HELMHOLTZ Energy

The Research Field Energy in Helmholtz.

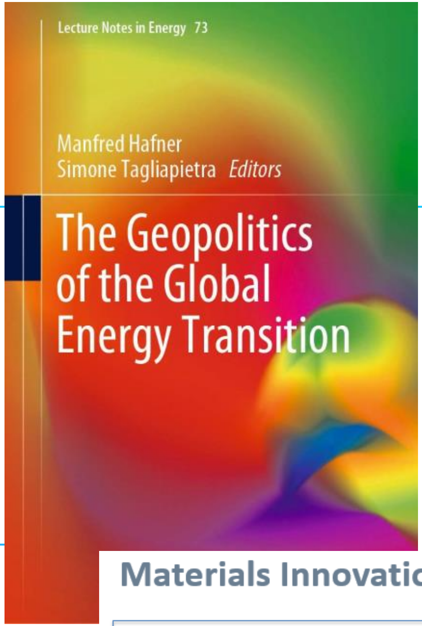
Mission Innovation: **Materials for Energy -M4E**

Holger Ihssen

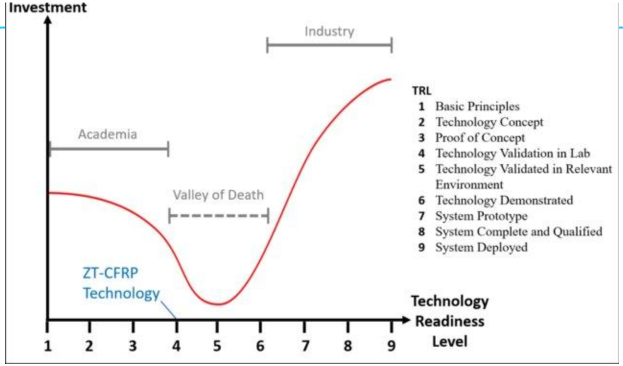
M- ERA-net Meeting in Paris **17.09.2024**

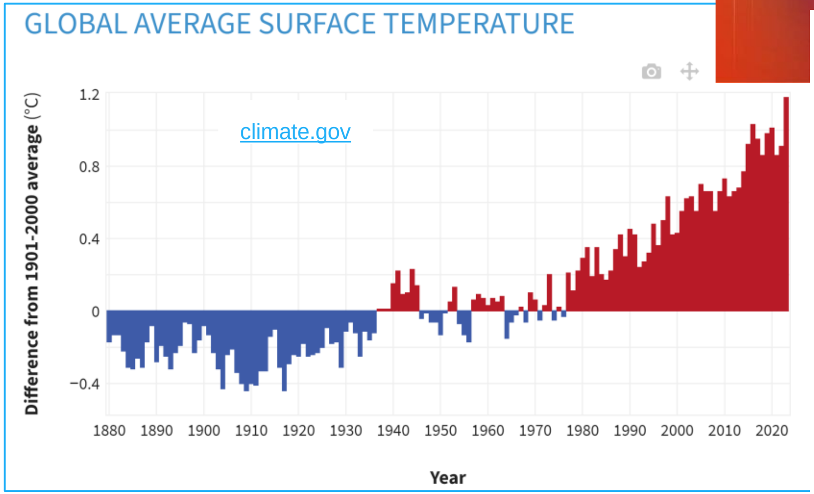
Global Drivers

- Climate change mitigation
- Sustainability and circularity
- Economic resilience
- Geopolitical context

