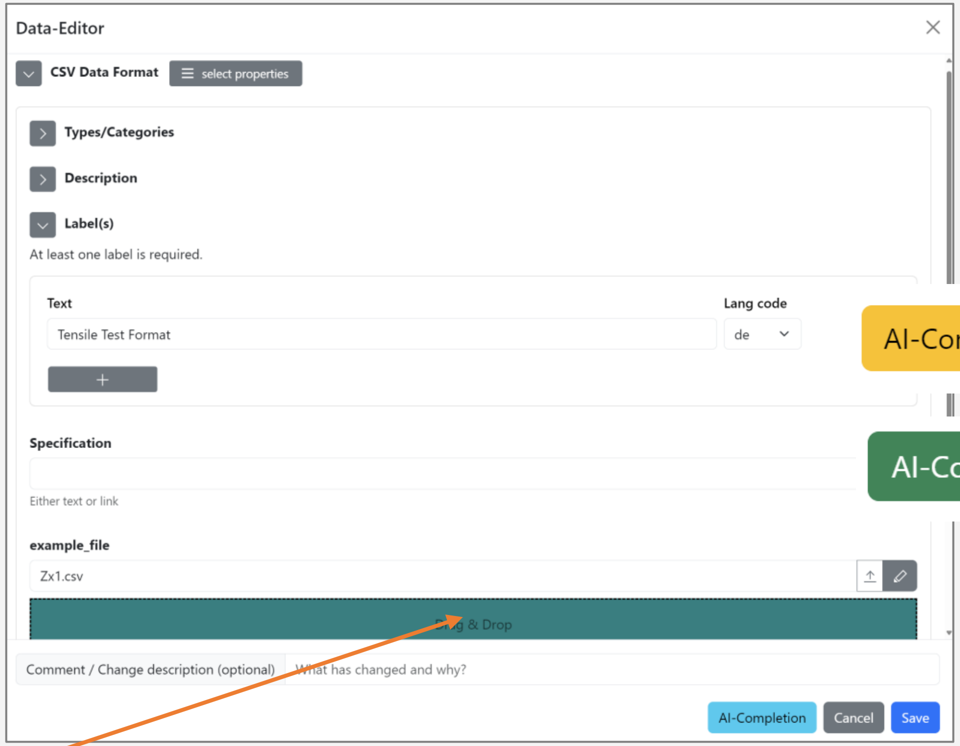

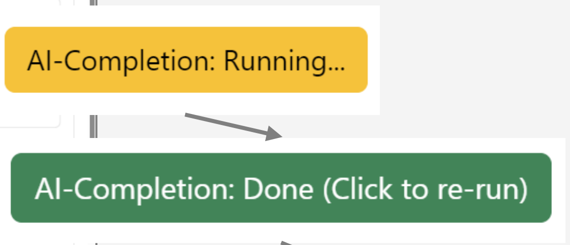

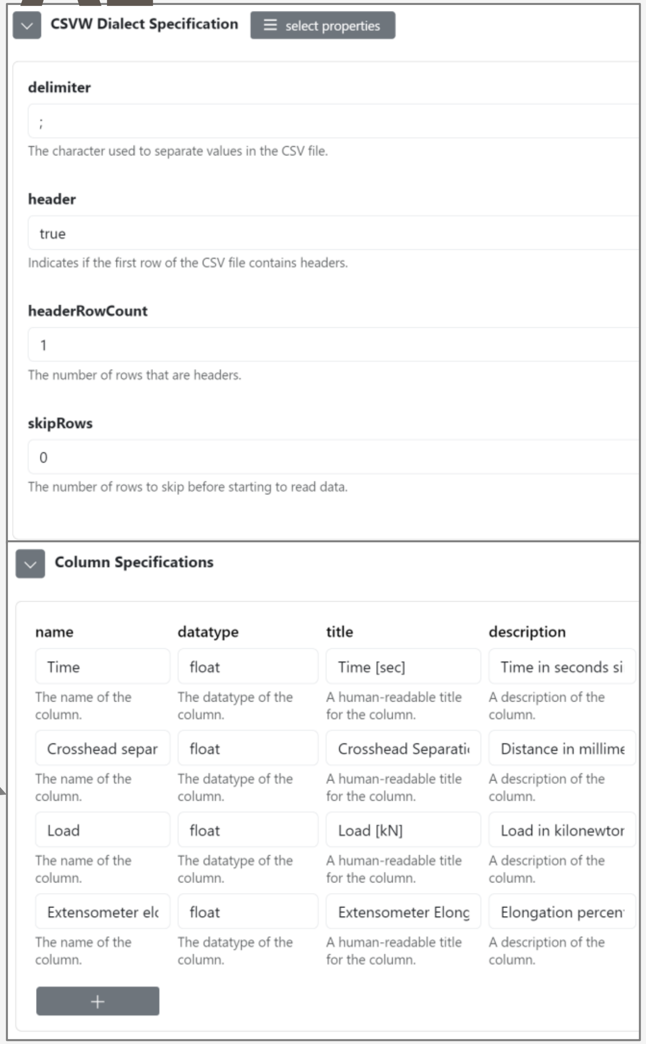

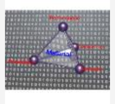

Developed within Mat-o-Lab

