DIGITALIZATION OF BATTERIES FOR SMART ENERGY AND TRANSPORT SYSTEMS

Workshop co-organised by BATTERIES EUROPE, ETIP SNET and EGVIA

5 May 2021

Keynote speech

Cristobal Irazoqui
Policy Officer (DG ENER)

Saki Gerassis Davite
Policy Officer (DG MOVE)

Shaping the Energy Transformation in Europe with Digital Batteries (integrated in the energy system)

Maher Chebbo

Ctechnologys/Digitalization Task Force Chair Batteries Europe ETIP

European Commission

BATTERIES EUROPE

EUROPEAN **TECHNOLOGY** AND **INNOVATION** PLATFORM

What do these cities have in common ?

Denmark

Amsterdam

Paris

Helsinki

London

Barcelona

European Commission

Energy Transition investments

BATTERIES EUROPE
EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM

Climate investments

- *1 trillion € Green Deal*
- *30-35 B€ for Climate & Energy (out of 100 B€ Horizon Europe)*
- *10 B€ Innovation Fund*

EVs & Batteries

- *250 B$ annual market from 2025 (European Battery Alliance setup in 2017)*
- *60 B$ for producing Electrical Vehicles and Batteries secured in 2019 in EU*

Energy Efficiency

- *236 B$ Energy Efficiency investments in 2017*
- *29 B$ ESCO market*
- *27 B$ spending on Energy Efficiency Incentives in 16 major economies*

Energy as a Service (EaaS) for C&I : *70 B$ in 2017 growing to 250 B$ in 2026*

Energy Management Systems (EMS) : *44 B$ by 2020*

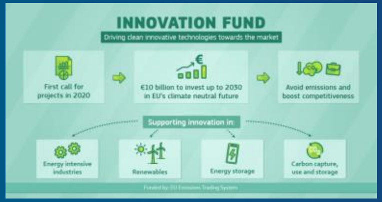
Residential IOT (including Smart Thermostats) : *$1.1B in 2016 growing to $4.4B in 2025 (CAGR 16.7%)*

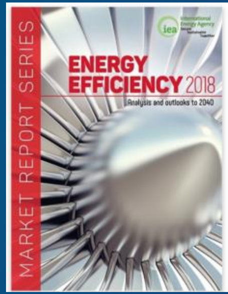
C&I and Residential IOT Platform : *40 B$ growing to 140 B$ in 2025*

DER : *110 B$ in 2017 growing to 375 B$ in 2026*

Smart Cities : *80 B$ in 2018 growing to 135 B$ in 2021 (IDC)*

Green Deal





2020 targets → 2030 targets → 2050 targets → Decarbonized

3D, Electrification & Impact on Technology

DECARBONIZATION

RENEWABLES **~60%** of installed capacity by 2026

IMPACT ON TECH

- Growing share of renewables an increasing challenge to the traditional power system model

DIGITIZATION

An Incremental **$2 Trillion** of value can be unlocked

IMPACT ON TECH

- Data integrity, cyber security, real time decision making, autonomous optimization

DECENTRALIZATION

~900MW Connected DER Capacity by 2026*

IMPACT ON TECH

- End users become active actors of the power system (Prosumer) growing grid complexity

ELECTRIFICATION

Electricity **~ 41%** total energy demand by 2050**

IMPACT ON TECH

- Step increase in electricity consumption, improve network capacity utilization through transactions

European Commission

DIGITAL & GREEN e-Mobility landscape

BATTERIES EUROPE
EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM

ROAD TRANSPORT LANDSCAPE

Jobs & Growth for Europe

ERTRAC
EPoSS European Technology Platform on Smart Systems Integration
ETIP SNET
alice Alliance for Logistics Innovation through Collaboration in Europe
EGVI European Green Vehicles Initiative

Green Mobility Goals

Electrification and Decarbonization

- Electric vehicles available to customers at similar cost level as conventional vehicles (TCO)
- Drop-in zero net carbon energy carriers for road transport
- Electrified vehicles with an active role on the electrical system

Batteries

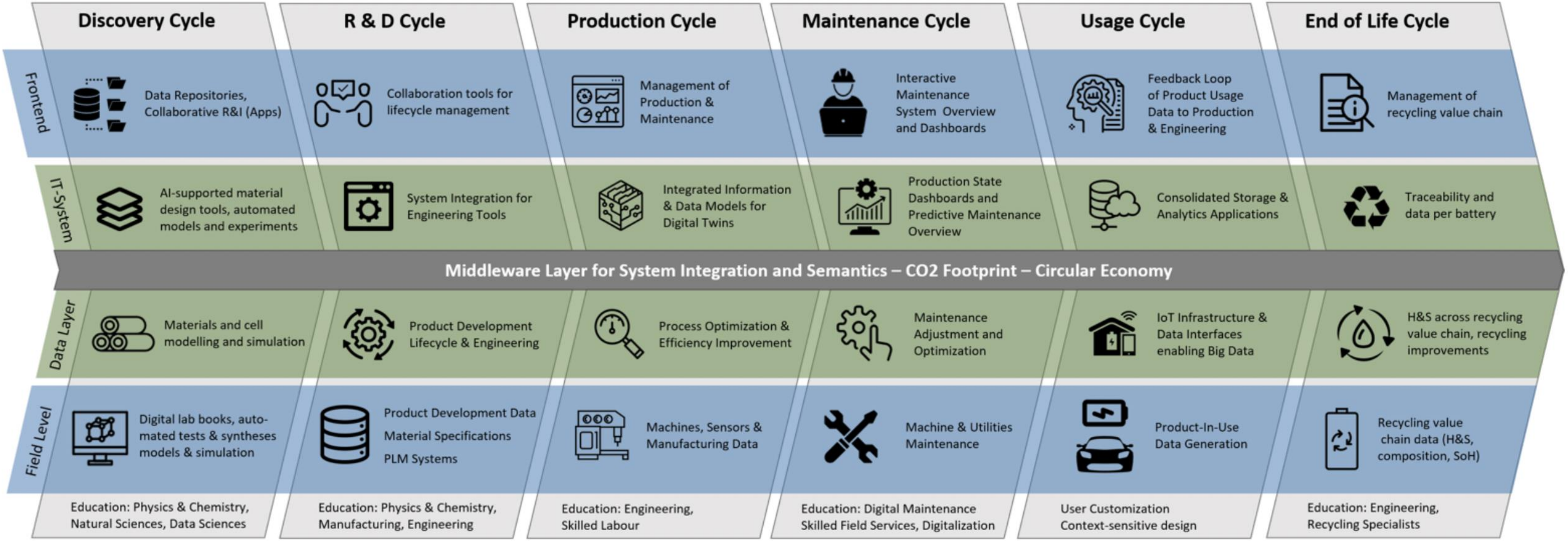
- Competitive and sustainable development and production of battery systems in Europe
- Decrease dependency on scarce raw materials
- Eco-design towards fully recyclable batteries

Connected Automated Driving and Safety

- Reaching automated driving level 4 for mass market
- Self driving vehicles for dedicated applications
- Improved overall traffic safety by using Connected Automated Driving technologies

Digital innovations across the Batteries Value Chain

BATTERIES EUROPE
EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM



Digital Batteries enabling technologies

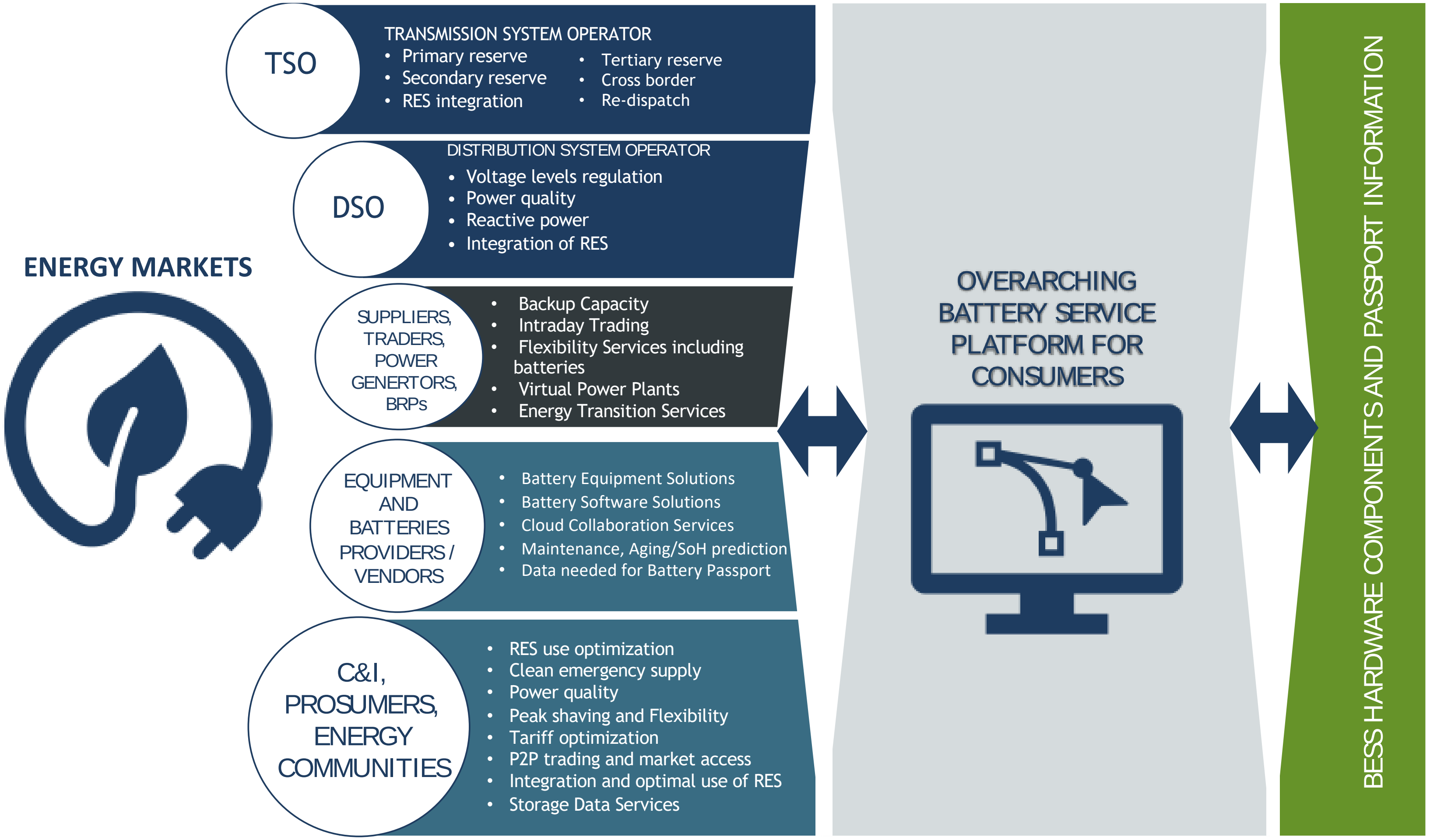
Technology	Readiness	EU Competitive Advantage	R&I Investment required	Budget	KPI example
CAE for Modelling & Simulation	++	++	++	40M€	% Model accuracy vs measurements, reduction in computational time and reduction in product time to market
Design of Experiments	++	++	+	15M€	#Relationships Established between parameters
ML Algorithms / AI	+	+++	++	40M€	% Level of prediction, reduction in time
Data Infrastructure	+	+++	++	25M€	#Test Data, #Organizations sharing information
(Big) Data Analytics	++	++	++	25M€	#Analytics programs, Amount of Data proceeded
Digital Twin[1]	+	+++	+++	60M€	% Accuracy of Digital Twins vs. real Batteries / Production Lines
Wireless Communication	++	+	+	15M€	#Data flow through wireless communication

Digital Batteries Use Cases

Use Case	Feasibility	Impact	R&I Investment required	Budget	KPIs Example
Automated materials discovery	+	++	+++	100 M€	- Number of new battery chemistries Discovered - Cost of Discovery and development of new battery materials - Number of materials developed in a time period - Lead time for material development
Green Battery Passport & digital referential	+++	+++	++	45M€	- % of batteries that go to the second life market - % of Savings in the Design and Development cycles - % of cost avoided related to health and safety along the whole battery value chain
Advanced methods for SoX now- and forecasting (sensors & big-data)	++	++	++	20M€	- Number and models of batteries with initialization problems - % of batteries with maintenance needs above the normal maintenance range
Hybridization of battery energy storage systems (BESS) into flexible portfolios	+++	+++	++	50M€	- % of use of renewable energy in BESS - % of battery users who monetize their energy storage
Accurate datasheet generator based on application specific Big Data Simulation Platform	++	++	++	30M€	- % of elements changed over original design in production phase - % of batteries with a lower life than the forecasted one
Digitalization of the battery cell production	+++	+++	++	50M€	- % savings in producing batteries with digital twin developed in the design and development phase vs without digital twin

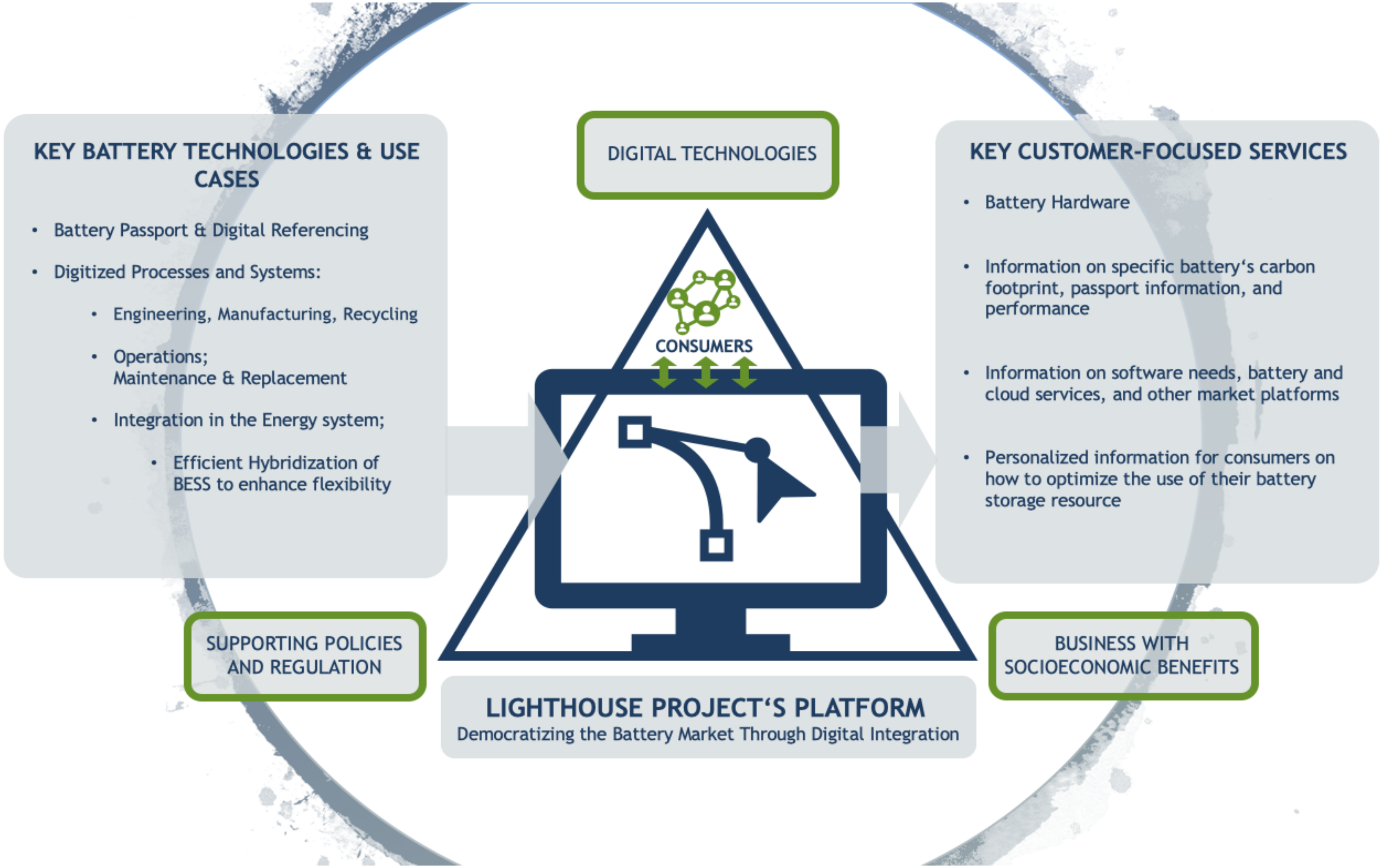
Digital Batteries integration in the Energy System

BATTERIES EUROPE
EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM



Digital Batteries Lighthouse Project

BATTERIES EUROPE
EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM



Digital Batteries socio-economic benefits

BATTERIES EUROPE
EUROPEAN **TECHNOLOGY** AND **INNOVATION** PLATFORM

- ✓ **European Battery Alliance** brings together **400 industrial** and **innovation actors**
- ✓ **EIB: battery projects** along the entire value chain remains among top investment priorities – with **loans amounting to € 1 billion** (2020), leveraging **B€ 4.7 in total**
- ✓ **Acceleration Plan** set to create up to **1 million jobs** in a **European battery ecosystem worth B€ 210 by 2022**
- ✓ **Demand** within the **battery sector** is expected to grow exponentially by 2030.
- ✓ The demand for **1.890 GWh in the electric mobility** and **280 GWh in stationary storage** necessitates a **digital platform** to facilitate the transactions for this marketplace.
- ✓ The electricity sector is ripe for realizing value from **rapid digital transformation**; it is estimated that there is **$1.3 trillion of value to be captured** globally, from 2016 to 2025
- ✓ **Renewable energy sector** employed **11 million people** in 2018 (IRENA)
- ✓ **Employment in energy efficiency** and **Renewable energy** expected to raise up to **250.000 jobs**

Achieving an accelerated adoption …

BATTERIES EUROPE
EUROPEAN **TECHNOLOGY**
AND **INNOVATION** PLATFORM

1. Start by the **Decarbonized, Decentralized & Digitalized Energy Transition** & **Batteries** needs
2. List the enabling **Technologies** and **Use Cases x-Sectors** : Maturity, Feasibility, Simplicity & Accessibility
3. Measure the **Value** generated through **Quick pilots** and then **Scaleup turnkey solutions**

Key to an accelerated energy transition

Regulation/Policy

Consortium/ Industry Collaboration

Pilot results & Technology Maturity Use Cases Feasibility

Value generated From Pilots to massive Scaleup with Turnkey solutions

European Dataspaces

Marco-Robert Schulz
Siemens Energy/ETIP SNET/Gaia-X

SIEMENS energy

Batteries Europe Event

ETIP SNET WG4

Implementation Plan 2021-2024,
Big Idea, Use Case Approach

GAIA-X

Short Overview

Presented by Marco-Robert Schulz
Siemens Energy, Gas & Power, Generation
Digitalization and IT - Service