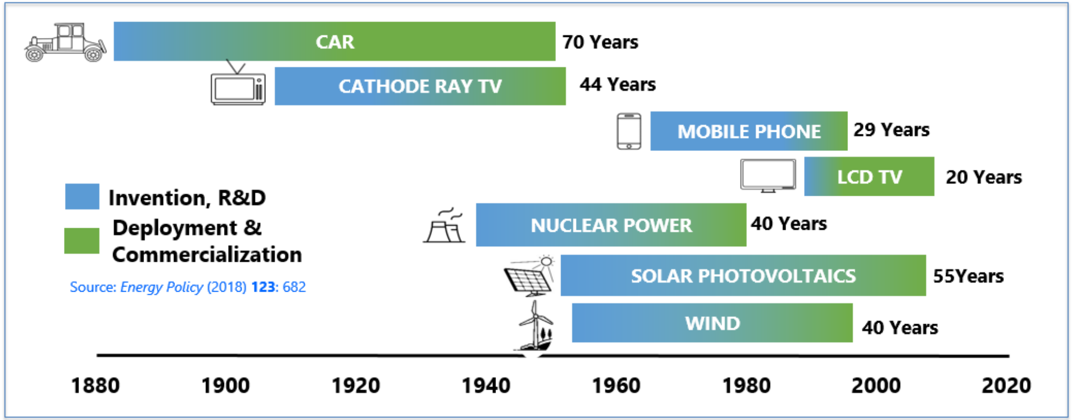


We need new **Solutions / Devices** much faster





Materials Innovation Cycles take Decades



Advanced Materials for Industrial Leadership

CHALLENGES TO BE ADDRESSED

- **Long innovation processes and an insufficient level of digitalisation**
- **A lack of testing and experimentation facilities**
- **Fragmentation of the R&I ecosystem**
- Increasing circularity and material efficiency needs
- Disconnect between innovative research and uptake in industry
- A lack of skills
- Increasing private investment needs
- Need for harmonised standards

Communication

Report

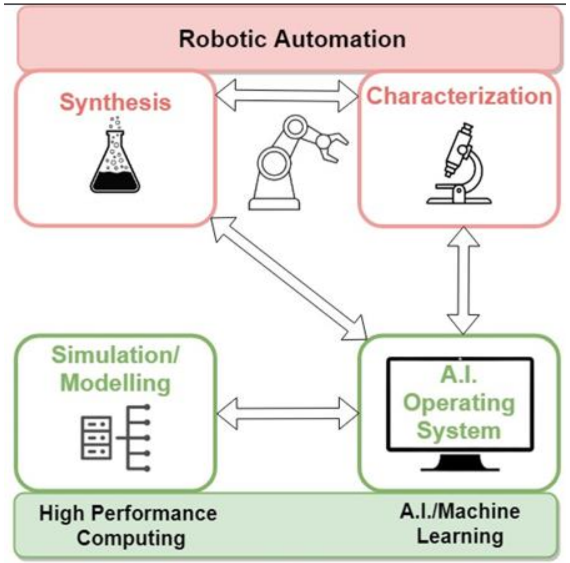
From 2024

- Mission Innovation (MI) was launched during COP21 under the United Nations Framework Convention on Climate Change, UN FCCC, 2015
- The Clean Energy Materials Innovation Challenge, IC6, was 1 of 8 innovation challenges to address climate change under MI, 2017
- IC6 became Materials for Energy, **M4E**, under the second MI mandate, 2021
  - **M4E** has the objective to accelerate energy materials **innovation** through **Materials Acceleration Platforms (MAPs)** – self-driving materials laboratories

ME4 has 3 Co-leads:

Materials Acceleration Platforms
Self-Driving/Autonomous Materials Laboratories

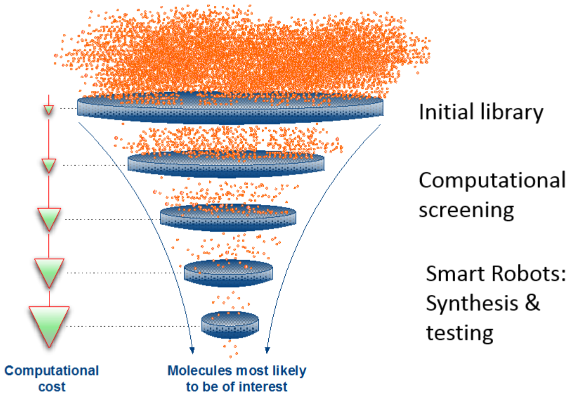
MISSION INNOVATION



ACCELERATION >10X

- Closed-loop characterization, synthesis and experimental planning
- Smart robotic automation
- Accelerated simulation/modeling through artificial intelligence