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10.12.2024

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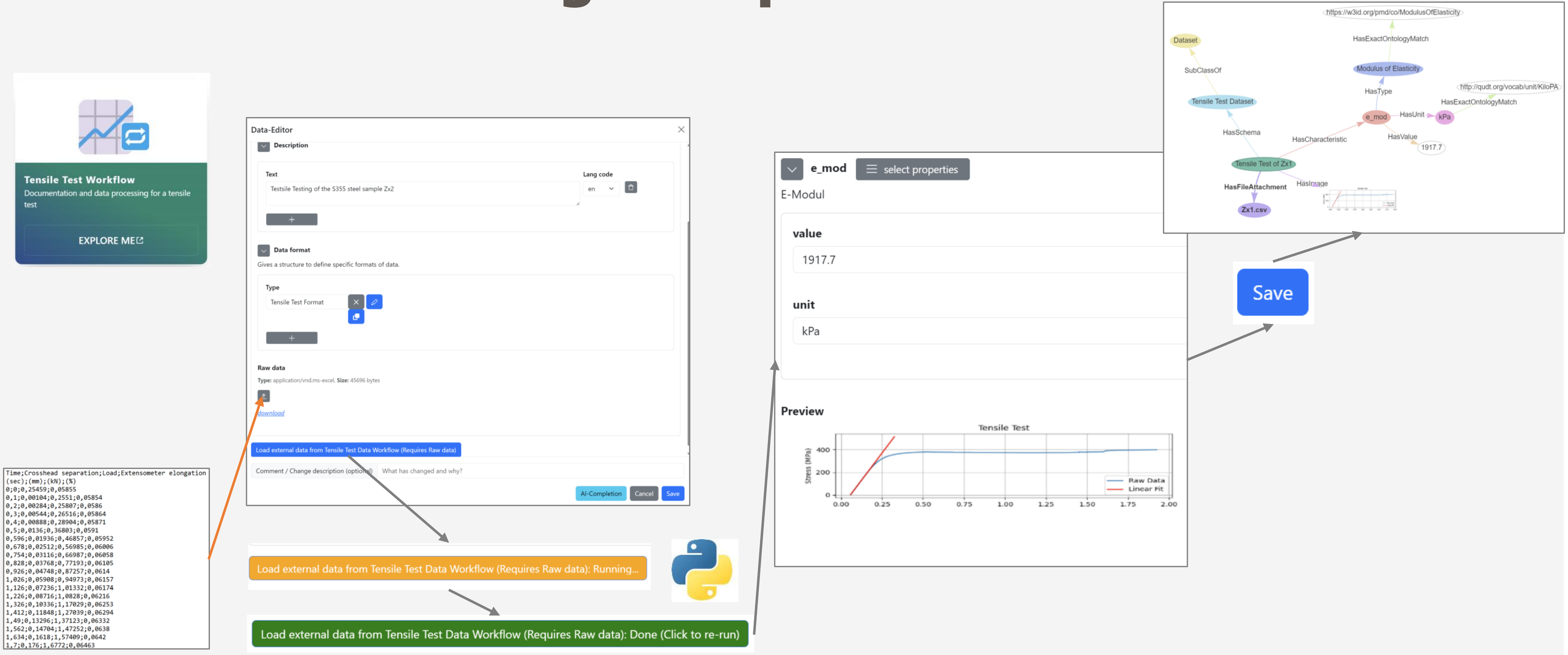
Build Knowledge Graphs within a few clicks