May 5th, 2021

European Commission

ETIP SNET

EUROPEAN TECHNOLOGY AND INNOVATION PLATFORM

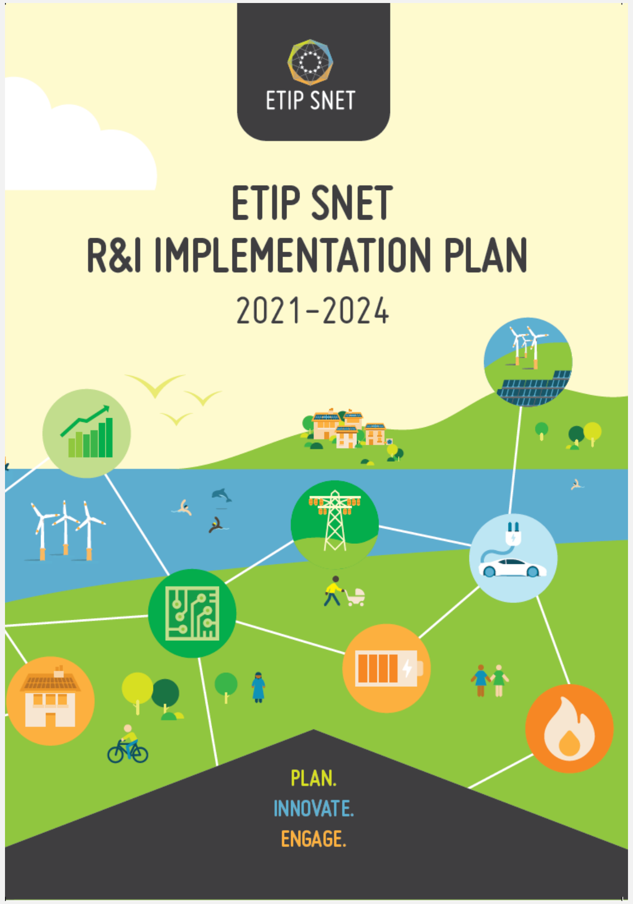
SMART NETWORKS FOR ENERGY TRANSITION

www.etip-snet.eu

Implementation Plan Research Areas and Topics 2021-2024

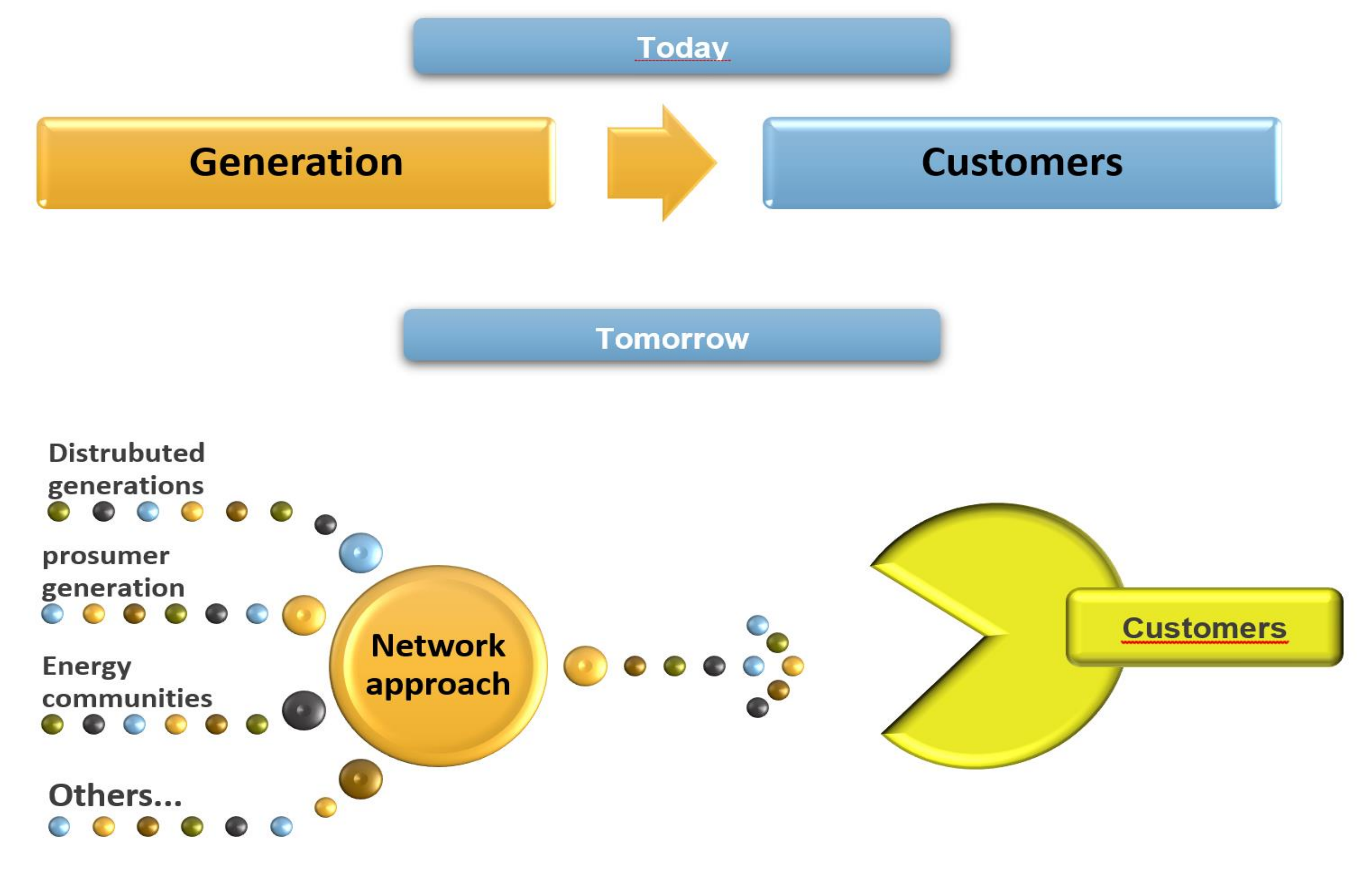
(with 6 research areas, 25 topics and approx.120 tasks)

https://www.etip-snet.eu/wp-content/uploads/2020/05/Implementation-Plan-2021-2024_WEB_Single-Page.pdf



Research Areas (RA)	TOPIC No.	
1. CONSUMER, PROSUMER and CITIZEN ENERGY COMMUNITY	1.1	Social campaigns and social studies (related to societal acceptance and environmental sustainabilty of energy infrastructures)
	1.2	Adaptive consumer/user behaviour incl. energy communities (Interaction, incentives by dynamic tariffs, etc)
	1.3	Consumer and prosumer device control
2. SYSTEM ECONOMICS	2.1	Business models (including Aggregators)
	2.2	Market design (Retail, Wholesale; Cross-border; Ancillary services; Flexibility markets; etc)
	2.3	Market governance (regulation, rules) and tariff design (capacity versus energy, etc)
3. DIGITALIZATION	3.1	Protocols, standardisation and interoperability (IEC, CIM, Information models, etc.)
	3.2	Data Communication (ICT) (Data acquisition, Smart Meter, Sensors (monitoring), AMR, AMM, smart devices, etc.)
	3.3	Data and Information Management (Platforms, Big Data, SW, IoT, etc.)
	3.4	Cybersecurity (vulnerabilities, failures, risks) and privacy
	3.5	End-to-end architecture (integrating market, automation, control, data acquisition, digital twin, end-users)
4. PLANNING - HOLISTIC ARCHITECTURES and ASSETS	4.1	Integrated Energy system Architectures (design including new materials)
	4.2	Long-term planning (System development)
	4.3	Asset management and maintenance (maintenance operation, failure detection, asset lifecycles, lifespan and costs, ageing, etc.)
	4,4	System Stability analysis
5. FLEXIBILITY ENABLERS and SYSTEM FLEXIBILITY	5.1	Demand flexibility (household and industry related)
	5.2	Generation flexibility (flexible thermal, RES (Hydro, PV and wind generators, etc.))
	5.3	Storage flexibility & Energy Conversion flexibility (PtG&H, PtG, GtP, PtL, LtP; PtW; WtP (W: Water), etc.)
	5.4	Network flexibility (FACTS, FACDS, smart transformers, etc.)
	5.5	Transport flexibility (VtG/EV; railway, trams, trolleybus, etc.)
6. SYSTEM OPERATION	6.1	State estimation and State supervision (basic control)
	6.2	Short-term control (Primary, Voltage, Frequency, etc)
	6.3	Medium and long-term control (Forecasting (Load, RES), secondary & tertiary control: LFC, operational planning: scheduling/optir
	6.4	Preventive control/restoration (Contingencies, Topology (incl. Switching) optimisation, Protection, Resilience)
	6.5	Control Center technologies (EMS, platforms, Operator training, Coordination among Control Centers)

Big Idea: From Push to Select



Big Idea: ONE STOP SHOP
for user friendly energy access and information

- **Commercial provision of services and technology solutions** to favour flexibility, sustainable energy access (on top of the technical analysis)

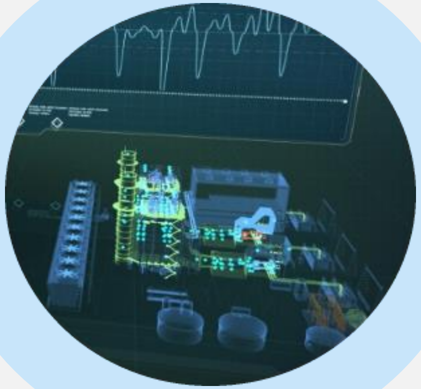
*** ESCOs
Retailers
Aggregators**

*APIs

*TSO
- **Joint planning**
- **Joint flexibility**

*APIs

*APIs



*DSO
Digital Twin

- **Advanced planning of the network based on accurate data**
- **Facilitating/speeding up current interactions**
- **Continuous sharing and visibility of the relevant data** and information
- **Enabling new services to all stakeholders and innovative resilience approaches** (cross sectorial activation)

**ONE STOP SHOP
Universal access platform**
for user-friendly energy access
(Harmonized experience of EU citizen)

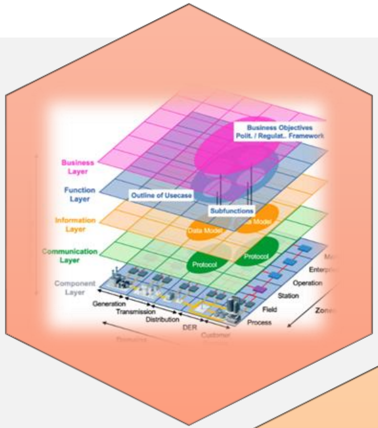
*APIs

Database owners (e.g. municipalities, cyber institutions, other utilities)

- **Up to date info on urban and rural mapping and cybersecure risks, weather prediction etc.**

* ESCO: Energy Service Company
* TSO : Transmission Service Provider
* DSO : Distribution Service Provider
* API : Application Programming Interface

Architechtures: Integration Options



SGAM

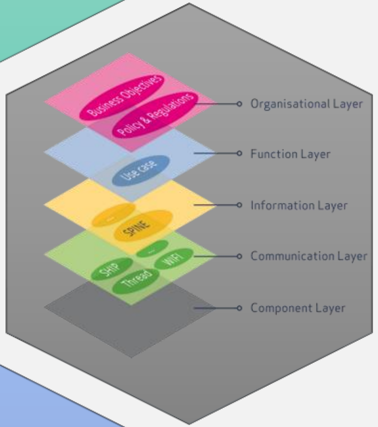
Smart Grid Architechture Model

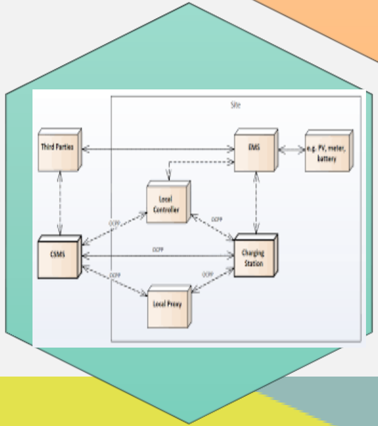
* CIM, TSO/DSO: local, national, regional, Pan European

Demand Response
Energy Efficiency

SAREF

Smart Applications REFerence Ontology





OCPP

Open Charge Point Protocol

Smart Charging
For EV

How to proceed towards integration of different ecosystems?

1 — **Multiple architecture and integrate *them through a common approach***

or

2 — **Multiple architectures and creating connection.** Integrating the operations and markets of different ecosystems

Connecting Multisided platform

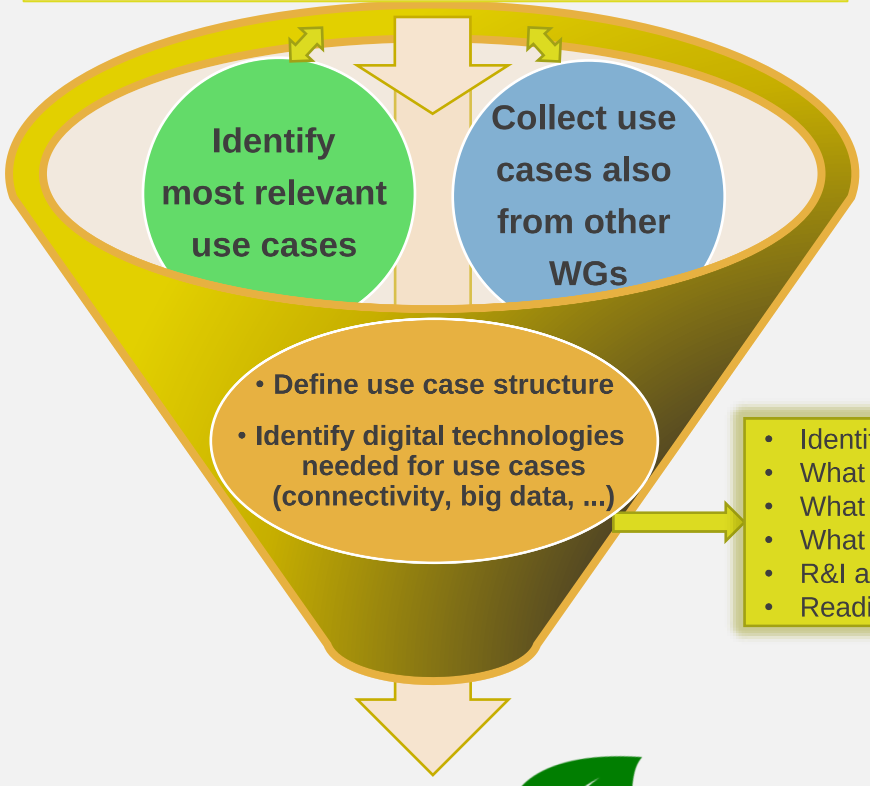
- *Buy and sell: services , products , information*
- *Simplified and integrated access (single interface) – hidden complexity*
- *Activation layer based on real time data*

* CIM : Common Information Model
* TSO : Transmission Service Provider
* DSO : Distribution Service Provider

5 to 10 Use Cases to be identified

Research Areas (RA)	TOPIC No.	
1. CONSUMER, PROSUMER and CITIZEN ENERGY COMMUNITY	1.1	Social campaigns and social studies (related to societal ac
	1.2	Adaptive consumer/user behaviour incl. energy commun
	1.3	Consumer and prosumer device control
2. SYSTEM ECONOMICS	2.1	Business models (including Aggregators)
	2.2	Market design (Retail, Wholesale; Cross-border; Ancillary
	2.3	Market governance (regulation, rules) and tariff design (c
3. DIGITALIZATION	3.1	Protocols, standardisation and interoperability (IEC, CIM,
	3.2	Data Communication (ICT) (Data acquisition, Smart Mete
	3.3	Data and Information Management (Platforms, Big Data,
	3.4	Cybersecurity (vulnerabilities, failures, risks) and privacy
	3.5	End-to-end architecture (integrating market, automation
4. PLANNING - HOLISTIC ARCHITECTURES and ASSETS	4.1	Integrated Energy system Architectures (design including
	4.2	Long-term planning (System development)
	4.3	Asset management and maintenance (maintenance opera
	4,4	System Stability analysis
5. FLEXIBILITY ENABLERS and SYSTEM FLEXIBILITY	5.1	Demand flexibility (household and industry related)
	5.2	Generation flexibility (flexible thermal, RES (Hydro, PV an
	5.3	Storage flexibility & Energy Conversion flexibility (PtG&H
	5.4	Network flexibility (FACTS, FACDS, smart transformers, et
	5.5	Transport flexibility (VtG/EV; railway, trams, trolleybus, e
6. SYSTEM OPERATION	6.1	State estimation and State supervision (basic control)
	6.2	Short-term control (Primary, Voltage, Frequency, etc)
	6.3	Medium and long-term control (Forecasting (Load, RES),
	6.4	Preventive control/restoration (Contingencies, Topology
	6.5	Control Center technologies (EMS, platforms, Operator tr

➢ **Sources and synergies to be used**:
- ❖ Use cases from others ETIP SNET WGs
- ❖ Use cases repository developed in BRIDGE
- ❖ Use cases developed by GAIA-X Initiative



- Identify the budget,
- What are the impacts
- What are the KPIs
- What is the EU competitiveness
- R&I advantages
- Readiness

5 to **10** use cases to be identified !

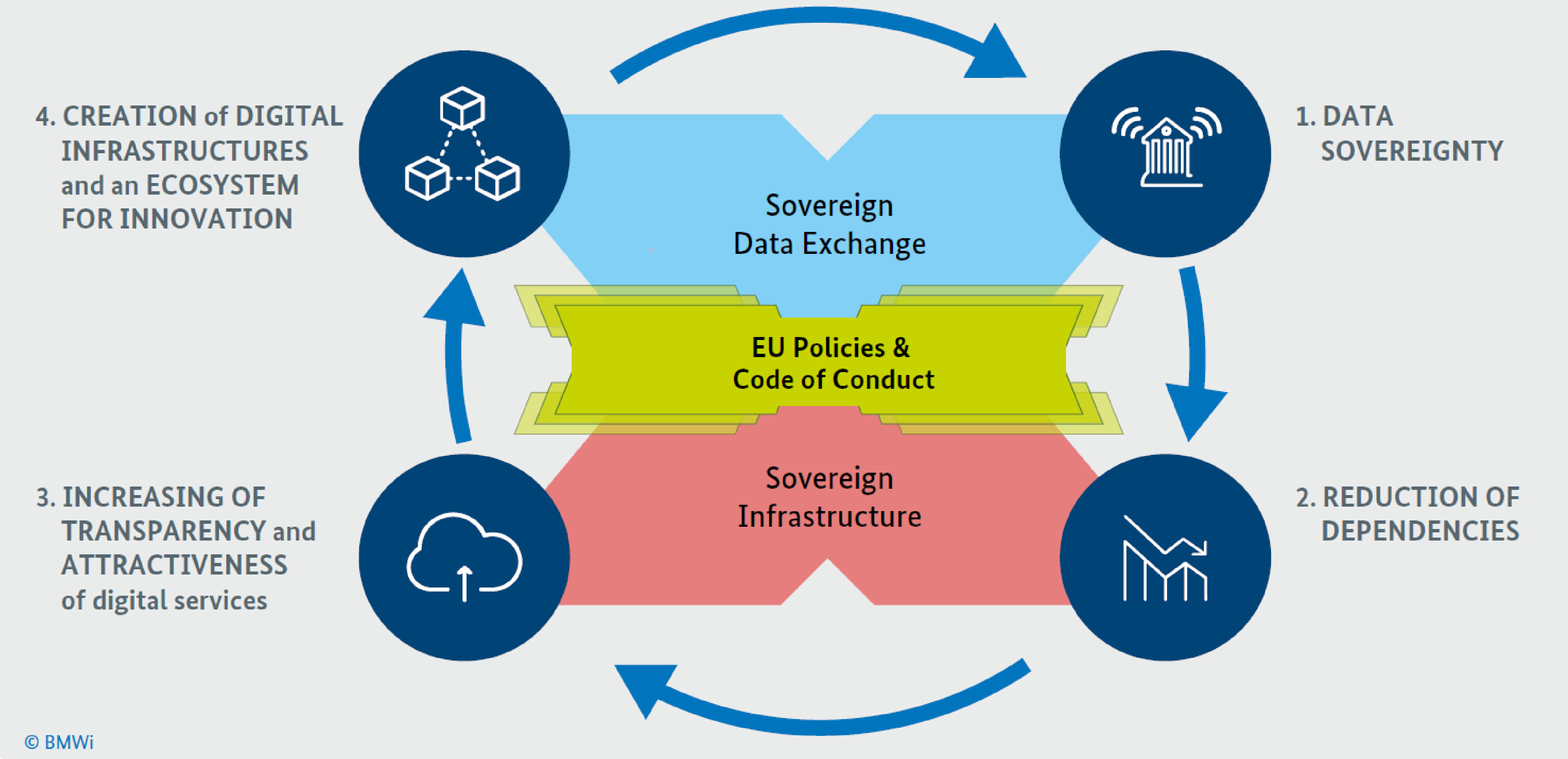
GAIA-X

gaia-x

https://www.bmwi.de/Redaktion/EN/Dossier/gaia-x.html

https://www.gaia-x.eu/

Gaia-X aims at building a trusted, sovereign digital infrastructure for Europe



Source: BMWi, gaia-x-driver-of-digital-innovation-in-europe.pdf / July 2020 | ETIP SNET, 2021