- Develop novel materials and devices



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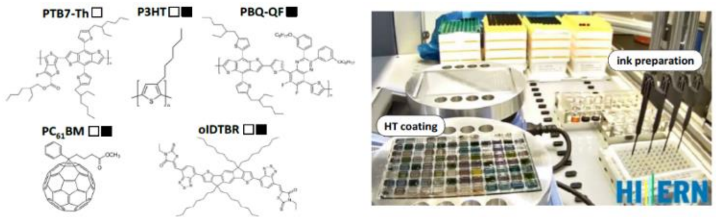
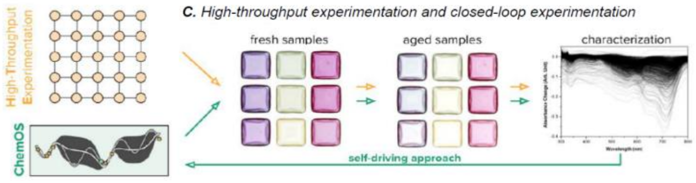
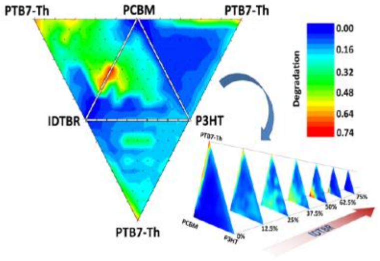
AMANDA

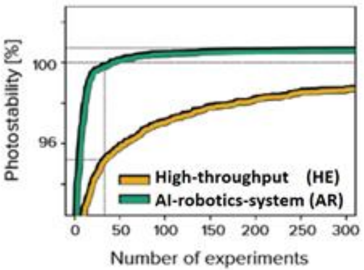
- Autonomous Materials and Device Application Platform
  - Optimization of OPV light stability







S. Langner, *et al*., **Beyond Ternary OPV: High-Throughput Experimentat and Self-Driving Laboratories Optimize Mu Component Systems**. (20
[arXiv:1909.03511](https://arxiv.org/abs/1909.03511)



	HE	AR	Advantages
Samples	1022	30	34 x faster
Throughput	2 blends/week	9 blends/week	4.5 x faster
Consumption	ca. 15 mg material ca. 100 ml solvent	ca. 0.9 mg material ca. 6 ml solvent	16.7 x material savings

GERMAN-CANADIAN MATERIALS ACCELERATION CENTRE

- 5-year bilateral collaborative project (2021-26)
- Ongoing impactful materials science to push key technologies discovery to scale-up, across 5 work packages
  - Electrolysers for H_2 production and CO_2 conversion
  - Education & Training
- Focus on accelerated materials discovery and development – as imagined in the Clean Energy Materials Innovation Challenge of Mission Innovation
- GCMAC initiated several new MAP activities in academia and industry

€6M Program value

40+ Experts & talent pool

5 Technical work packages

5 Online Workshops

5 Internal review & advisory board meetings

1 German –Canadian Industry Days Event

2 Summer Schools

3 Key accelerated technology demonstrations

7 Partner Institutions

21 HQP and Trainees

7 Broader network linkages

Funded by Bundesministerium für Bildung und Forschung

JÜLICH Forschungszentrum

KIT Karlsruher Institut für Technologie

Natural Resources Canada

Canada

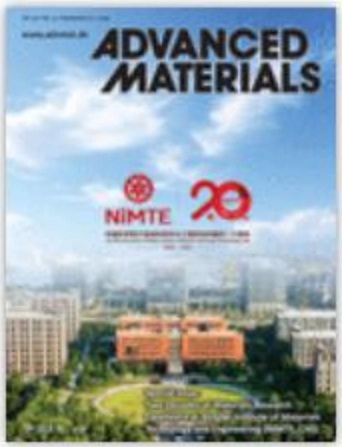
NRC·CNRC

Energy

Community Publication on MAPs is Discussing

- Advantages of MAPs
  - Closed loop and FAIR data => Also process information is stored.
    => All results are reproducible.
  - Decentralized and modular => Allows a global community to contribute.
    => **A complete new way of research and innovation management.**
- List many research projects and initiatves
- Academic and industry research frameworks
- Building blocks // hardware, software, protocols, interfaces, HPC and community
- Impact
- Gaps
  - Compatible infrastructure, data structures and sharing
  - Standardized software for distributed MAPs
  - Make existing labs „MAP“ ready
  - Education & Training
  - IP ownership