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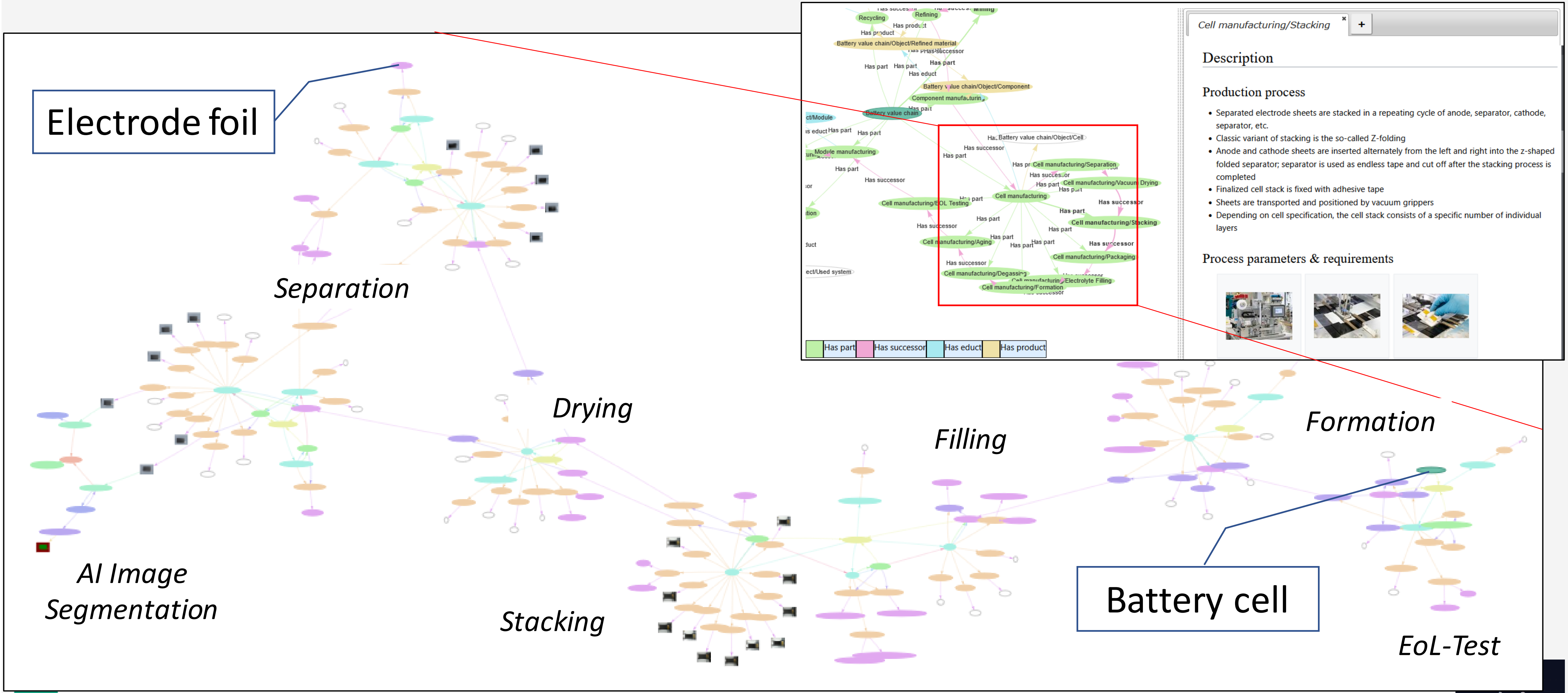
Large Knowledge Graphs from reuseable patterns