The Gaia-X ecosystem of services and data

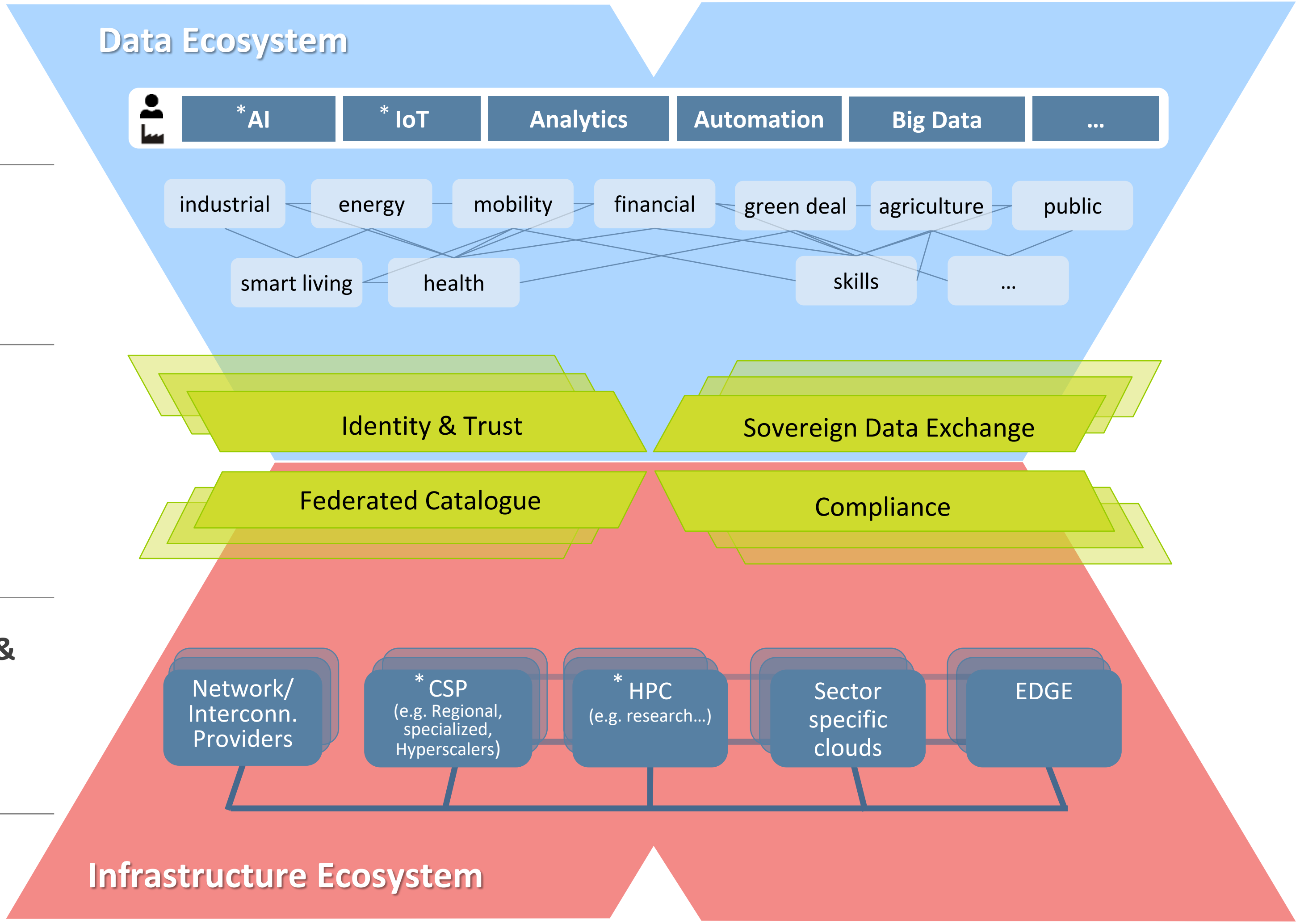
Advanced Smart Services
(Cross-) Sector Innovations /
Market places / Applications

Data Spaces
Interoperable & portable (Cross-)
Sector data-sets and services

GAIA-X Federation services
Federated & distributed for
interoperability Trust & Sovereignty
services

Portability, Interoperability & Interconnectivity
Technical: Architecture of Standards
Commercial: Policies

Compliance
Legal: Regulation & Policies



* AI : Artificial Intelligence
* IoT : Internet of Things
* CSP : Cloud Solution Provider
* HPC : High Performance Computing

All domains share common requirements

gaia-x

Energy	Finance	Agriculture	Health	Industry 4.0/SME	Mobility	Public Sector	Smart Living

Common cross-domain requirements

Gaia-X as enabler

Federated Identity Management

Algorithms for data monetisation

Trusted Relationship Management

Data Custodianship as a business principle

Open to adapt of all market participants - and systems

Authorisation and data usage control by the data owner

Uniform definition of protection classes for data and services for all participants

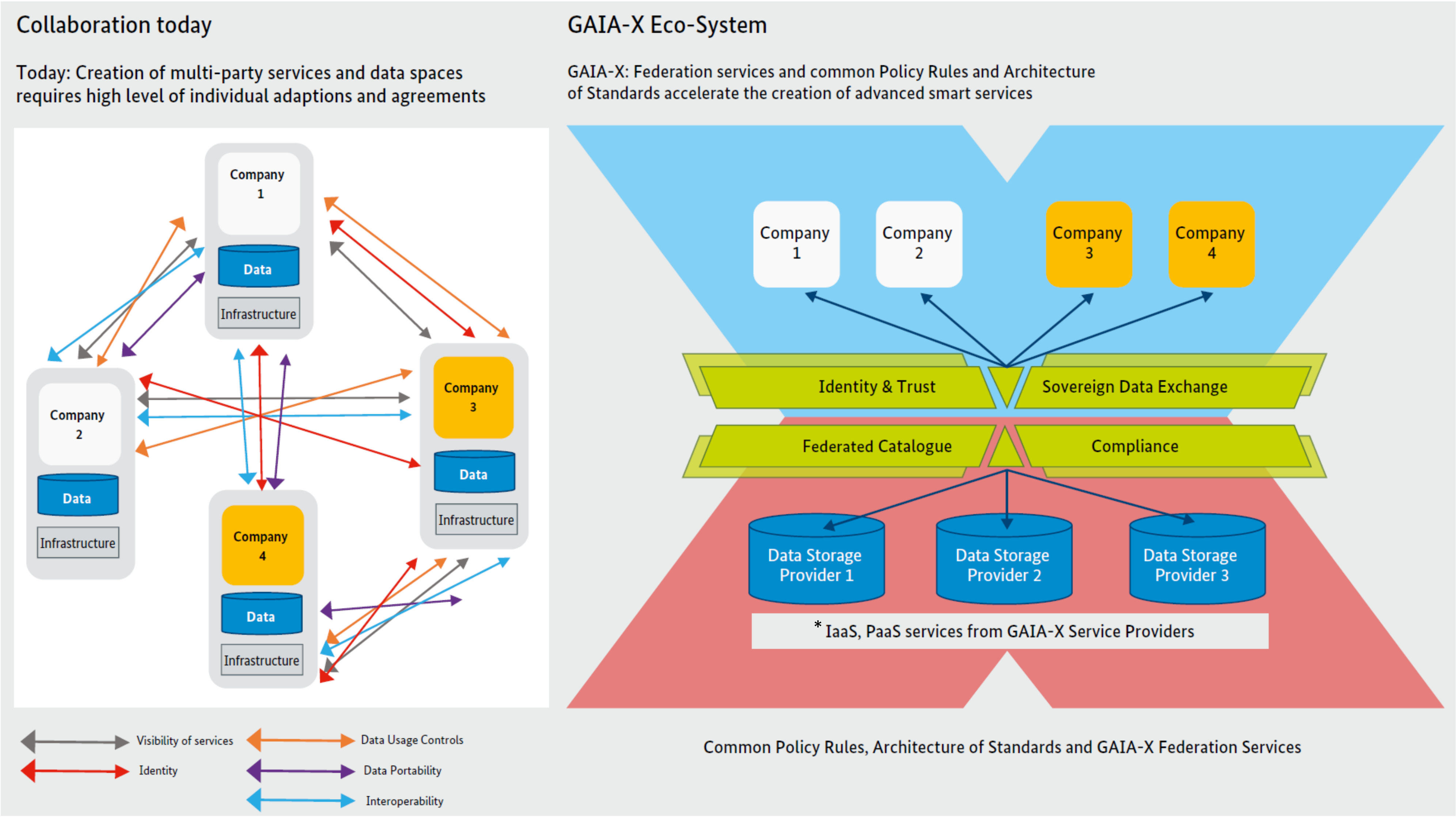
Selectable Geography and Legislation for data storage and service offering (locally/centrally)

Hybrid Cloud Scenario through distributed implementation (vertically and horizontally) across many vendors

+

Additional domain-specific requirements

Collaboration Today (left) and Tomorrow (right)



* IaaS : Information as a Service
* PaaS : Platform as a Service

Source: BMWi, gaia-x-driver-of-digital-innovation-in-europe.pdf / July 2020 | ETIP SNET, 2021

Gaia-X will add value to the European digital economy

gaia-x

Data-based business models

Enabling self-determined data-based business models from an entrepreneurial perspective.

Raise the value of data

Supporting innovative collaborations across industries to aggregate and raise the value of data.

Fairness and transparency

Promoting fair and transparent business models by providing the rules for such collaborative approaches, including the legally compliant use of data.

gaia-x

Data commercialisation

Providing common data monetisation schemes, sharing models and respective enforcement rules. As such, the commercialisation of data becomes less complex and costly.

Interoperability

Enabling collaboration across industries to create federated, interoperable services on the infrastructure layer.

Data protection

Supporting the detection and preservation of data protection classes and confidentiality rules even in the case of “mixed” data allocations. Hence, the value leakage of enterprise data sets is prevented.

Infrastructure

Easing access to trustworthy next generation IT infrastructure, which will provide a productivity boost for software engineering teams.

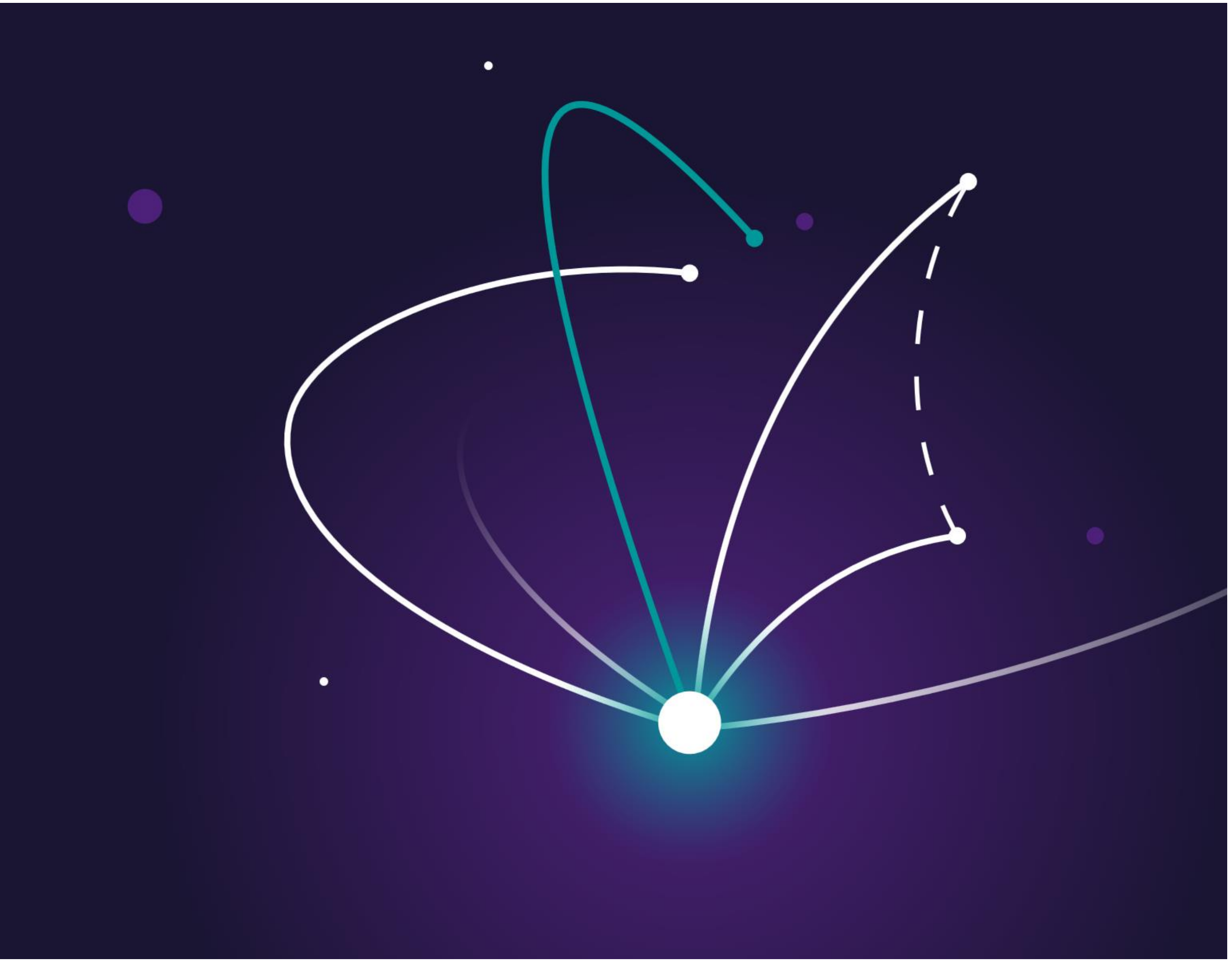
Be part of **gaia-x** and **create**
a **future** that is both **open** and **fair**!

We are **happy** to **have you with us**
and **welcome you**.

gaia-x
standard
presentation

PDF Document

Thank you for your attention !



Presented by

Marco-Robert Schulz

Siemens Energy
Gas & Power, Generation
Digitalization and IT - Service
SE GP G DIG IT SV 2
Huttenstrasse 12-16
10553 Berlin
Germany

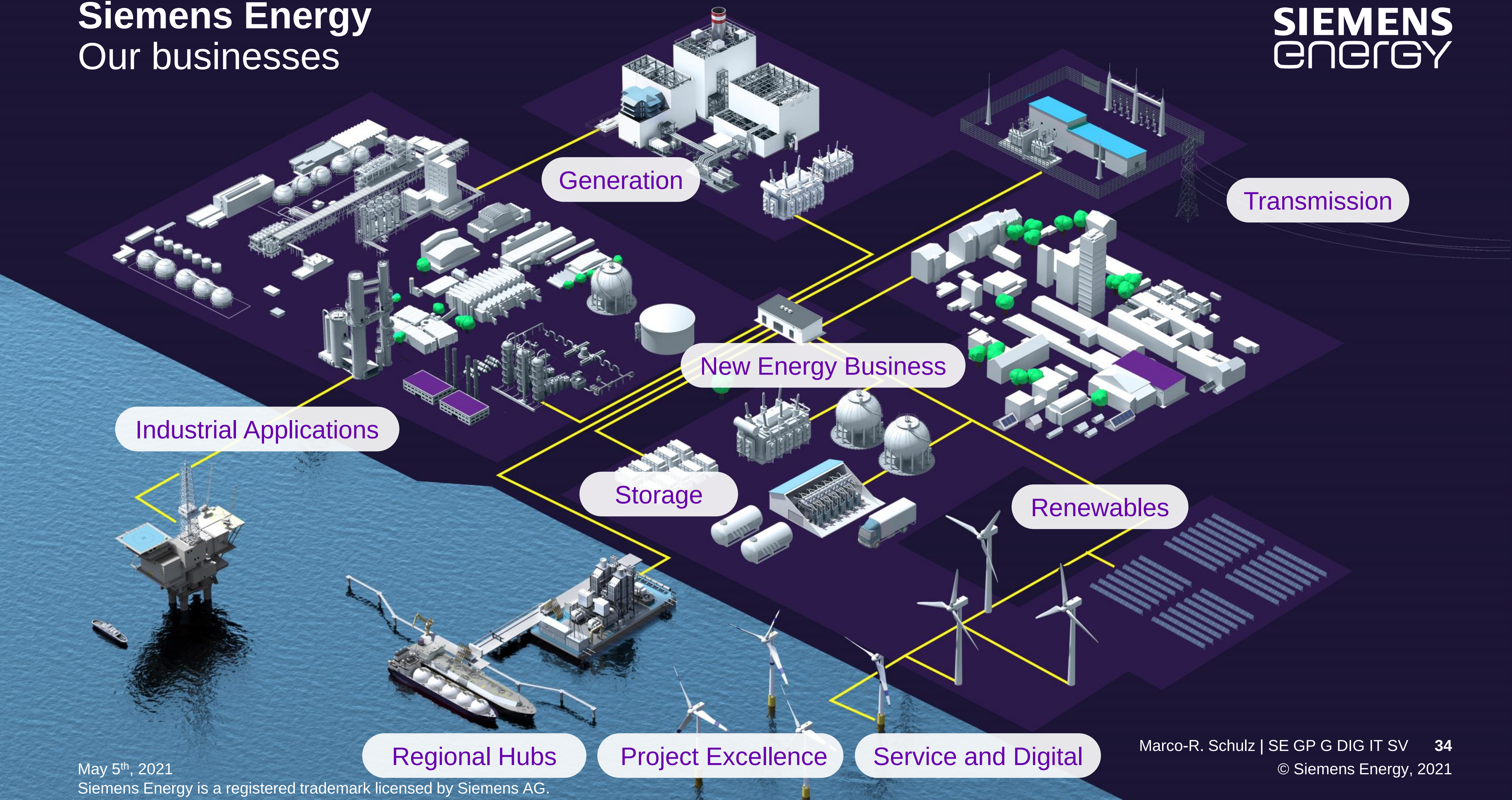
M +49 174 34 70 250
E marco-robert.schulz@siemens-energy.com
W https://www.siemens-energy.com/global/en.html

Siemens Energy

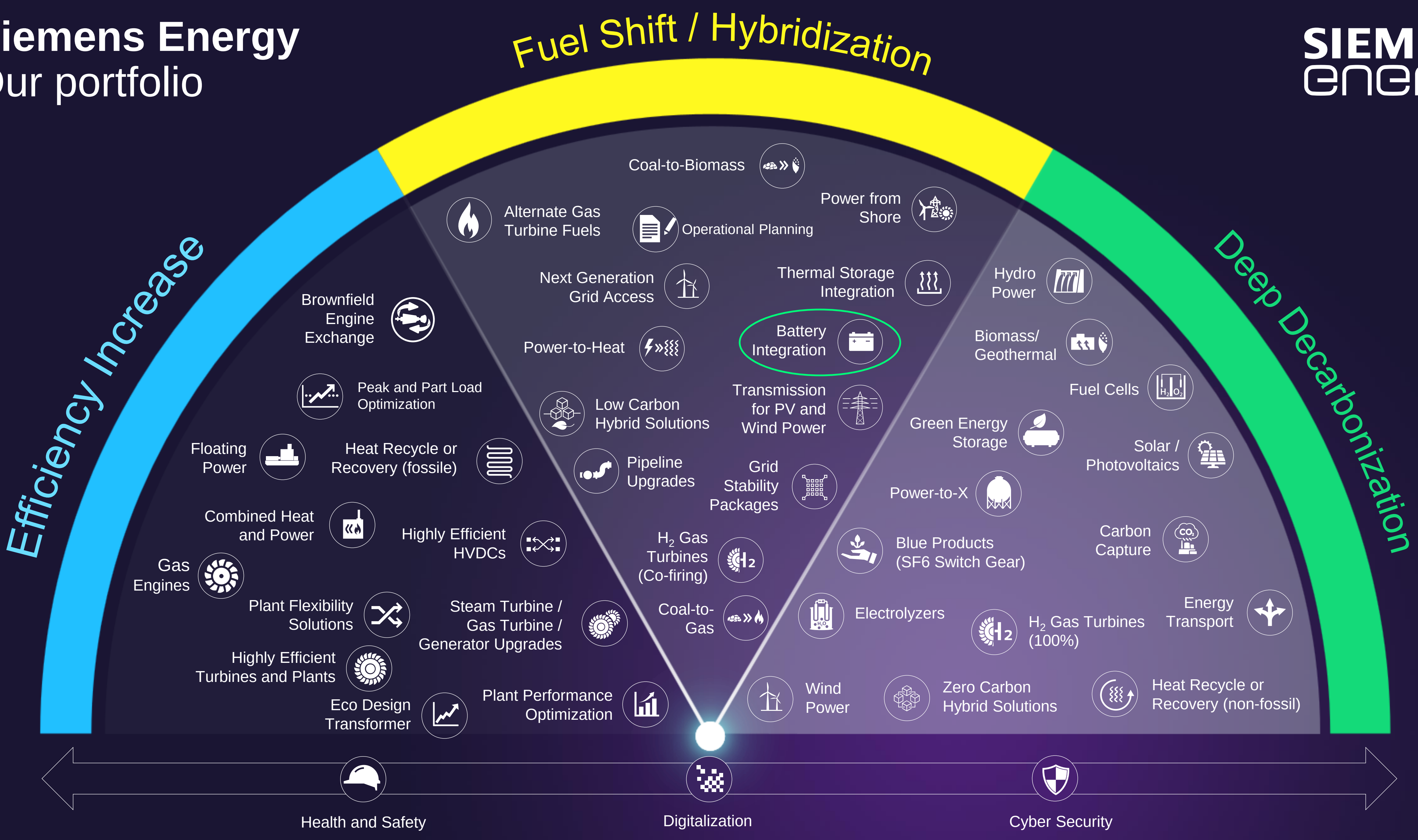
SIEMENS energy

Partner and Driver of the Energy Transition

Siemens Energy
Our businesses



Siemens Energy
Our portfolio



Energy storage is the key to deep decarbonization

SIEMENS energy

Energy Market & Storage Market Trends

- Increasing energy demand
- Decarbonization
- Decentralization

- Increasing share of renewables
- Decreasing cost of storage tech.
- Increasing demand flexibility
- Regulations