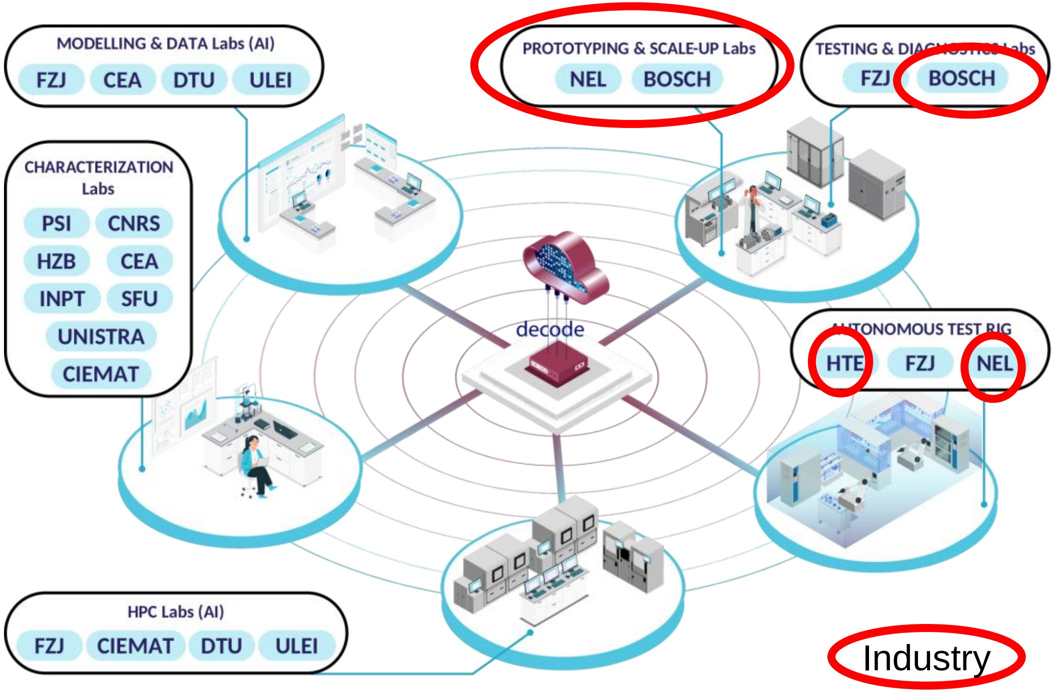
https://onlinelibrary.wiley.com/doi/10.1002/adma.202407791



The next Step : The DECODE project

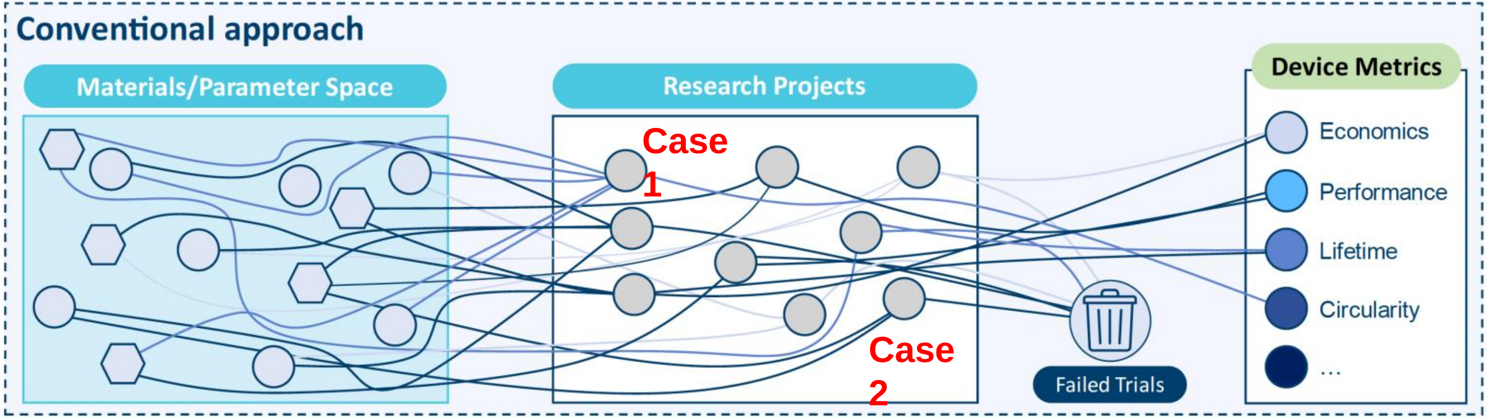
- **DECODE** aspires to revolutionize the process, by which **materials for clean energy technologies** are developed, **integrated**, and **assessed**.