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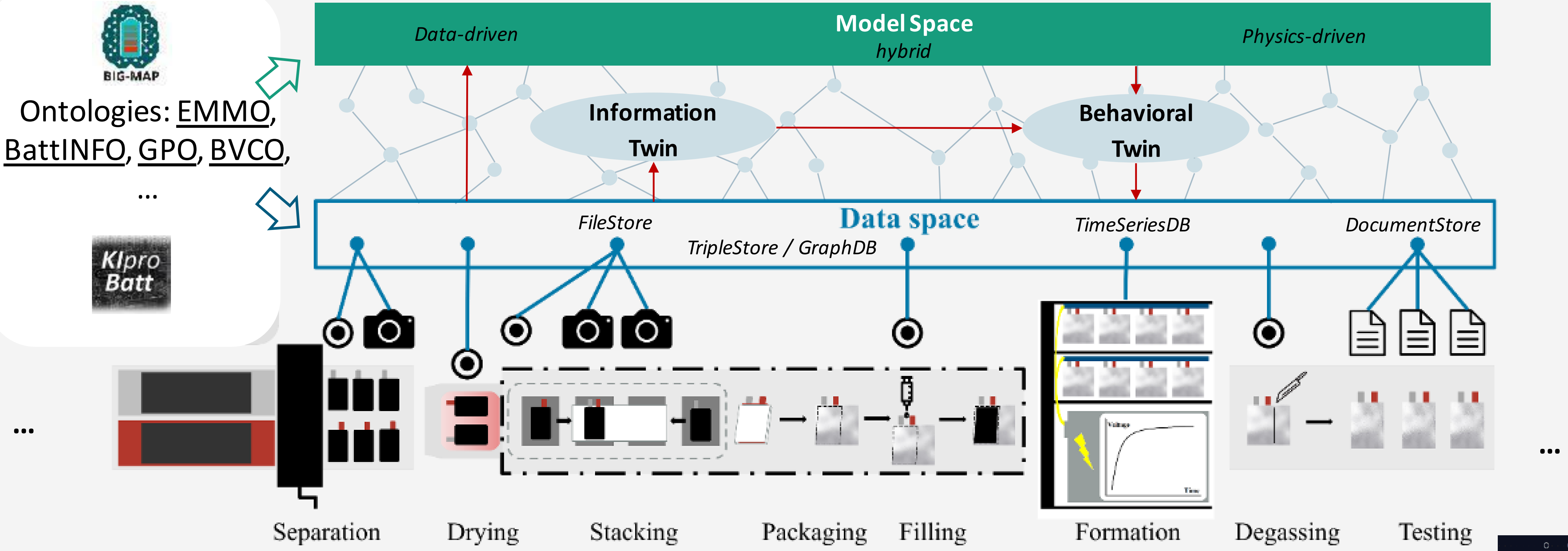
Usecase: Comprehensive Semantic Information Structure in the Battery Value Chain

- Provides the foundation for a seamless coupling of *informational* and *behavioral* digital twin & enables efficient creation and validation of Digital Twins