Bloomberg energy outlook (NEO2018):

World is on track to miss 2°C warming target due to insufficient decarbonization

Even fast coal phase-out combined with more gas and renewables **not enough to close the gap**

Wind and solar PV cheapest ways of electricity producing worldwide until the 2030s (BNEF)

Battery Energy Storage Systems

Reliable battery storage systems are required also on large and medium scale level to combine the global energy demand and climate protection goals:

- Increased **availability of renewable energy sources**, hence supporting **decarbonization**
- **Supply-Load balancing** in case of high share of **volatile renewable energy sources**
- Higher overall **energy system efficiency** through using **excess energy**

Siemens Energy's Battery Storage Systems

SIEMENS energy

Customer segment

- Conventional Generation
- Renewable Generation
- Transmission and Distribution
- Indust. Producers & Consumers
- Offshore Applications

Battery energy storage systems

Instant and zero carbon energy

Revenue streams

- Capacity Firming
- Flexibility & efficiency
- Decarbonization
- Virtual grid expansion
- Non-Sync. Grid stabilization
- Decentral power generation
- Electrical peak shaving
- Industrial power generation

SIESTART ™ - May 2019
BASF Schwarzheide Germany

SIEMENS energy

Project

Siemens Energy to modernize industrial power plant from BASF in Germany with key components

Customer

BASF Schwarzheide GmbH

BASF We create chemistry

Location

Schwarzheide, Germany

Partner

FLUENCE A Siemens and AES Company

Project Scope

- Replacement of gas turbine from another OEM with an SGT-800
- Installation of a SIESTART battery storage solution for black start capability
- Customized solution requires comprehensive engineering expertise

Use case

- **Non. Sync. Grid stabilization** - Provide blackstart capability

Advantages

- Siemens Energy will install a SIESTART battery storage solution that will enable the entire power plant to start-up independently of an external power supply
- Reduced CO_2 Emission compared to blackstart diesel or gas motors

SIESTART ™ - April 2020
HKW Leipzig Süd
Germany

SIEMENS energy

Project Scope
- 2 x SGT-800 gas turbines
- 2 x Sgen-100A generators
- SIESTART™ battery energy storage system

Use case
- **Non. Sync. Grid stabilization** - Provide blackstart capability

Advantages
- Siemens Energy will install a SIESTART battery storage solution that will enable the entire power plant to start-up independently of an external power supply
- Reduced CO_2 Emission compared to blackstart diesel or gas motors

Project

Siemens Energy to provide Leipzig with a climate neutral power supply.

Customer

Stadtwerke Leipzig GmbH

Stadtwerke Leipzig

Location

Leipzig, Germany

Partner

FLUENCE A Siemens and AES Company

Utilization and Monetization of Stationary Batteries Flexibility

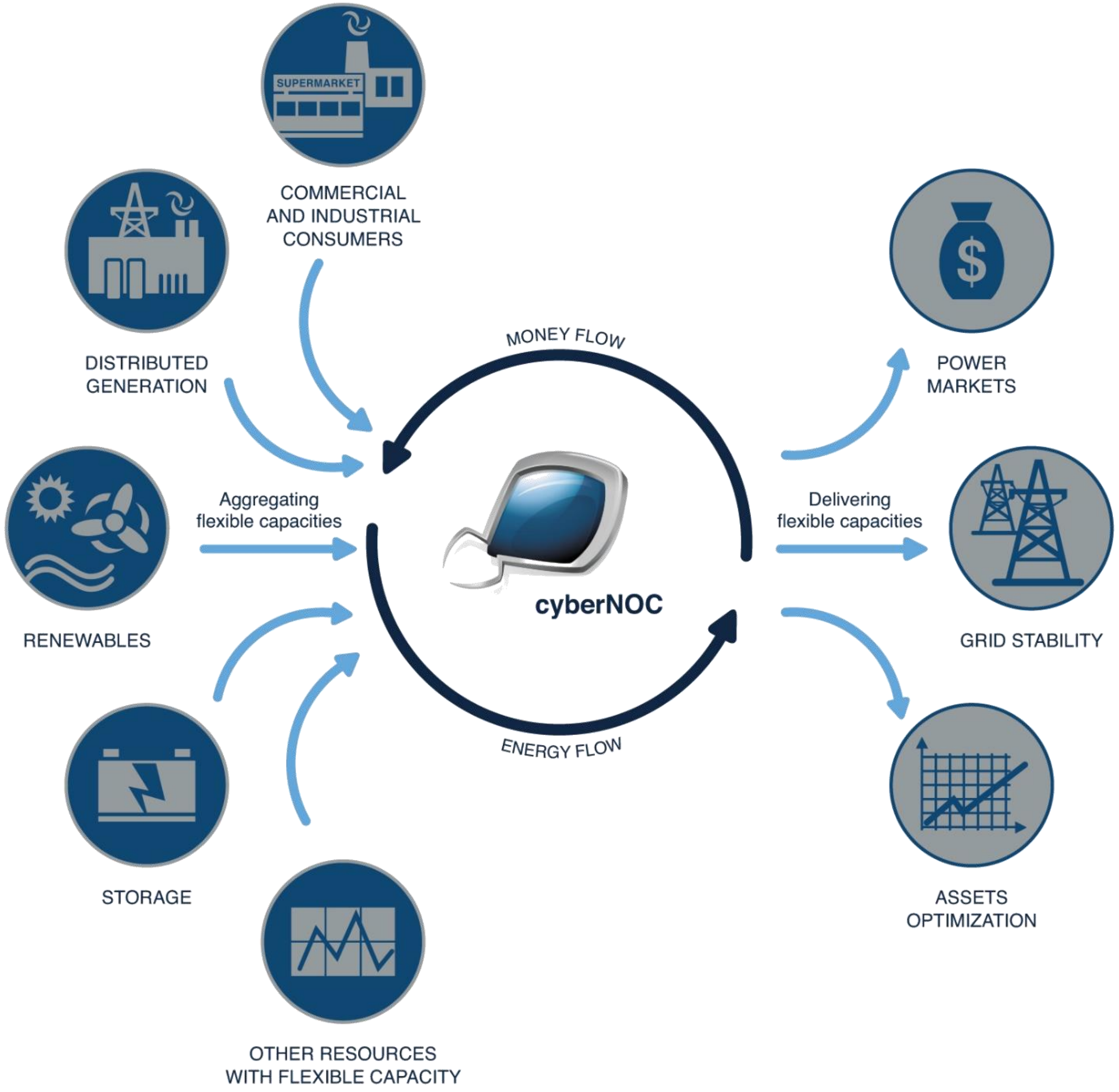
Peter Nemcek

CyberGrid/ETIP SNET

Utilization and monetization of stationary batteries‘ flexibility

Peter Nemcek, M.Sc.

Flexibility Utilization and Monetization



Example of ICT system

Vision

Utilization and monetization of Battery Energy Storage Systems (BESS) should be seamless:

1. Connect with the electrical grid.
   (GRID)
2. Register with a flexibility service provider (e.g. aggregator).
   (ICT)
3. Start offering flexibility services to several different markets.
   (MARKET)

R&D challenges

- Interoperability:
  - Plug and play
  - Standardization of data exchange at all 5 SGAM layers
- Hybridization:
  - Pairing with other flexibilities (loads, RES, EV charging, etc.)
  - Portfolio based utilization and monetization
  - Baselines – measurement and verification methodology
- Multi-service:
  - Local (behind the meter)
  - Community (asset sharing)
  - Balance group (imbalance management)
  - DSO (non-frequency system services)
  - TSO (frequency system services)

Thank you! Questions?

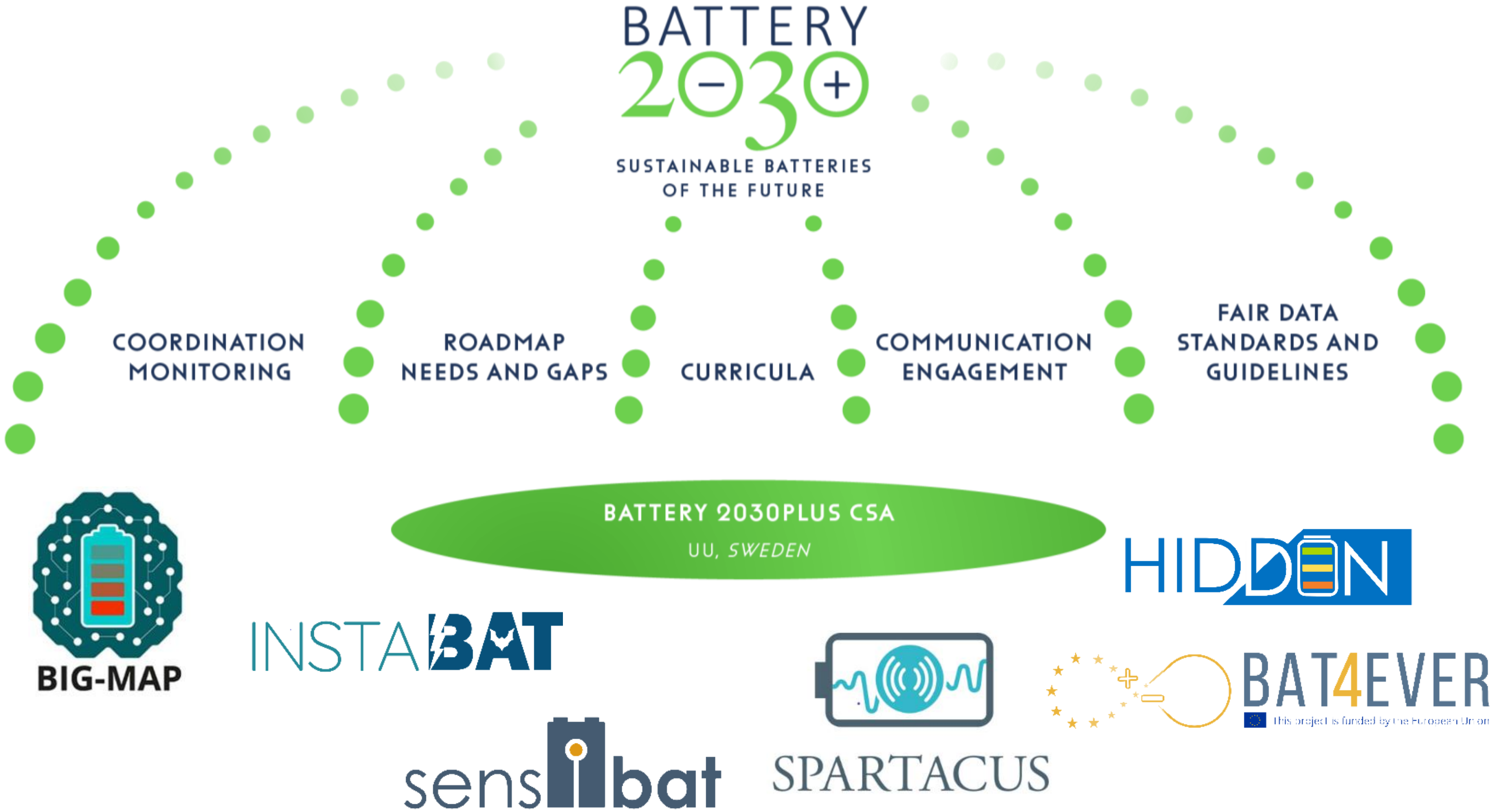
BIG-MAP: Accelerating Battery Discovery with a Common Digital Representation

Tejs Vegge

DTU/ Battery 2030+

BIG-MAP: Accelerating battery discovery with a common digital representation

LARGE-SCALE RESEARCH INITIATIVE



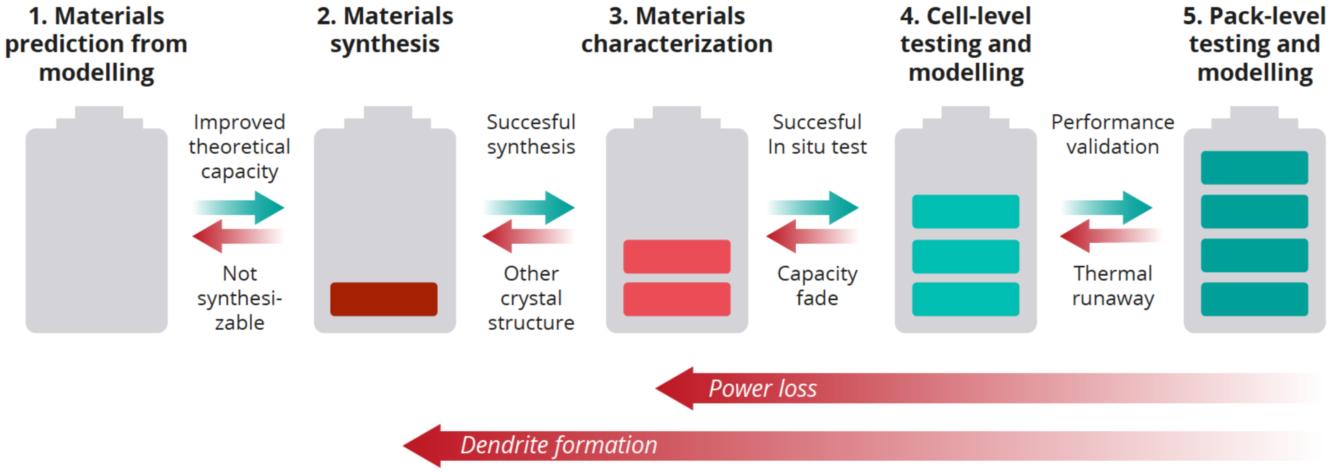
Tejs Vegge (big-map@dtu.dk, @BIGMAP_EU, www.big-map.eu, www.battery2030.eu)

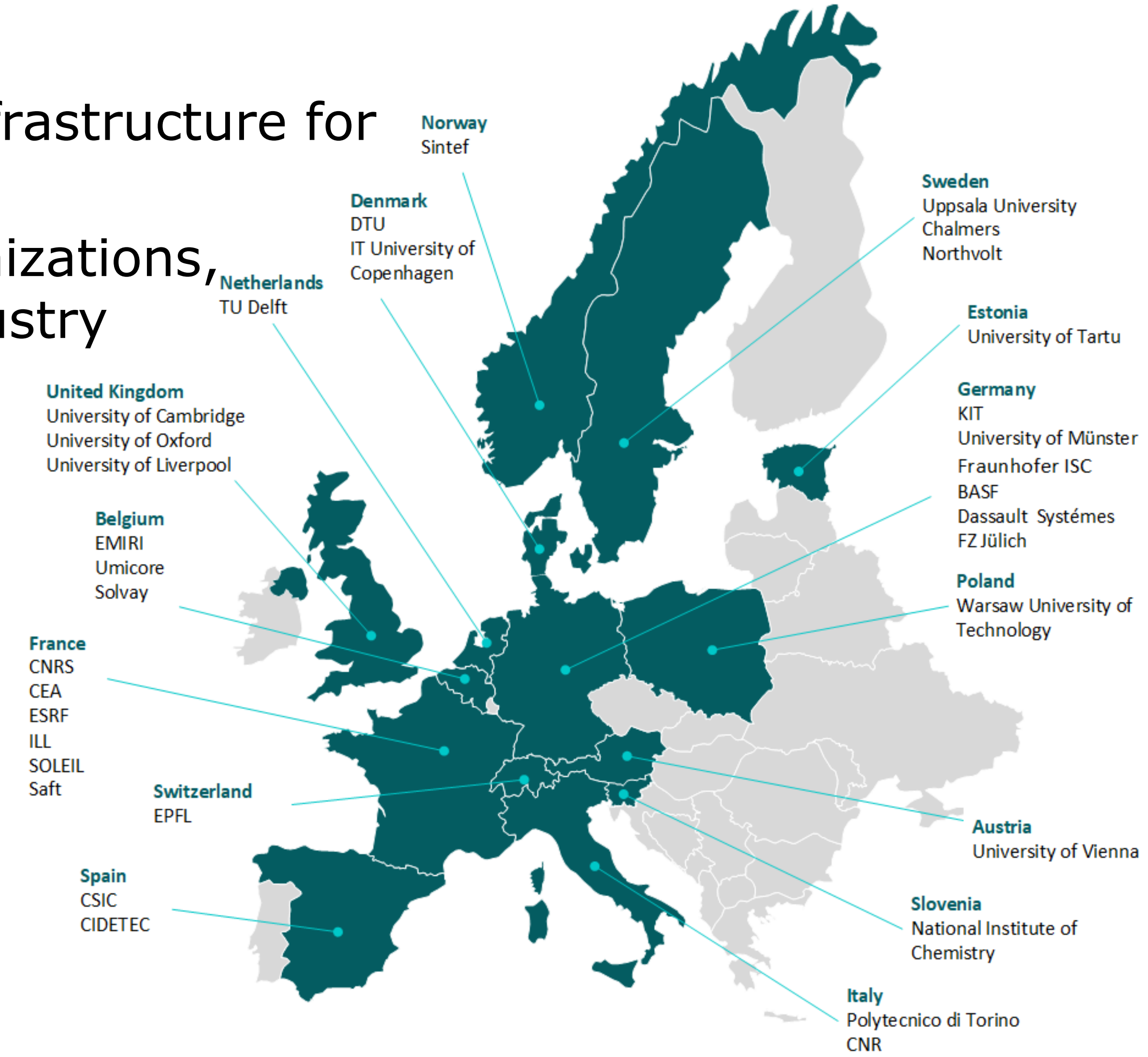
DTU Energy, Technical University of Denmark Technical University of Denmark

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 957189

BIG-MAP: Battery Interface Genome – Materials Acceleration Platform

- *Reinventing the way we invent batteries*
- Developing an AI-accelerated digitalized infrastructure for the European Battery Community
- 34 partners from academia, research organizations, large-scale research infrastructure and industry
- Read more: www.big-map.eu