- **DECODEs main focus is on PEM electrolysers.**

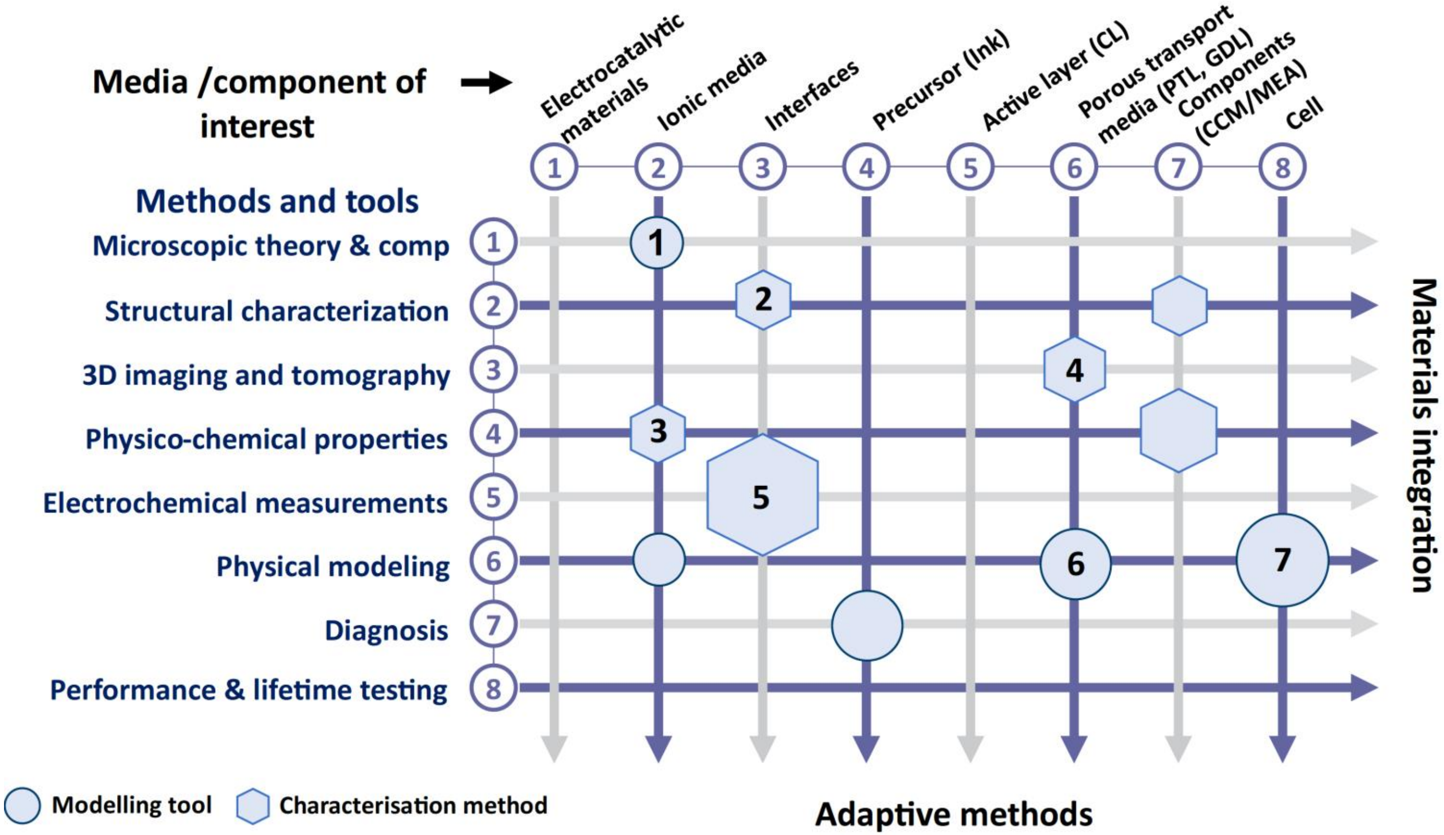


- **Computing infrastructure, RI** and **TRI** are needed
- **Industry is of key importance !**