BIG-MAP

Ontologies: EMMO, BattINFO, GPO, BVCO, …

KIpro Batt



https://kiprobatt.de/wiki

https://doi.org/10.1002/ente.202301305

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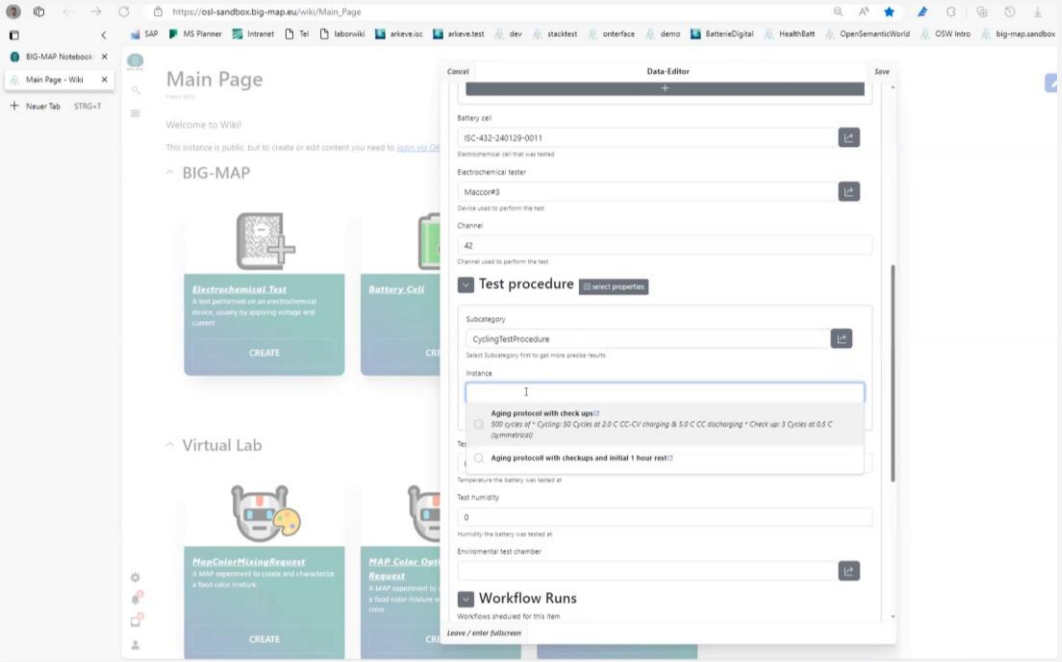
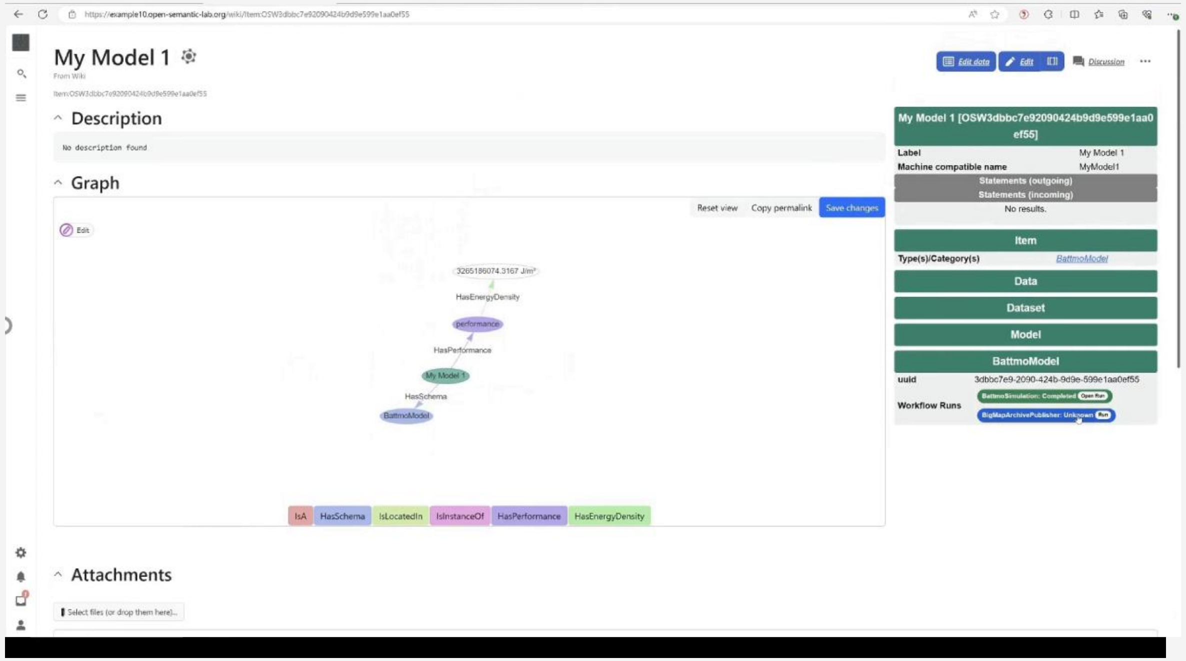
Demonstration





OpenSemanticLab LIMS & ELN Battery Research & more
Video: https://doi.org/10.5281/zenodo.11582036

Run simulations & optimizations
https://onterface.open-semantic-lab.org
Video: https://doi.org/10.5281/zenodo.11582014