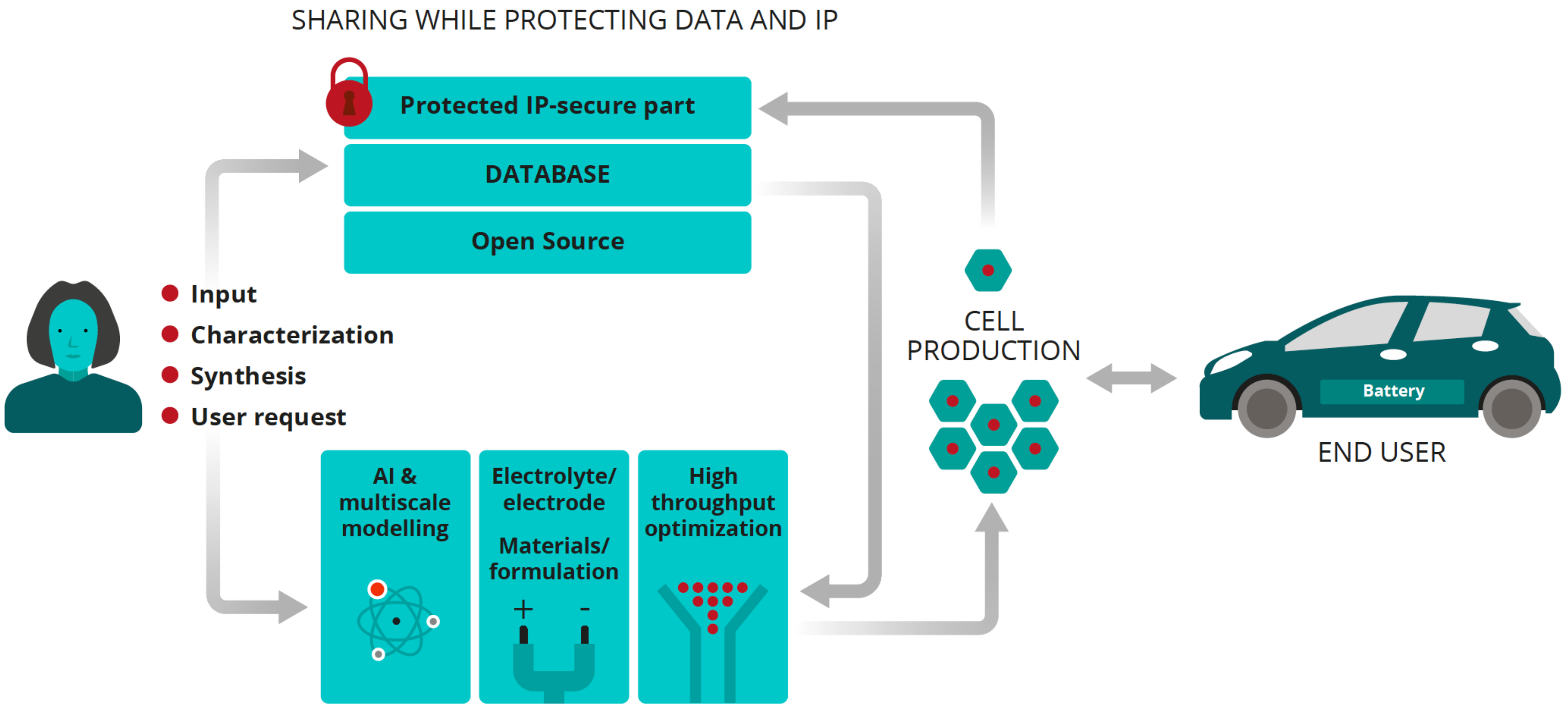


DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

Accelerated Battery Development Processes

- **Vision**: A modular and chemistry neutral platform for 5-10x accelerated closed-loop discovery using digitalization, AI-accelerated models & procedures

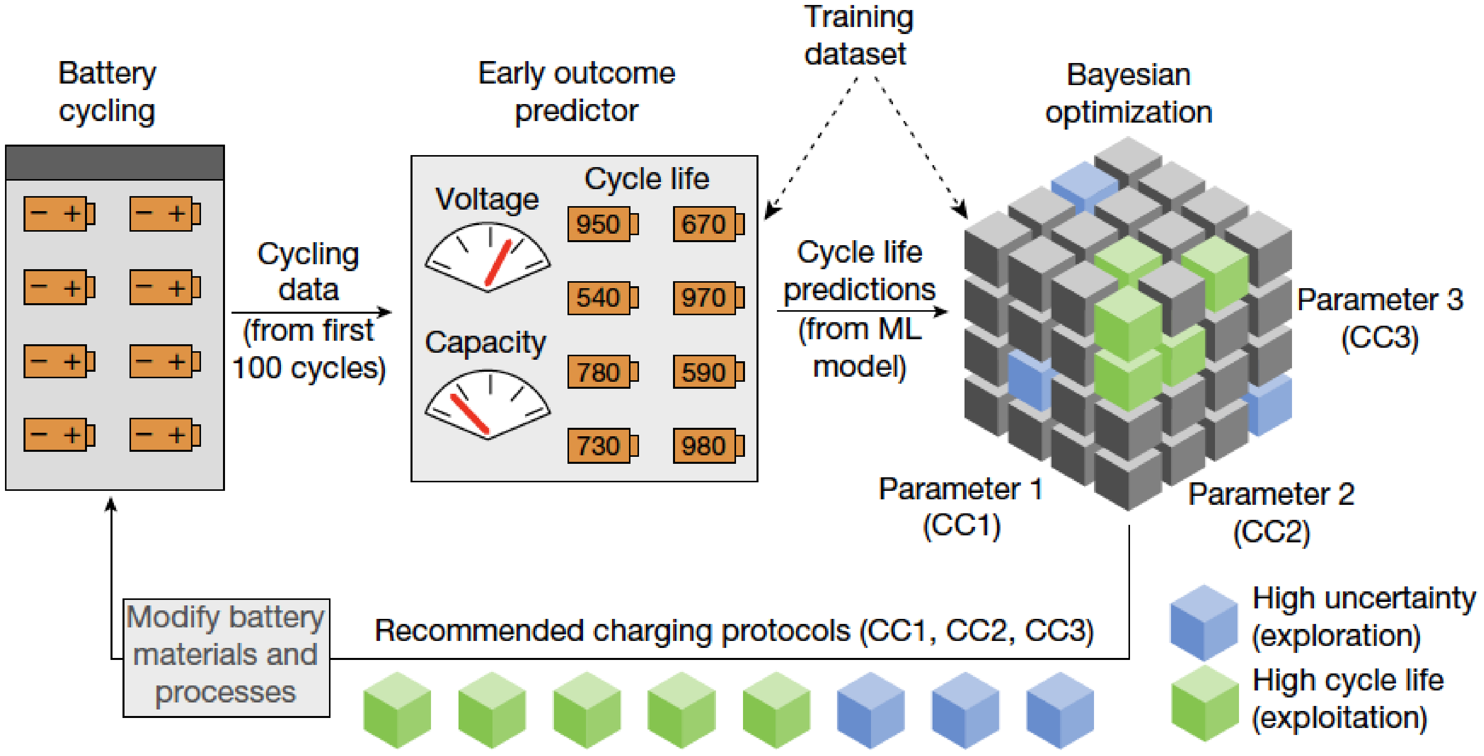


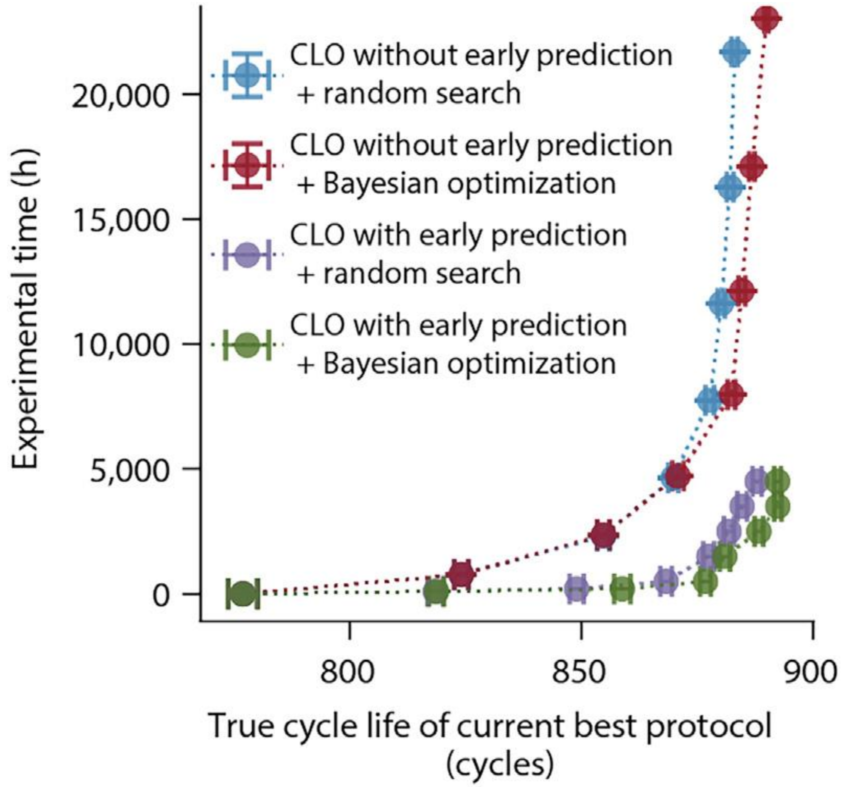
DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

Why digitalize the battery discovery process?

- Digital optimization of battery performance and utilization with machine learning
- Developing new insights into the limiting processes





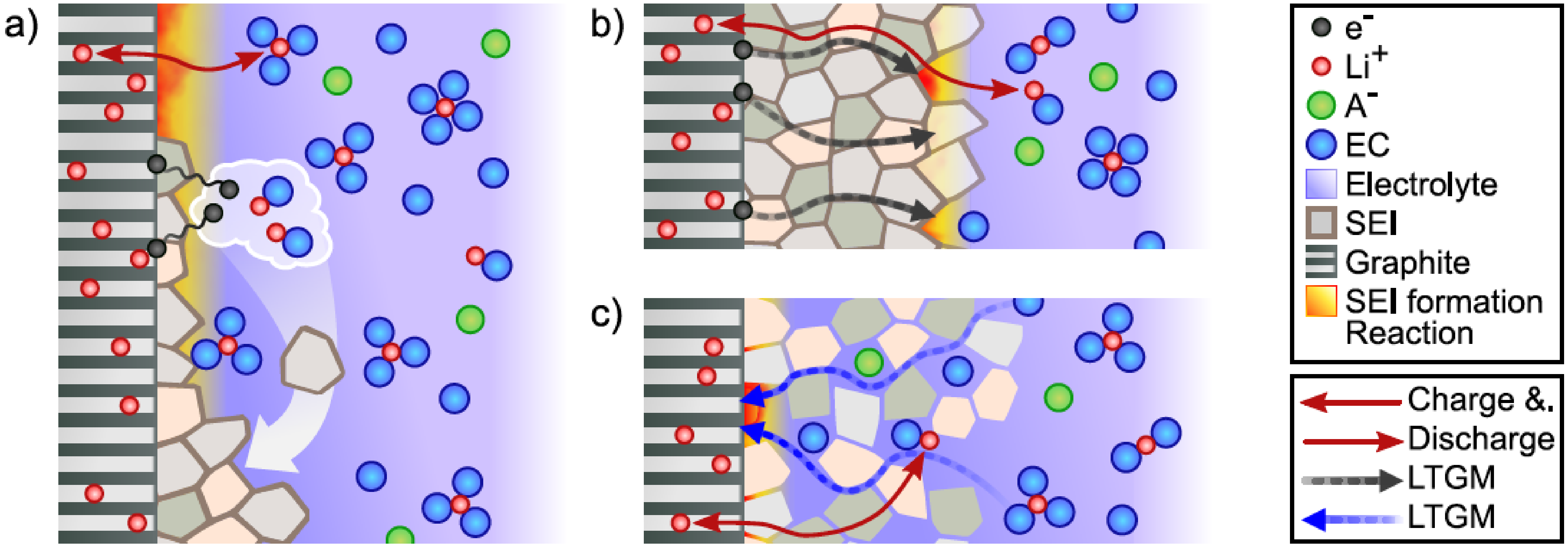
Attia, Chueh et al., Nature 578, 397–402 (2020)

Bhowmik, Vegge, Joule 4, 717-719 (2020)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

BIG: Understanding & Controlling Interfaces

- Interfaces and interphases play a critical role in all battery technologies
- Develop hybrid physics and data-driven models for accelerated discovery



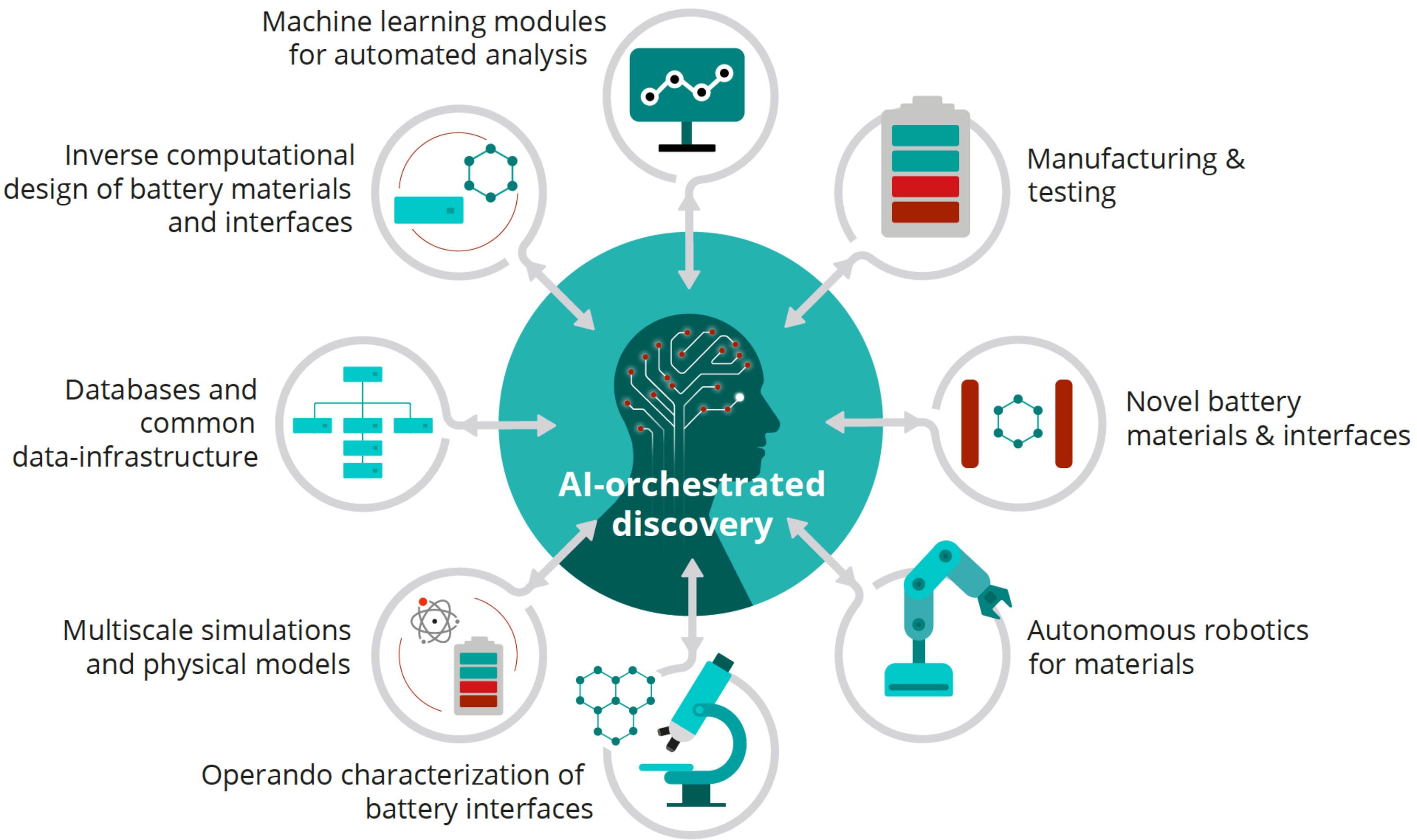
Horstmann, Single, Latz, Current Opinion in Electrochemistry 13, 61-69 (2019)

DTU Energy, Technical University of Denmark

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 957189

MAP: An AI-orchestrated Discovery Process

- **Mission**: Enabling automated data acquisition, analysis, prediction and utilization

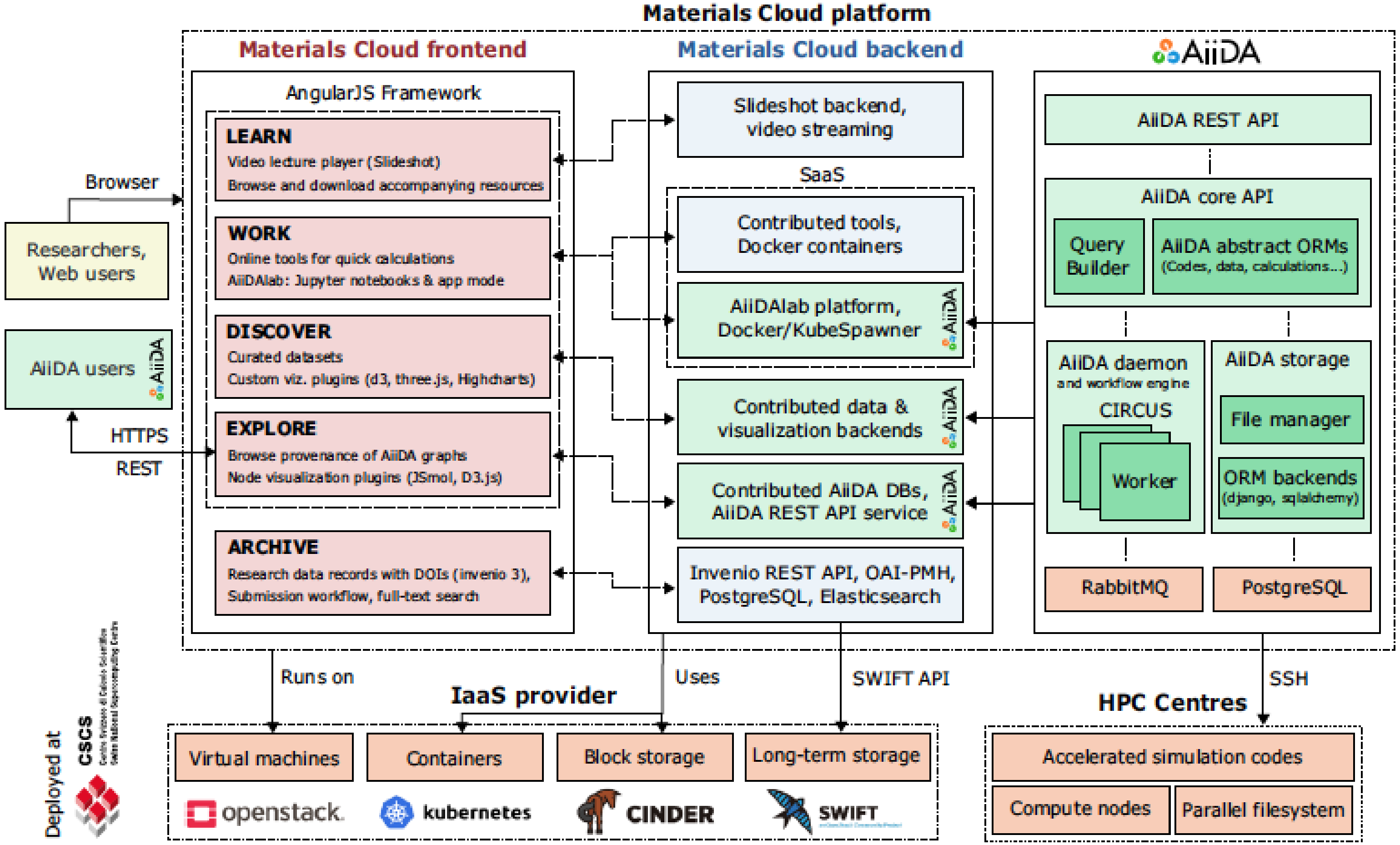


DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

Shared Data Infrastructure & Interoperability

- A shared FAIR data-infrastructure spanning research data, simulation codes, scales, experiments and domains



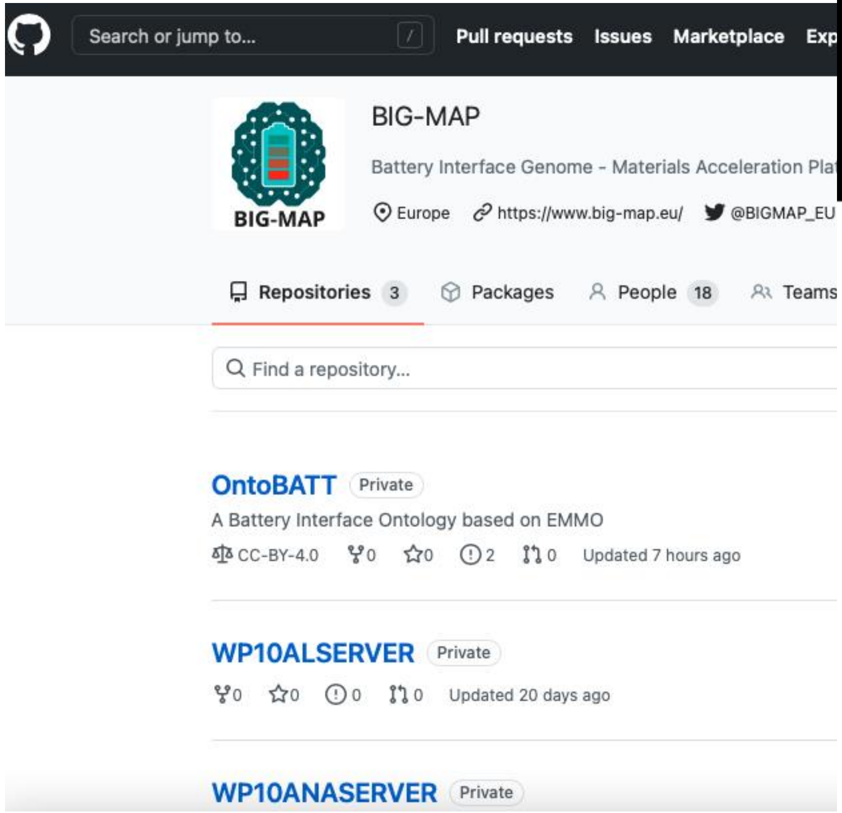
Talirz et al., Scientific Data 10.1038/s41597-020-00637-5 (2020); Huber et al., Scientific Data 10.1038/s41597-020-00638-4 (2020)