From Conventional Approach …

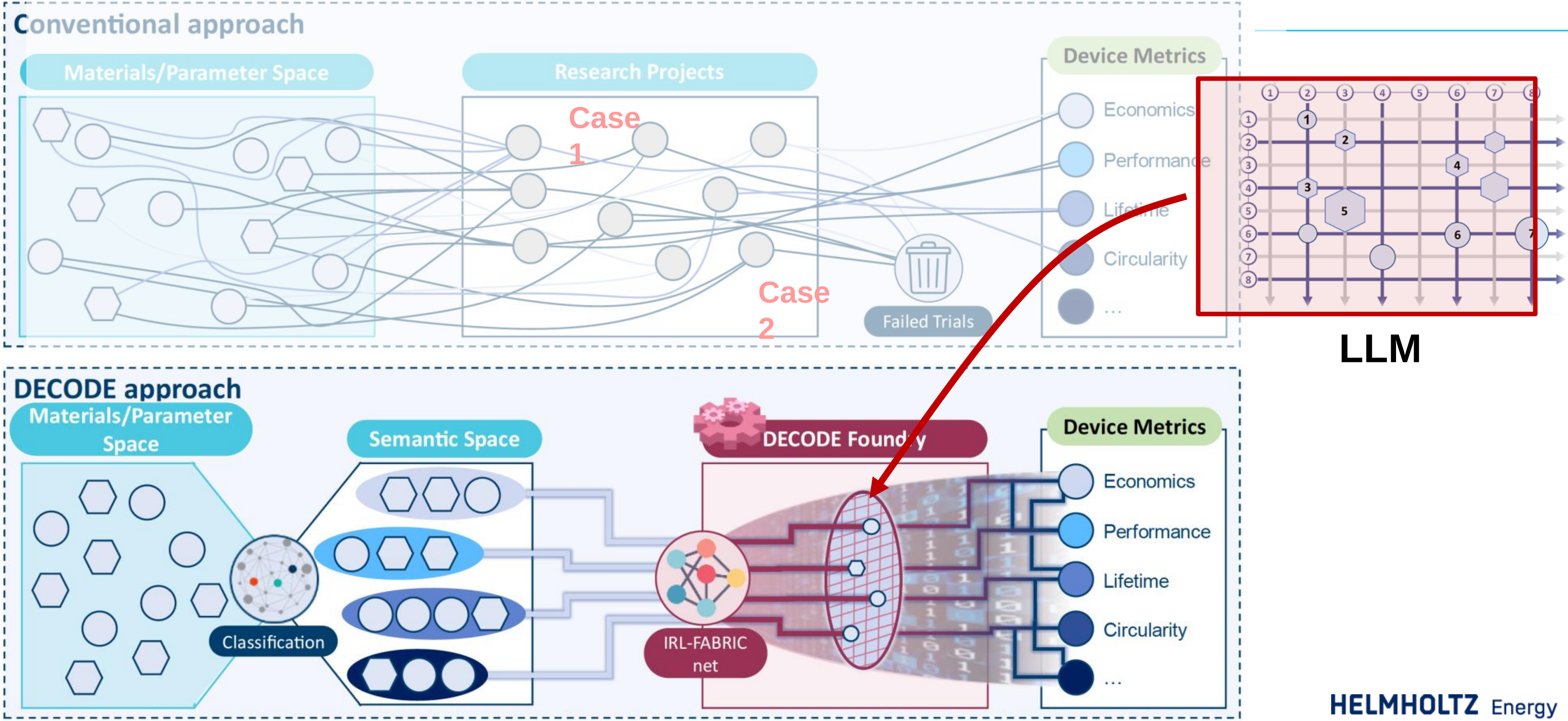


How to not get lost in integration and scale-up?