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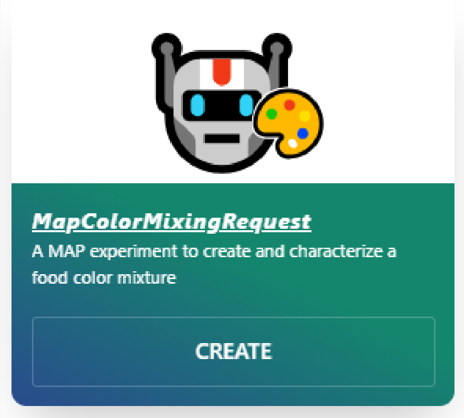
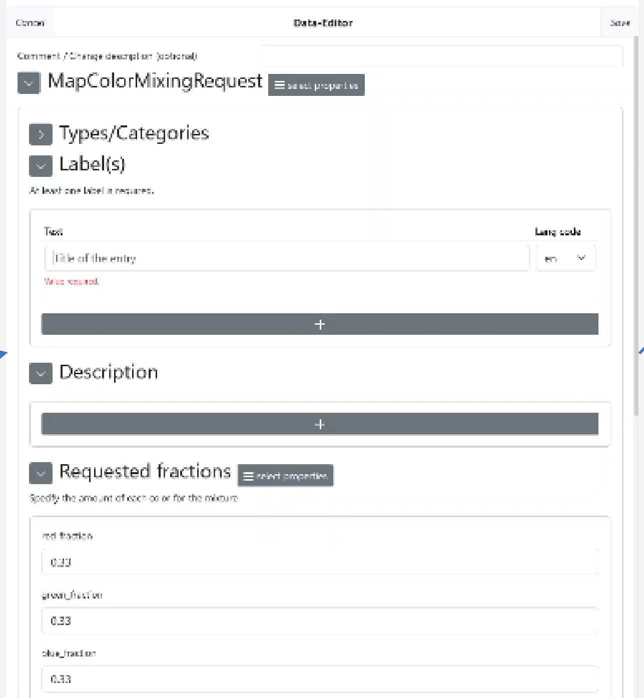
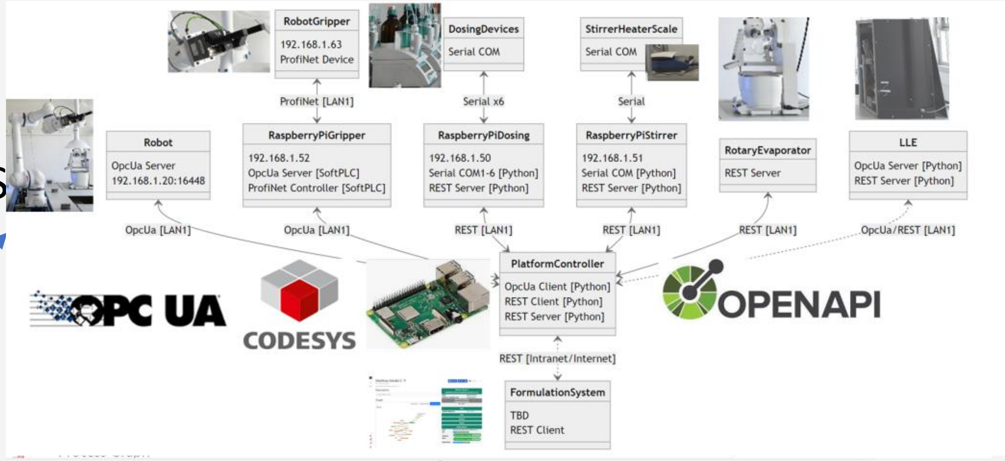
Head of Digital Transformation @ Fraunhofer ISC

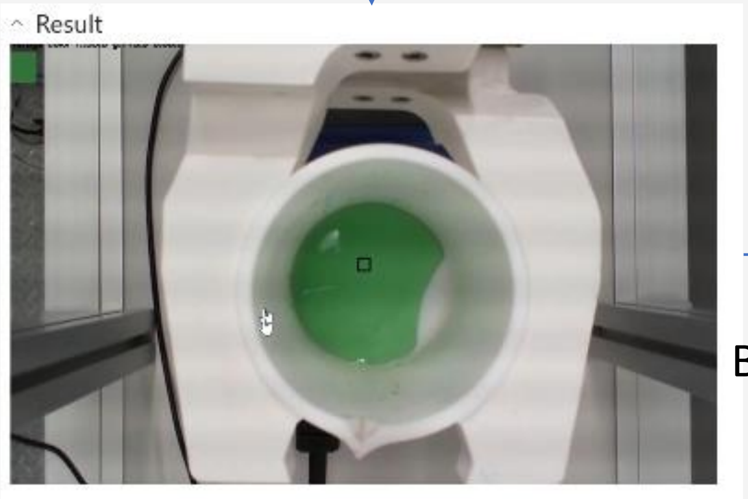
Software-Integration: OpenSemanticLab as MAP-ELN