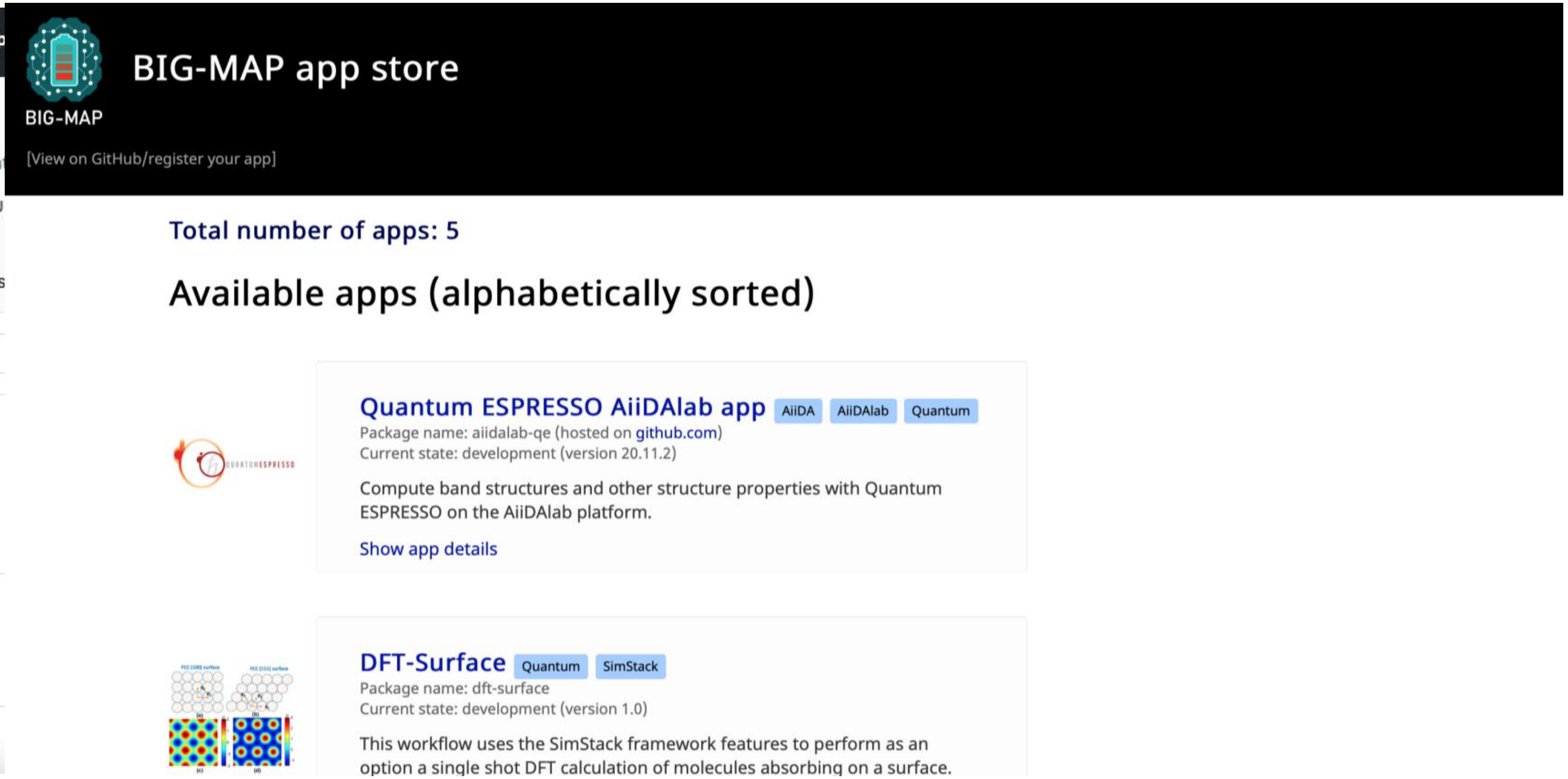
DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

BIG-MAP App Store and GitHub repository

- Developing externalizable tools, apps and workflows for the European battery community
- We've created a BIG-MAP repository (GitHub) and a BIG-MAP App Store



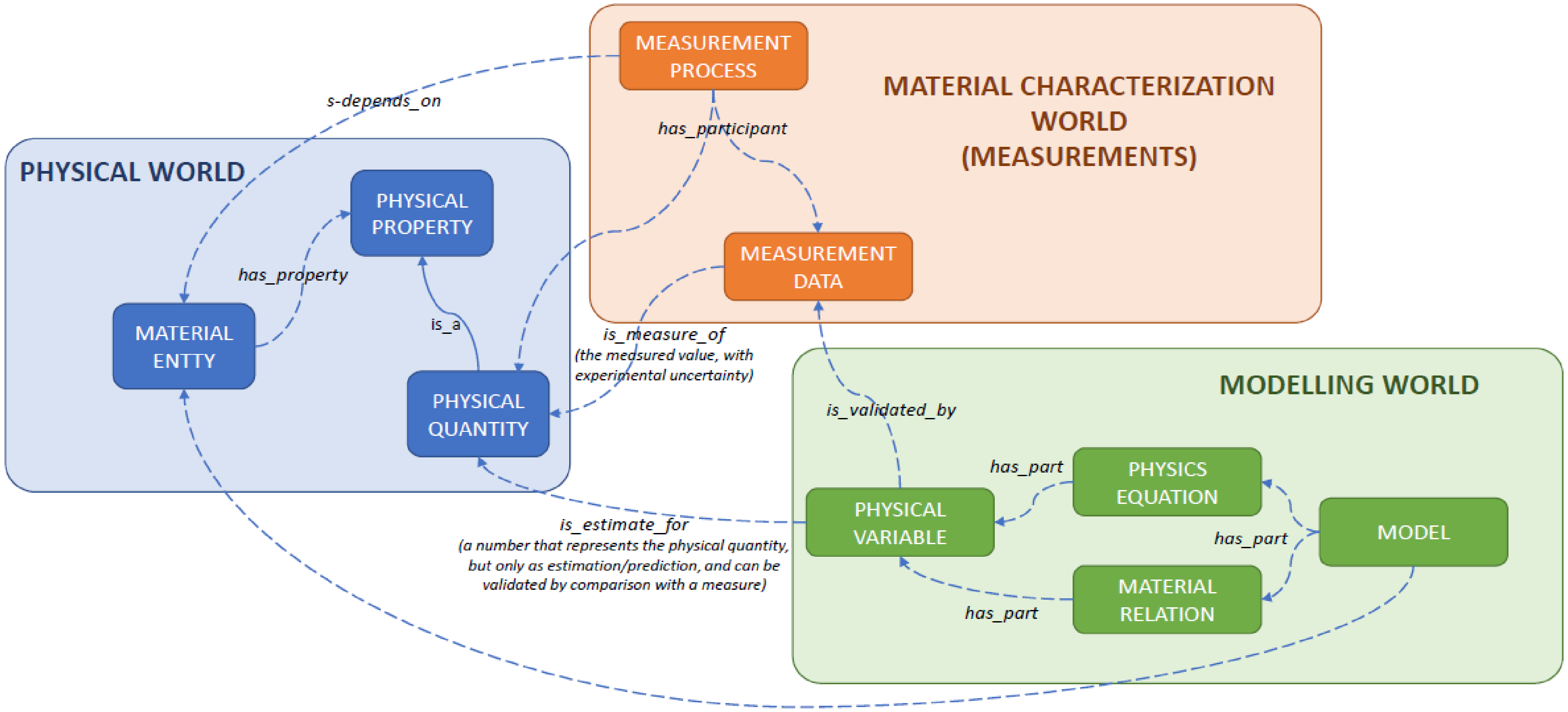


DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

BattINFO: the Battery Interface Ontology

- Creating the digital representation to connect the different battery worlds
- Read more about the BattINFO ontology at the website or watch the video

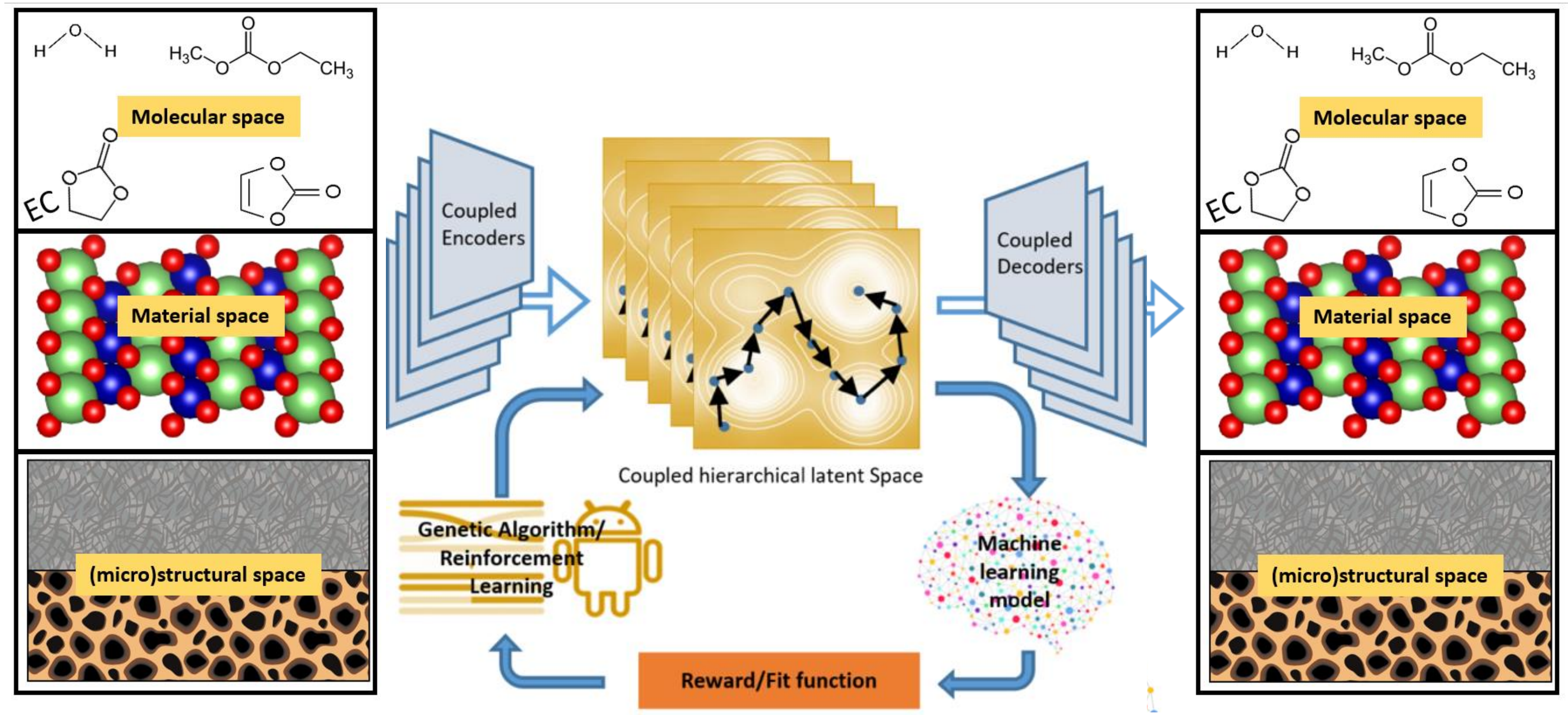


Simon Clark, Jesper Friis and others (SINTEF)

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 957189

Identifying Dynamic Interface Descriptors

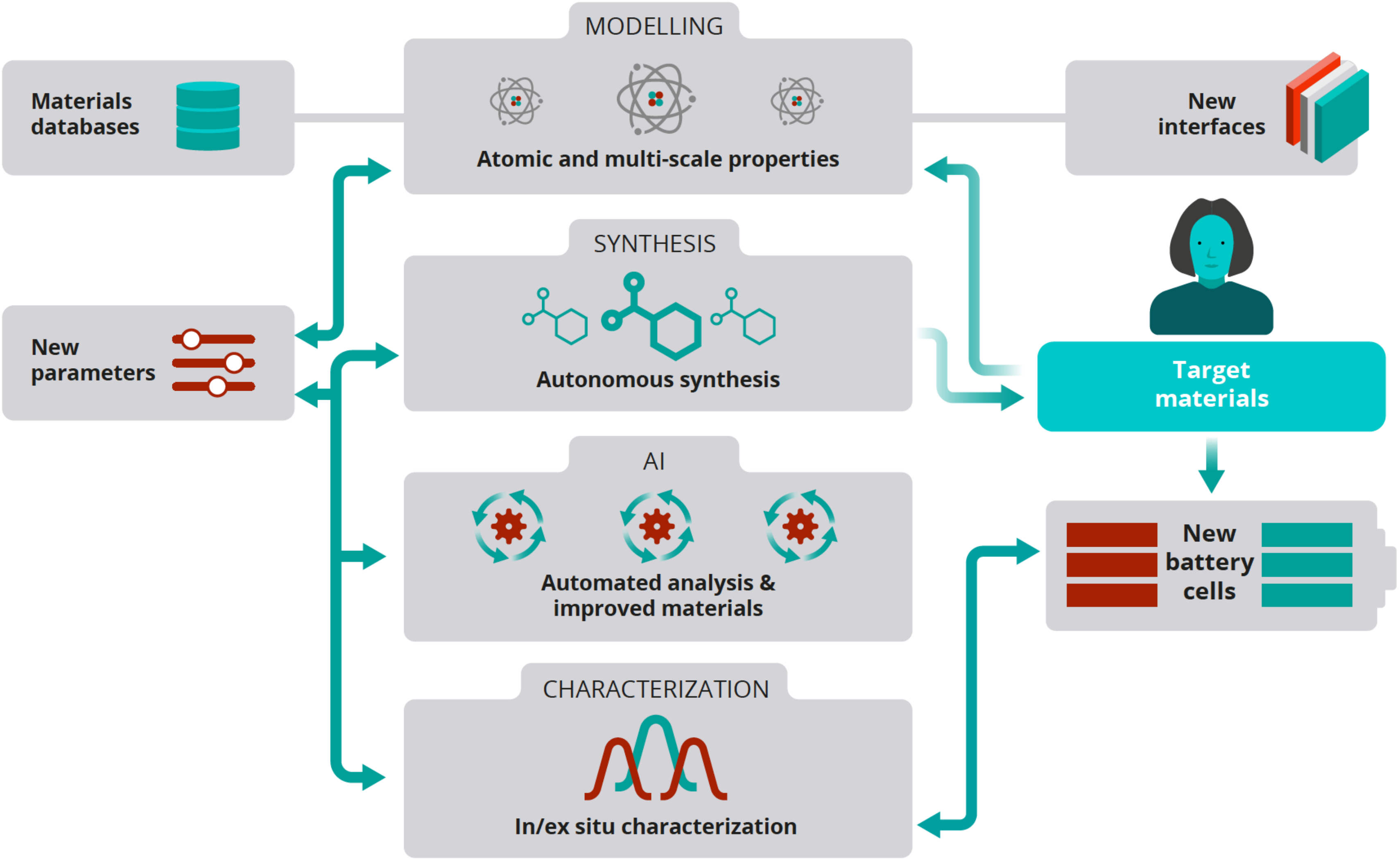
- Inverse design of battery interfaces with spatio-temporal multiscale models
- Generative deep learning to identify dynamic interface descriptors



Bhowmik, Castelli, Garcia-Lastra, Jørgensen, Winther, Vegge, Energy Storage Materials 21, 446-456 (2019)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

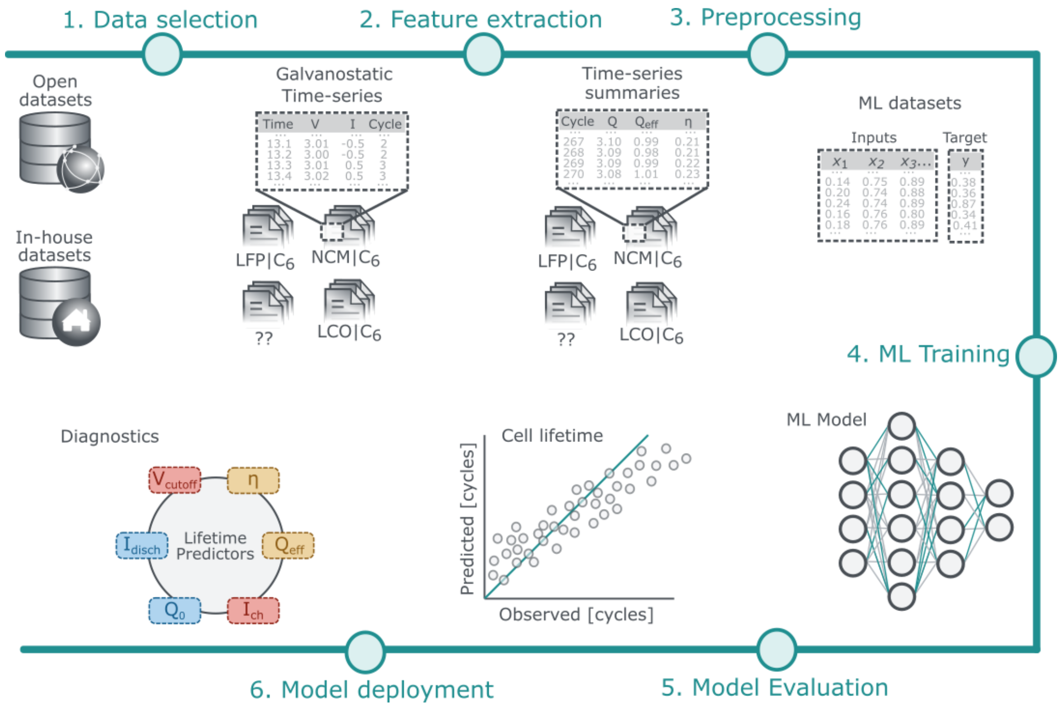
Integrated Autonomous Discovery Workflows



DTU Energy, Technical University of Denmark
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

Outlook

- Improving battery performance and utilization with digital twins
- Acceleration the battery discovery and development process by digitalization



Bhowmik, Vegge, Joule 4, 717-719 (2020)

Rieger, Flores, Bhowmik, et al. (2021)

PerSpective

ADVANCED ENERGY MATERIALS

www.advenergymat.de

Toward Better and Smarter Batteries by Combining AI with Multisensory and Self-Healing Approaches

Tejs Vegge, Jean-Marie Tarascon,* and Kristina Edström**

With an exponentially growing demand for rechargeable batteries, the development of new ultra-performant, fully scalable, and sustainable battery technologies and materials must be accelerated. Creating a holistic, closed-loop infrastructure for materials discovery, manufacturing, and battery testing that utilizes a common data infrastructure and autonomous workflows to bridge big data from all domains of the battery value chain, can pave the way for a transformative reduction in the required time to discovery. By embedding multisensory and self-healing capabilities in future battery technologies and integrating these with AI and physics-aware machine learning models capable of predicting the spatio-temporal evolution of battery materials and interfaces, it will, in time, be possible to identify, predict and prevent potential degradation and failure modes. This will facilitate enhanced battery quality, reliability, and life, for example, by preemptively changing the battery charging conditions or releasing self-healing additives from the separator membrane, akin to preemptive medicine, and form the basis for inverse design of new battery materials, interfaces, and additives. The large-scale and long-term European research initiative BATTERY 2030+ seeks to make this longer-than ten-year vision a reality through the development of a versatile and chemistry neutral "Battery Interface Genome—Materials Acceleration Platform" infrastructure (BIG-MAP).