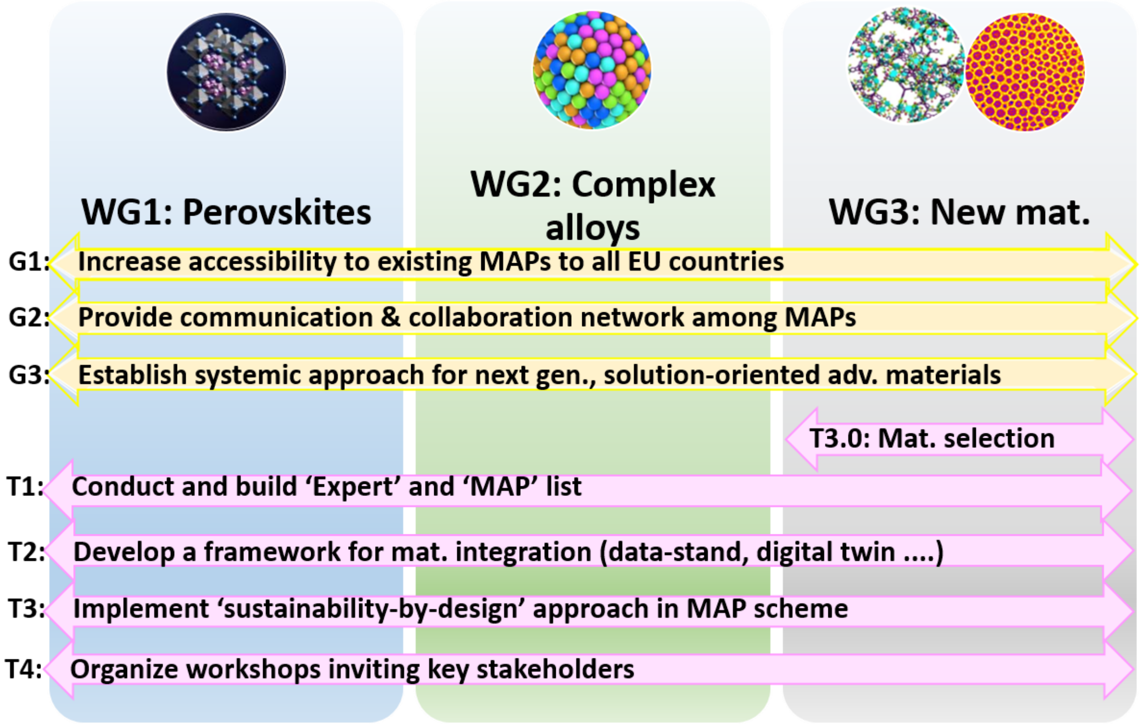


Develop and implement an orchestrated process

From Conventional Approach to DECODE



Network Development I
COST Project : European Materials Acceleration Center for Energy



Focus on ITC countries

Network Development II
RISEnergy : Research Infrastructure Services for Renewable Energy

RISEnergy

EXTENDED NETWORK

84 Research infrastructures from 69 Institutions

- in 8 renewable Energy Technologies and 2 Cross-Cutting areas.

Consortium:

- 17 Partner, 37 Affiliated Entities und 15 Subcontractors

Energy technologies:

- photovoltaics (PV), concentrated solar power/solar thermal energy (CSP/STE), hydrogen, biofuels, offshore wind, ocean energy (waves and tides), integrated grids and energy storage,

Cross technology areas:

- materials research
- information and communication technologies

Budget: 14,5 M€, 2/3 on transnational and virtual access

[Homepage - (risenergy-project.eu)](risenergy-project.eu)

International Cooperation, Transnational Access

- Organizations:

EERA European Energy Research Alliance
eera-set.eu/

eu-mace COST Action CA22123

RISEnergy
eera-energystorage.eu

StoRIES
https://www.storiesproject.eu/

FRANCE 2030 PROGRAMME DE RECHERCHE MATÉRIAUX ÉMERGENTS

EMIRI
emiri.eu/

Materials for Energy, M4E

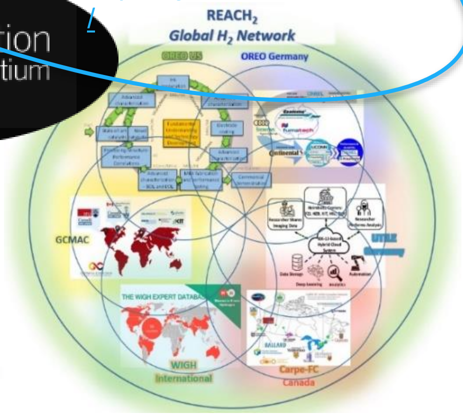
AMI2030 ADVANCED MATERIALS INITIATIVE
https://www.ami2030.eu/

IAM-I

EurA®
eura-ag.com/

gcmac GERMAN-CANADIAN MATERIALS ACCELARATION CENTRE
https://gcmac.ca/

Acceleration Consortium



- Industry:

MIRU smart technologies

BC RESEARCH

TELESCOPE INNOVATIONS

ATINARY ENABLING SELF-DRIVING LABORATORIES

hte

NSF National Science Foundation

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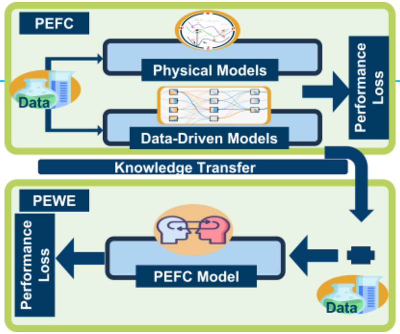
Thank You for Listening