FINALES





Prefect

BIG-MAP Archive

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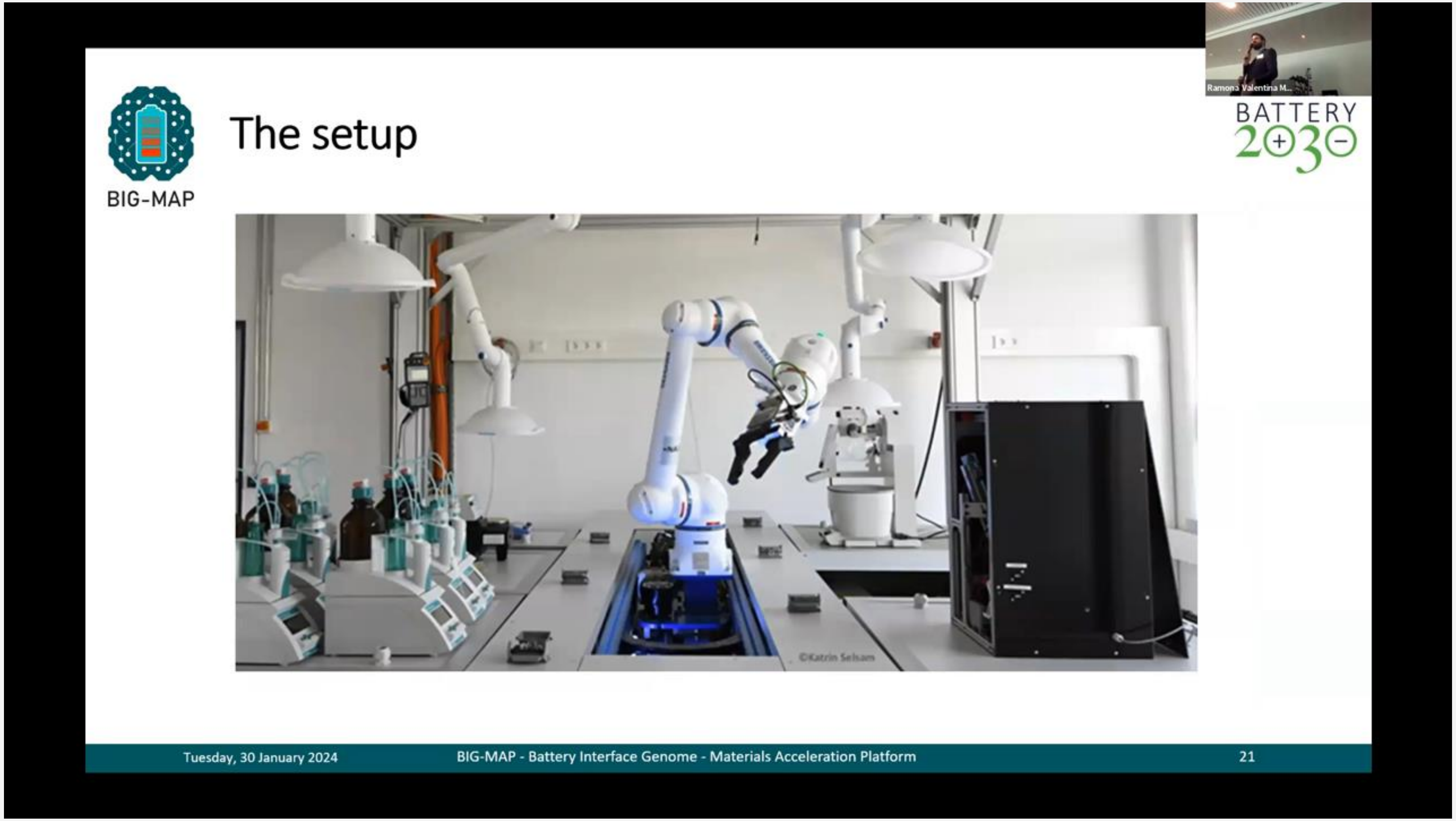
Live Demo during the BIG-MAP Data Workshop in Grindelwald



Video: https://zenodo.org/records/11653808

Building Blocks

Community

- **Governance**: Standards, quality control, and management of automated labs.
- **Create Awareness**: Dissemination of knowledge and success stories.
- **Training and Education**: Adapting R&D programs and ensuring high-quality software and automation modules.
- **Technology Transfer**: Ecosystem for startups and corporations to adopt technology.