1. Introduction

The concurrent transformations of the automotive sector toward e-mobility and the applicability of data-driven approaches in science and energy technology,[1] provides a synergistic opportunity to accelerate the battery discovery and manufacturing processes and to optimize the performance and lifetime of battery cells.[2]

As new high-performance battery materials, chemistries, and cell designs emerge to compete with existing Li-ion batteries,[3] they face a common challenge in controlling the complex dynamic processes occurring at battery interfaces, which span a multitude of time- and length scales.[4] Developing a versatile and chemistry neutral infrastructure that is capable of monitoring, predicting, and controlling the dynamic properties and evolution of these interfaces and interphases like the solid-electrolyte interphase (SEI), is a cornerstone of the long-term roadmap of the large-scale European initiative BATTERY 2030+[5] and the BIG-MAP project in particular.

Vegge, Tarascon, Edström, Advanced Energy Materials 10.1002/aenm.202100362 (2021)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

Scale Bridging Methodologies for Higher Fidelity Engineering Models and SoX Observers of Batteries

Tomaž Katrašnik

University of Ljubljana/EGVIA

Scale bridging methodologies for higher fidelity engineering models and SoX observers of batteries

Tomaž Katrašnik
University of Ljubljana
Faculty of Mechanical Engineering
Laboratory for Internal combustion engines and electromobility
http://lab.fs.uni-lj.si/LICeM/

and

National Institute of Chemistry

Objectives

Objectives of 2Zero Partnership*

General objectives of the partnership:

- Contribute to Europe having the first carbon-neutral road transport system by 2050;
- Technology leadership supporting economic growth and safeguarding jobs, creation all over Europe;
- Ensure European competitiveness thanks to solutions for an integrated carbon-neutral road transport ecosystem;
- Improve the health and quality of life of EU citizens and ensure mobility for people and goods.

Specific objectives of the partnership:

- Develop zero tailpipe emission, affordable user-centric solutions (technologies and services) for road-based mobility all across Europe and accelerate their acceptance to improve air quality in urban areas and beyond;
- Develop affordable, user-friendly charging infrastructure concepts and technologies that include vehicle and grid interaction;
- Demonstrate innovative use cases for the integration of zero tailpipe emission vehicles and infrastructure concepts for the road mobility of people and goods;
- Support the development of life-cycle analysis tools and skills for the effective design, assessment and deployment of innovative concepts in products/services in a circular economy context.

Message

- **Batteries are one of the key enablers to achieve listed objectives.**

Objectives of Batt4EU*

- Increase energy density
- Increase power density
- Improve cycle lifetime
- Ensure battery safety
- Implement BAT in manufacturing and recycling operations
- Improve sustainability and circularity
- Reduce battery cost

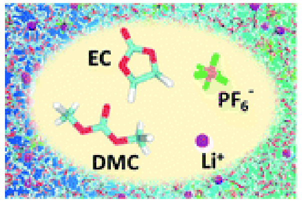
*might be subjected to changes.

University *of Ljubljana*
Faculty *of Mechanical Engineering*

Process

(sub)Nanoscale [~nm]

www.neicorporation.com

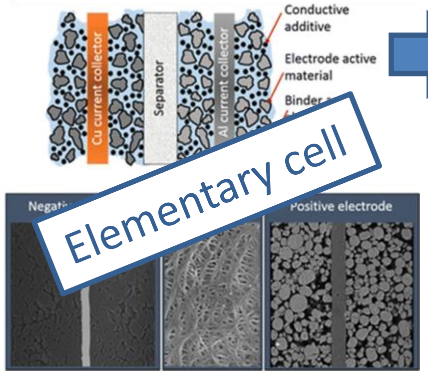


pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05140e#!divAbstract

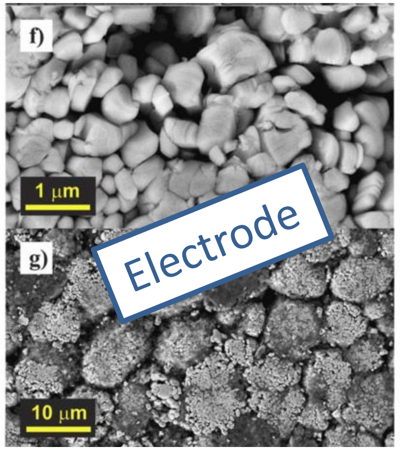
Materials

....

Microscale [~µm]

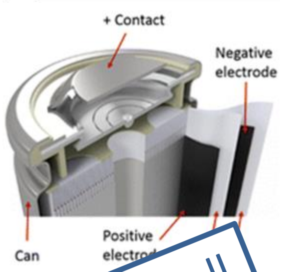


Elementary cell



Electrode

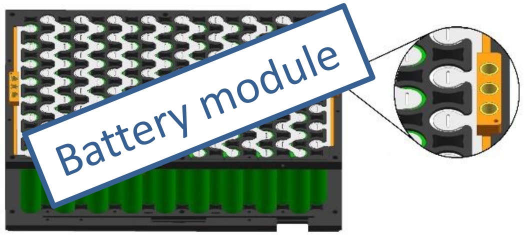
I. Mele ... T. Katrašnik, I, Journal of The Electrochemical Society, 2020 167 060531



Battery cell

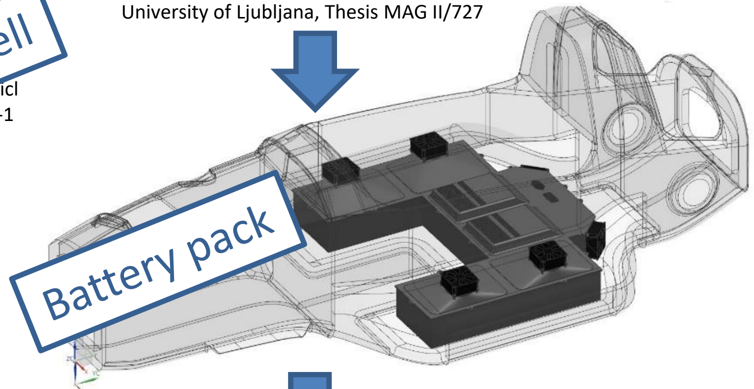
https... e/10.1... ...018-0196-1

Macroscale [> ~100 µm, >>]

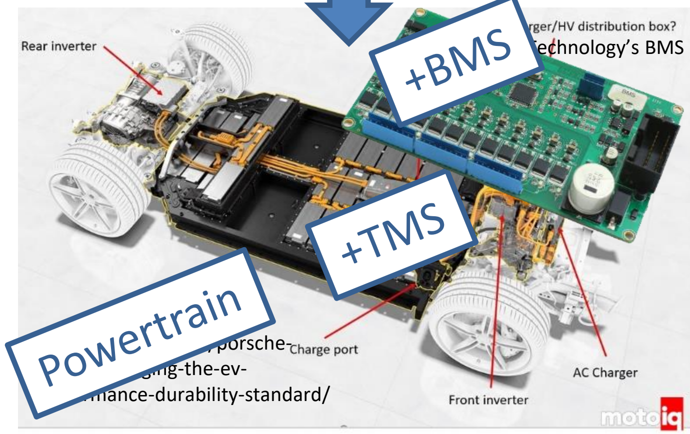


Battery module

University of Ljubljana, Thesis MAG II/727



Battery pack



+BMS

+TMS

Powertrain

...porsche-...ng-the-ev-...mance-durability-standard/

Cloud

www.bosch-presse.de

fs...i.eu

Charging infrastructure

Objectives of Batt4EU

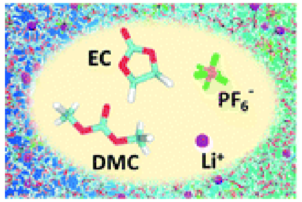
- Increase energy density
- Increase power density
- Improve cycle lifetime
- Ensure battery safety
- Implement BAT in manufacturing and recycling operations
- Improve sustainability and circularity
- Reduce battery cost

University of Ljubljana
Faculty of Mechanical Engineering

Process

(sub)Nanoscale [~nm]

www.neicorporation.com

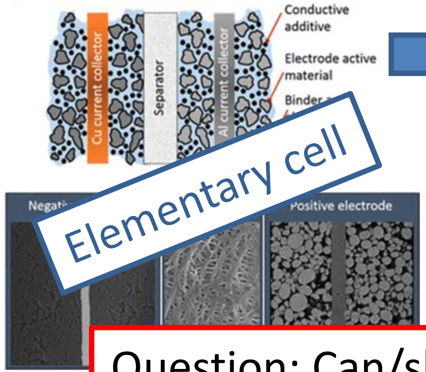


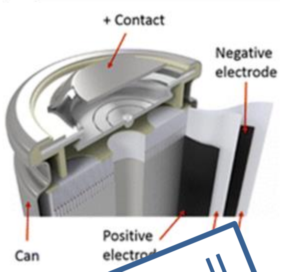
pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05140e#!divAbstract

Materials

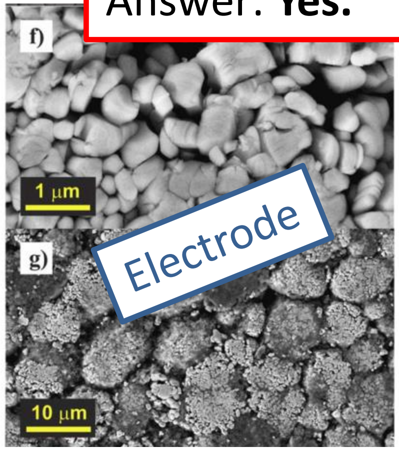
....

Microscale [~µm]



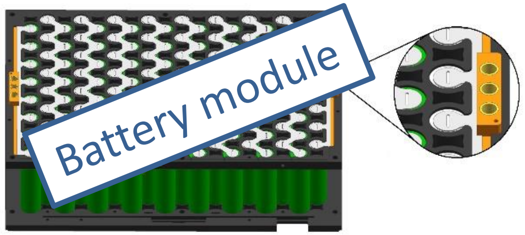


https:// ... articl e/10.1 ... 018-0196-1

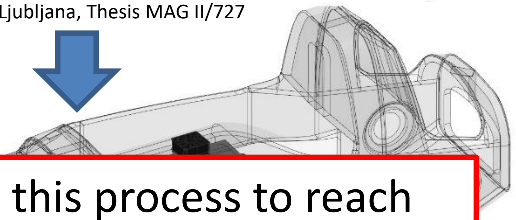


I. Mele ... T. Katrašnik, I, Journal of The Electrochemical Society, 2020 167 060531

Macroscale [> ~100 µm, >>]

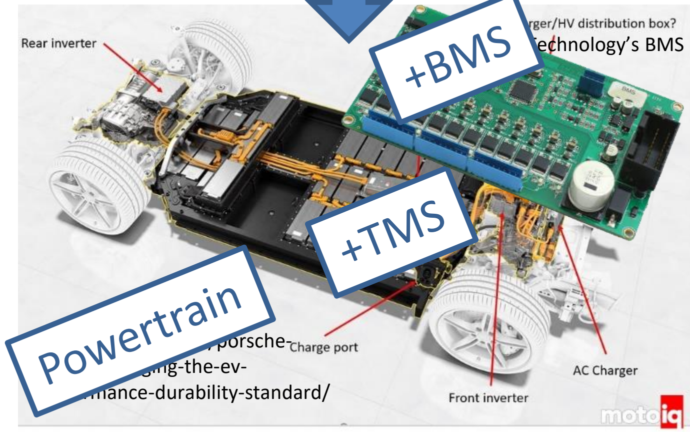


University of Ljubljana, Thesis MAG II/727



Question: Can/should we further improve this process to reach listed objectives and deliver beyond State-of-the-Art products?

Answer: **Yes.**



...porsche-...ng-the-ev-...mance-durability-standard/

www.bosch-presse.de

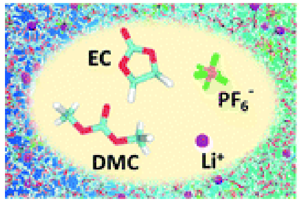
Objectives of Batt4EU

- Increase energy density
- Increase power density
- Improve cycle lifetime
- Ensure battery safety
- Implement BAT in manufacturing and recycling operations
- Improve sustainability and circularity
- Reduce battery cost

Modelling

Electronic/atomistic models

www.neicorporation.com

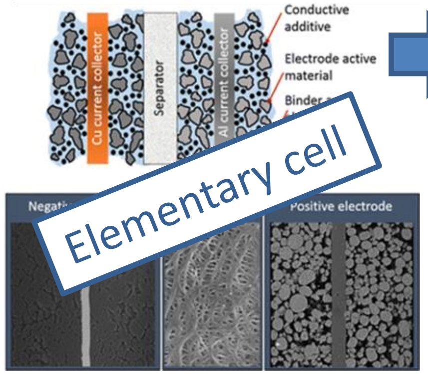


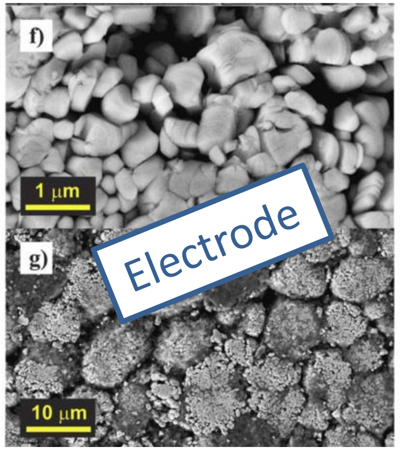
pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05140e#!divAbstract

Materials

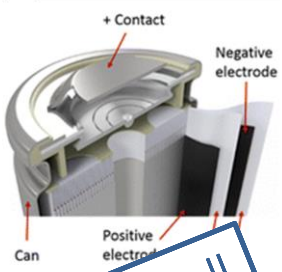
....

Mesoscopic models



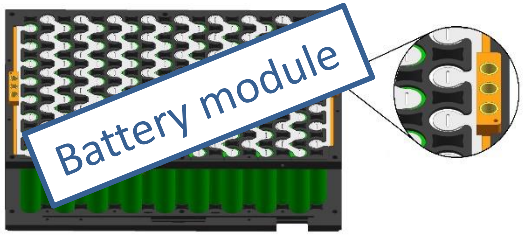


I. Mele ... T. Katrašnik, I, Journal of The Electrochemical Society, 2020 167 060531

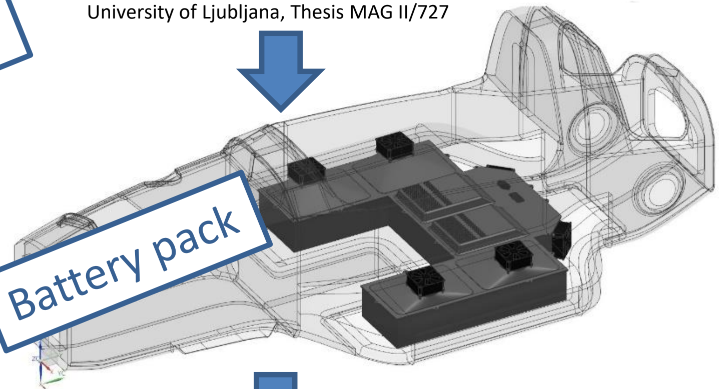


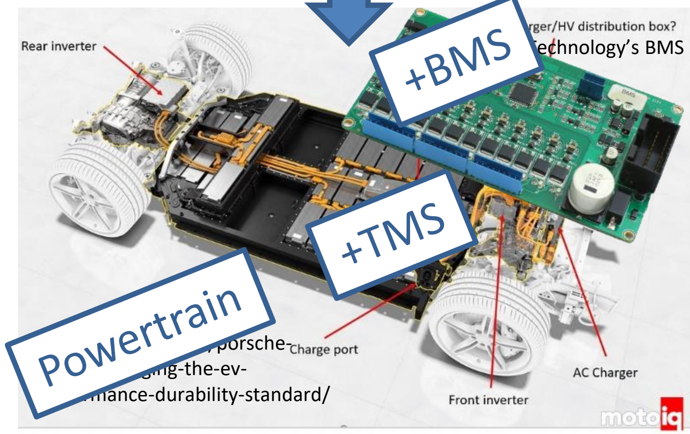
https ... articl
e/10.1 ... 018-0196-1

Continuum models



University of Ljubljana, Thesis MAG II/727





...porsche-...
...ging-the-ev-
...mance-durability-standard/

www.bosch-presse.de

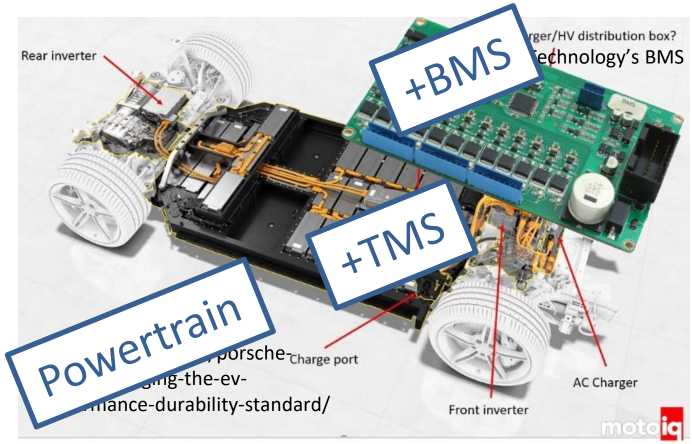
fs... ...i.eu

Modelling

Continuum models

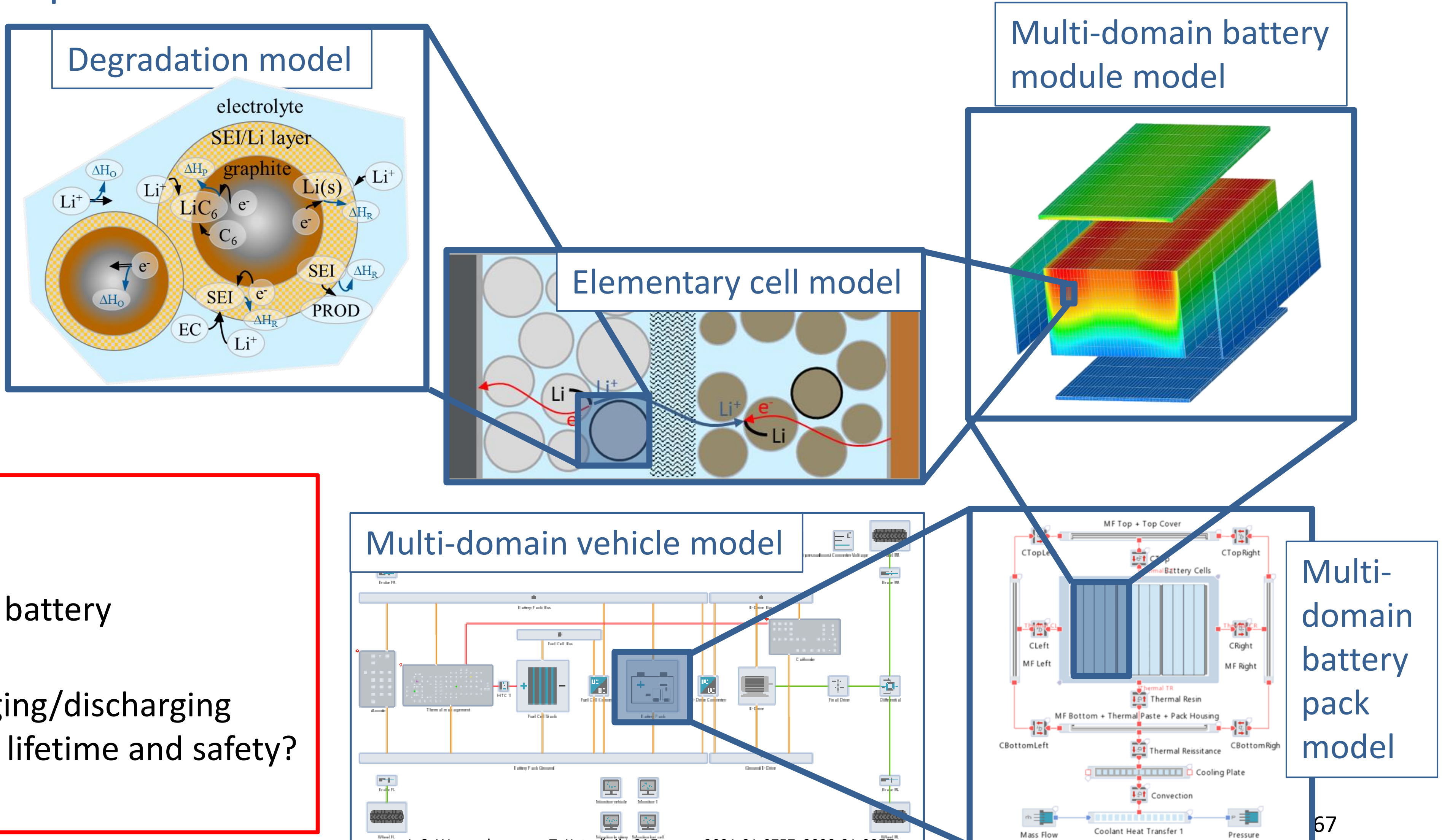
Questions (a few examples):

- Which cells?
- Which type and topology of battery thermoregulation system?
- Which are the limiting charging/discharging powers to ensure envisaged lifetime and safety?
- ...