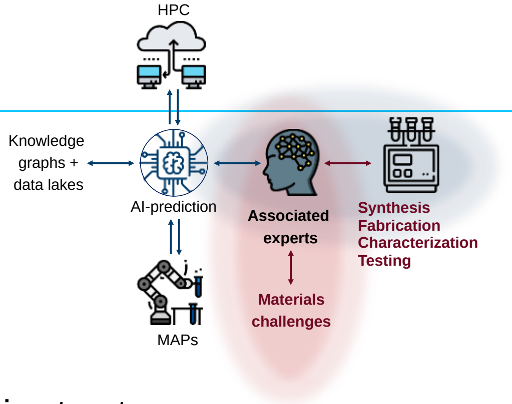
Closing the loop on energy materials



lifetime-performance evaluation

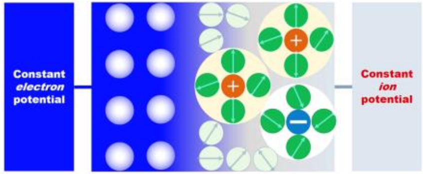
Device modeling

artificial materials intelligence



Ab initio simulations

atomistic structure and dynamics

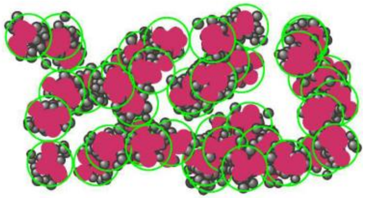


Classical simulations

self-organization: films, phases, interfaces

Mean-field theory

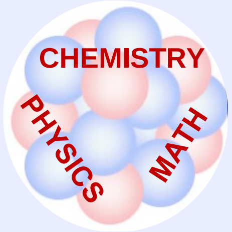
microstructure vs. properties



Statistical physics

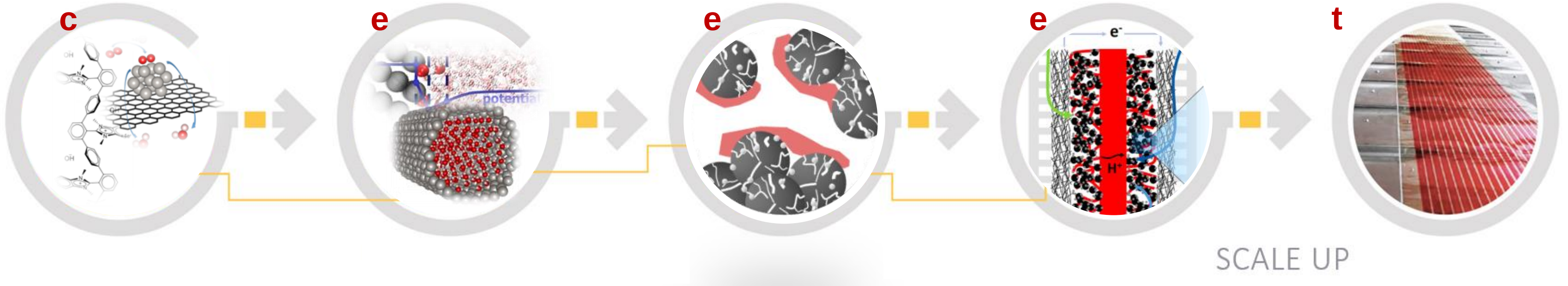
diagnostic methods and tools

Continuum modeling



Acceleration: where and how?

Intrinsic | Microscale | Mesoscale | Macroscale | Device/Product



Integration

scale-to-scale | component-to-component | lab-to-lab

- theory, modeling & simulation
- autonomous labs
- AI-enabled materials design
- automated fabrication & characterization
- data handling and workflow orchestration

Diverse Energy Materials of Interest

- **Organic thin films**: hole transport materials (organic solar cells)
- **High temp materials:** thermoelectric materials, high entropy alloys, etc.
- **Electrocatalysts, electrolysers**: O_2, H_2 production and CO_2 conversion
- **Batteries**: Lithium and alternative formulations
- **Thermal storage:** phase change materials / thermochemical materials
- **Additive manufacturing:** metal powder/wire 3D printing
- **Structural materials:** aluminum, steel cement and concrete
- **Traditional electrochemistry:** Corrosion/Electroplating
- **Thin Film PVD:** multi-metal target systems
- **Magnetic materials:** Neodymium replacements
- **Structural joining:** welding, brazing, soldering, adhesives