Examples of MAP initiatives: BIG-MAP, DIADEM, PSDI, GC-MAC, EU-MACE, EuMINe, M4E, Acceleration Consortium, REACH2, MRS Meetings …

Impact

Scope	Description
Synthesis	High-throughput synthesis using thin films, micro/milli-fluidic tools, and pixelized annealing/sintering for efficient material processing.
Catalysis	Lowering energy costs and reducing waste in material production through improved catalytic materials and processes.
Biotechnology	Enhancing strain engineering speed and efficiency for sustainable product and process development in chemicals and pharmaceuticals.
Bio-sourced Polymers, Hybrids, and Composites	Accelerating monomer discovery and polymer production with advanced functionalities, focusing on recycling and sustainability.
Health, Pharma, and Bio-medicine	Increasing productivity in drug discovery and development through AI-based data analytics and high-throughput approaches.
Energy Materials	Developing novel materials for sustainable energy production and storage to meet increasing demand.
Photovoltaics	Improving efficiency and cost-effectiveness of solar panels through new material development and optimization.
Metamaterials	Accelerating design and fabrication of metamaterials for diverse applications like electrochemistry, membranes, and photonics.
High Entropy Alloys and Oxides	Using automated thermodynamic modeling and high-throughput probing for advanced functionalities in complex material systems.
Materials for Additive Manufacturing	Extending additive manufacturing to diverse material classes and integrating digital twins for enhanced process control.
Per- and Polyfluoroalkyl Substances (PFAS)	Finding alternatives to PFAS in various industries due to health and environmental regulations.
Recycling Processes	Promoting circular economy by optimizing recycling processes for polymers and precious metals to maintain product properties and improve material recovery.

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Impact

- Synchronize material innovation and end-product development
- Enable innovation that maximizes the use of existing assets
- Turn open innovation into societal impact

- **Processing and Manufacturing**
  - Synthesis
  - Additive Manufacturing
  - Recycling Processes (Polymers, Precious Metals)
- **Biotechnology and Health**
  - Bio-sourced Polymers, Hybrids, and Composites
  - Biotechnology
  - Health, Pharma, and Bio-medicine
- **Energy and Catalysis Materials**
  - Energy Storages
  - Photovoltaics
  - Catalysis, CO_2 / H_2
- **Advanced and Functional Materials**
  - Metamaterials
  - High Entropy Alloys and Oxides
  - Per- and Polyfluoroalkyl Substances (PFAS)

- Reduce dependency on raw materials
- Technology Sovereignity
- Green and digital Transition

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Gaps

- **Technological and Organizational Gaps**: Initial implementations of MAPs show potential but face **hurdles in widespread adoption**, requiring coordinated regional, national, and international research strategies.
- **International Collaboration**: Strong international partnerships and collaborations are essential to accelerate materials discovery and innovation, requiring **standardized hardware, communication protocols and ontologies** for distributed MAPs.
- **Education and Training**: Increased awareness, training, and implementation of MAPs are needed to build a **multidisciplinary and collaborative skillset**, with initiatives like international postgraduate programs and specialized training schools.
- **Funding and Research Strategy**: Current funding is insufficient for sustainable MAP development; **dedicated funding programs** are needed to support the **meta-method level**, FAIR and OPEN research results, and the **integration of MAPs with conventional labs** and AI-ready data infrastructures.

Vision: Making Research and Technologie Infrastructure FAIR

… and therefore MAP-ready

Level 1 - **F**indable: Create a machine readable catalogue of available capabilities (services and competences)

Level 2 - **A**ccessible: Define a common protocol to submit requests and deliver results

Level 3 - **I**nteroperable: A common language to describe the request and results datasets

Reusable: Defined legal framework, IP management and automated digital contracts

- Accelerate every process stage

- Strong digital ecosystem with academics and industry

- Both within Europe…

- … and worldwide

R&D Dataspaces

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Thank you for your attention!

More Information: isc.fraunhofer.de/digitale-transformation
github.com/OpenSemanticLab

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