Modelling - State-of-the-Art (selected example of a multi-domain multi-scale model)

Mesoscopic models **Continuum models**



J. C. Wurzenberger … T. Katrašnik, SAE paper 2021-01-0757, 2020-01-0857

Questions (a few examples):

- Which cells?
- Which type and topology of battery thermoregulation system?
- Which are the limiting charging/discharging powers to ensure envisaged lifetime and safety?
- …

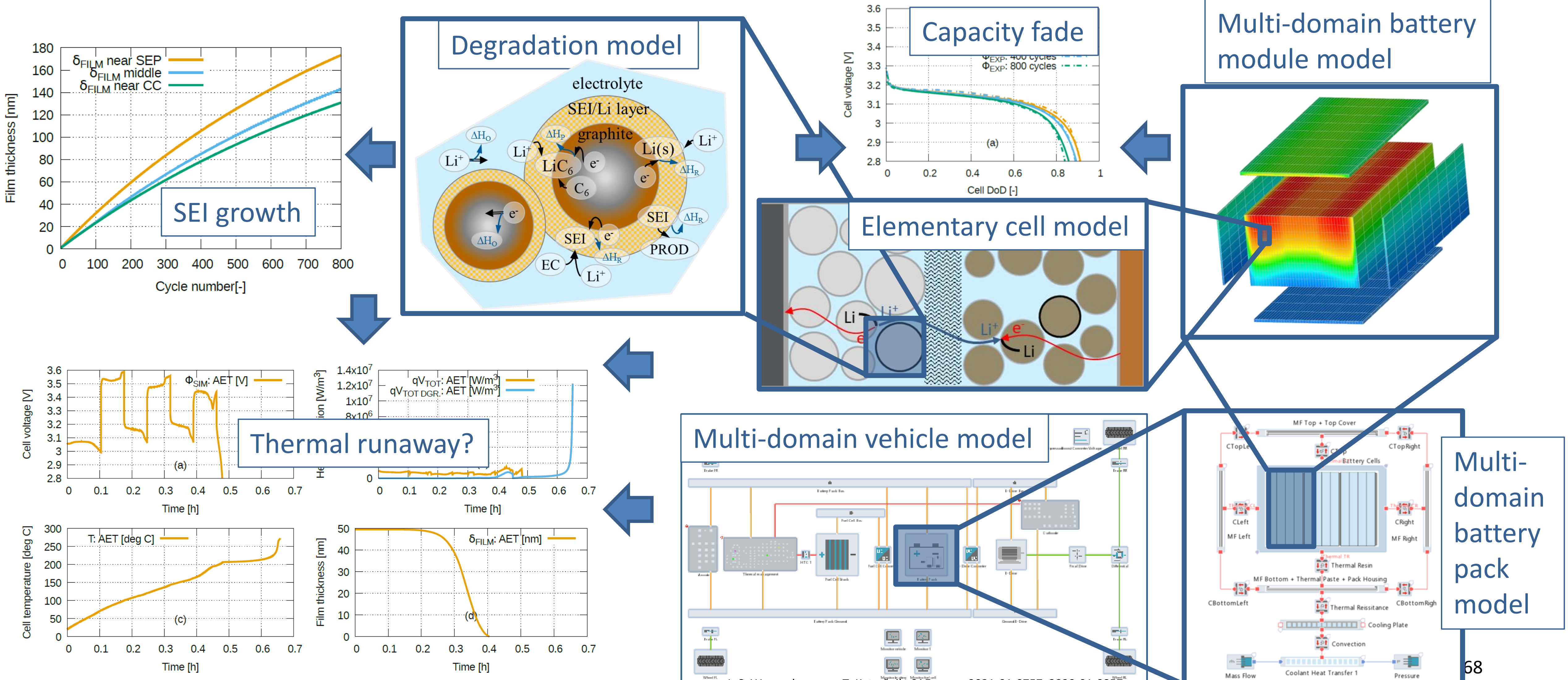
University of Ljubljana
Faculty of Mechanical Engineering

Asterics obelics Slovenian Research Agency

Modelling - State-of-the-Art (selected example of a multi-domain multi-scale model)

Mesoscopic models

Continuum models



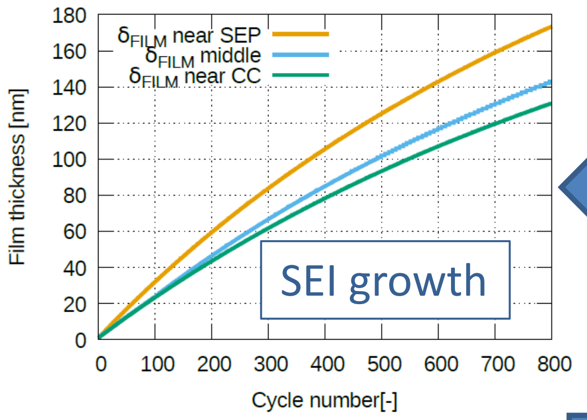
J. C. Wurzenberger … T. Katrašnik, SAE paper 2021-01-0757, 2020-01-0857

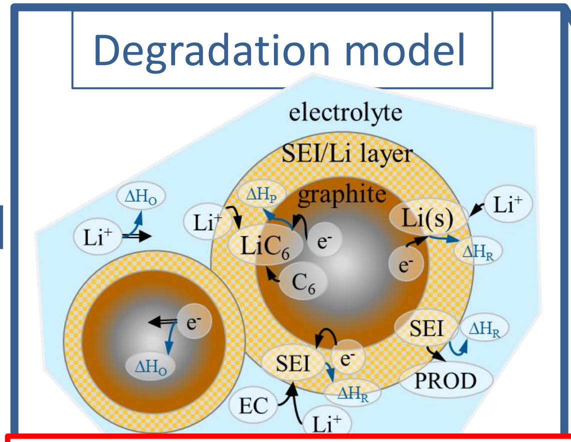
T. Katrašnik et al, Energy Conversion and Management 236 (2021) 114036

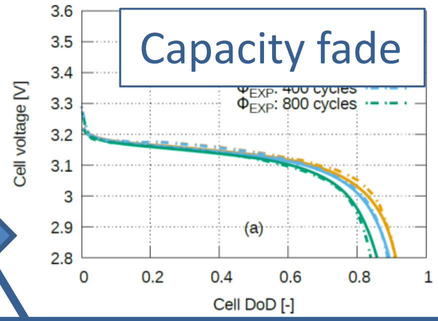
Modelling - State-of-the-Art (selected example of a multi-domain multi-scale model)

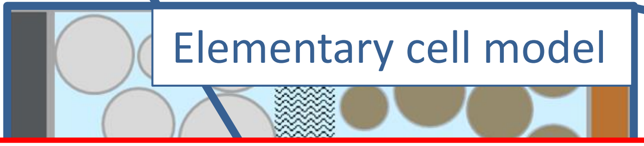
Mesoscopic models

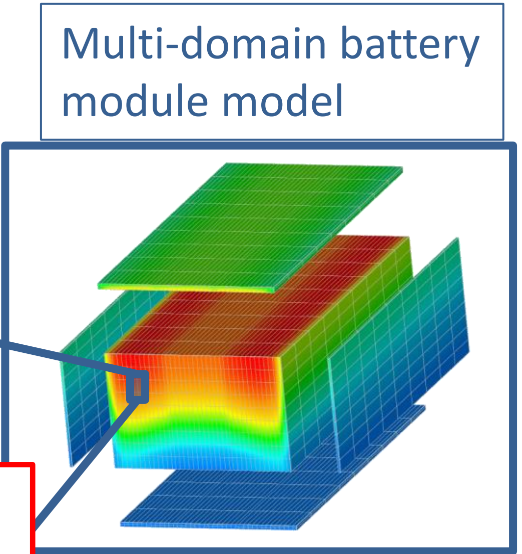
Continuum models



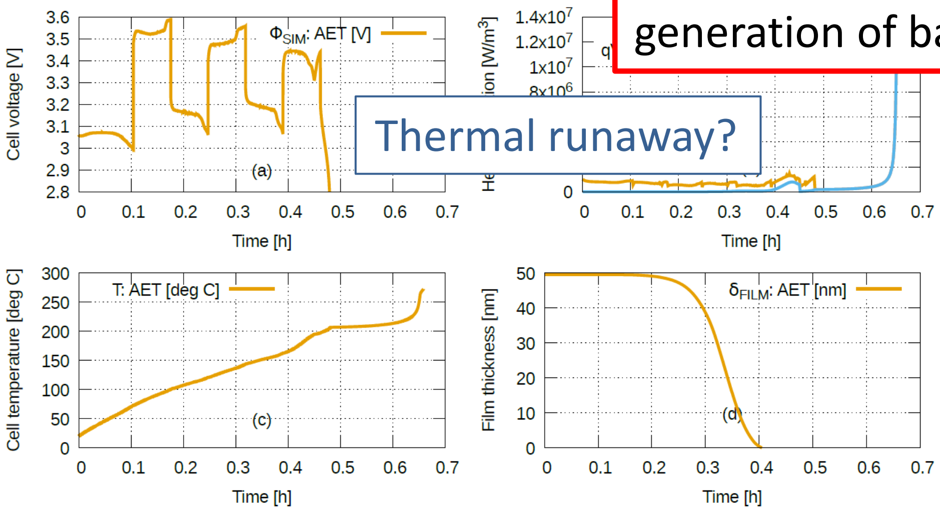


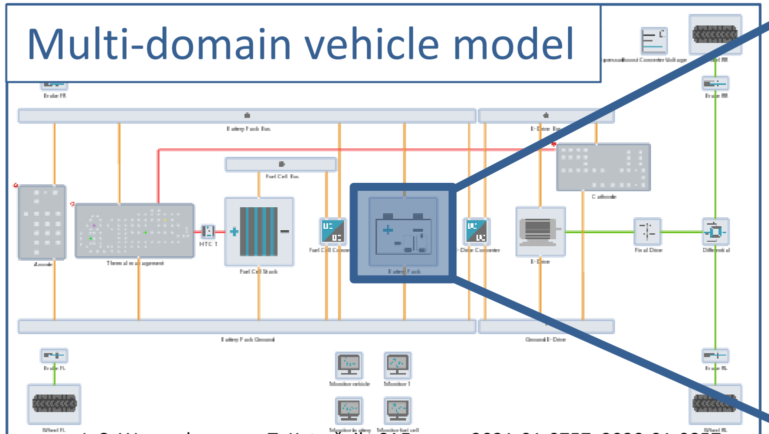


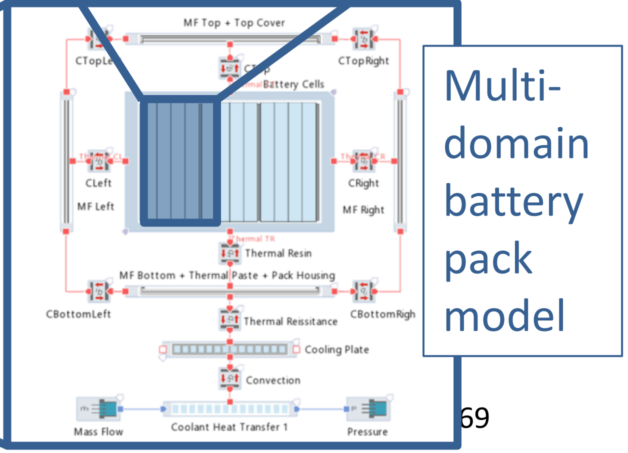




These recently developed multi-domain multi-scale models and other State-of-the-Art models will be utilized to develop next-generation of batteries and battery packs.







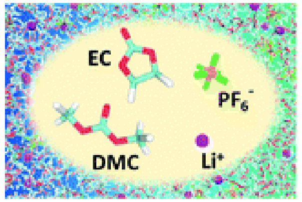
J. C. Wurzenberger … T. Katrašnik, SAE paper 2021-01-0757, 2020-01-0857

T. Katrašnik et al, Energy Conversion and Management 236 (2021) 114036

Why scale bridging?

Electronic/atomistic models

www.neicorporation.com

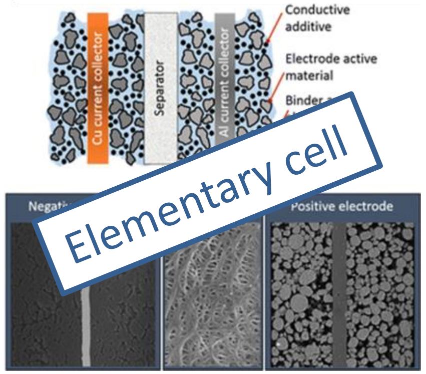


pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05140e#!divAbstract

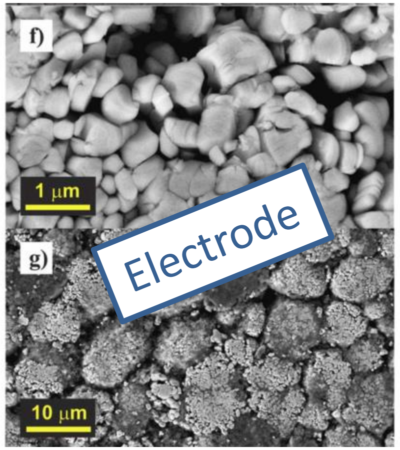
Materials

....

Mesoscopic models



Elementary cell



Electrode

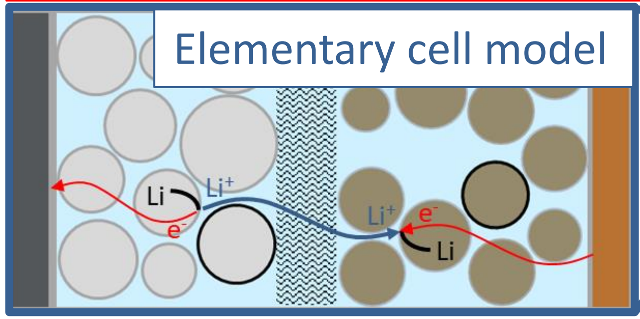
I. Mele ... T. Katrašnik, I, Journal of The Electrochemical Society, 2020 167 060531

Gap?

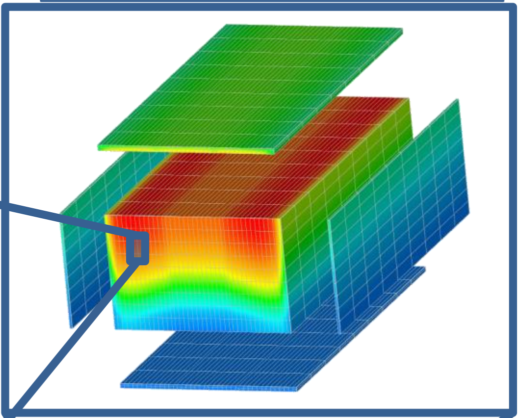
Continuum models

The elementary cell model is a key bridging model between lower scales models and higher scale engineering models of powertrain components.

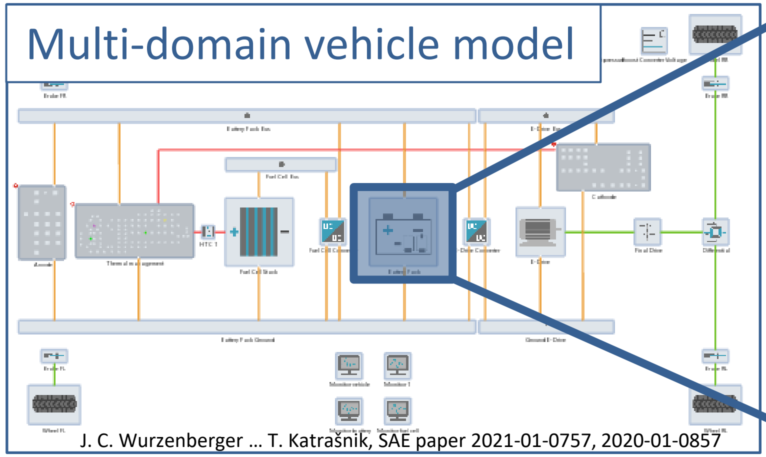
Elementary cell model



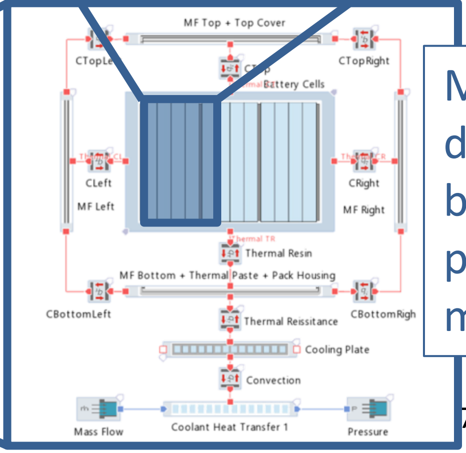
Multi-domain battery module model



Multi-domain vehicle model



Multi-domain battery pack model

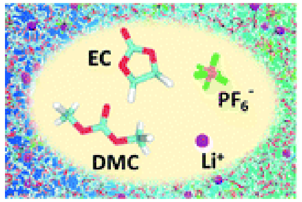


J. C. Wurzenberger ... T. Katrašnik, SAE paper 2021-01-0757, 2020-01-0857

Why scale bridging?

Electronic/atomistic models

www.neicorporation.com



pubs.rsc.org/en/content/articlelanding/2016/cp/c6cp05140e#!divAbstract

Materials

....

Mesoscopic models

Continuum models

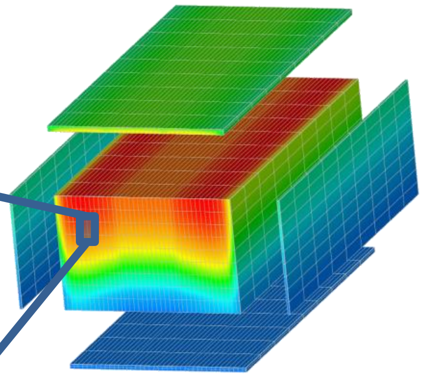
The elementary cell model

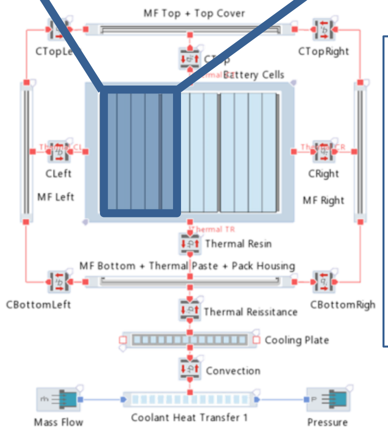
Questions (a few examples):

- Is it possible to ***model*** from atoms to the battery pack? *or* Is it possible to ***predict*** the performance/degradation/safety parameters of cells/packs that are virtually assembled utilizing new virtually designed materials and/or different manufacturing techniques or process parameters and/or different cell, module and stack designs?
- Is it possible to ***mechanistically determine root-cause relations*** of battery degradation and safety critical phenomena? and Is it possible to provide clear guidelines for enhanced material synthesis, the manufacturing of electrodes and elementary cells, battery cells, modules, packs and their optimal control to mitigate or minimize these critical phenomena?
- Are SoX observers, in particular State-of-Health observer, in BMSs ***capable of pinpointing*** specific degradation/safety relevant phenomena and mitigate them?

Answer: **Not (yet).**

Multi-domain battery module model



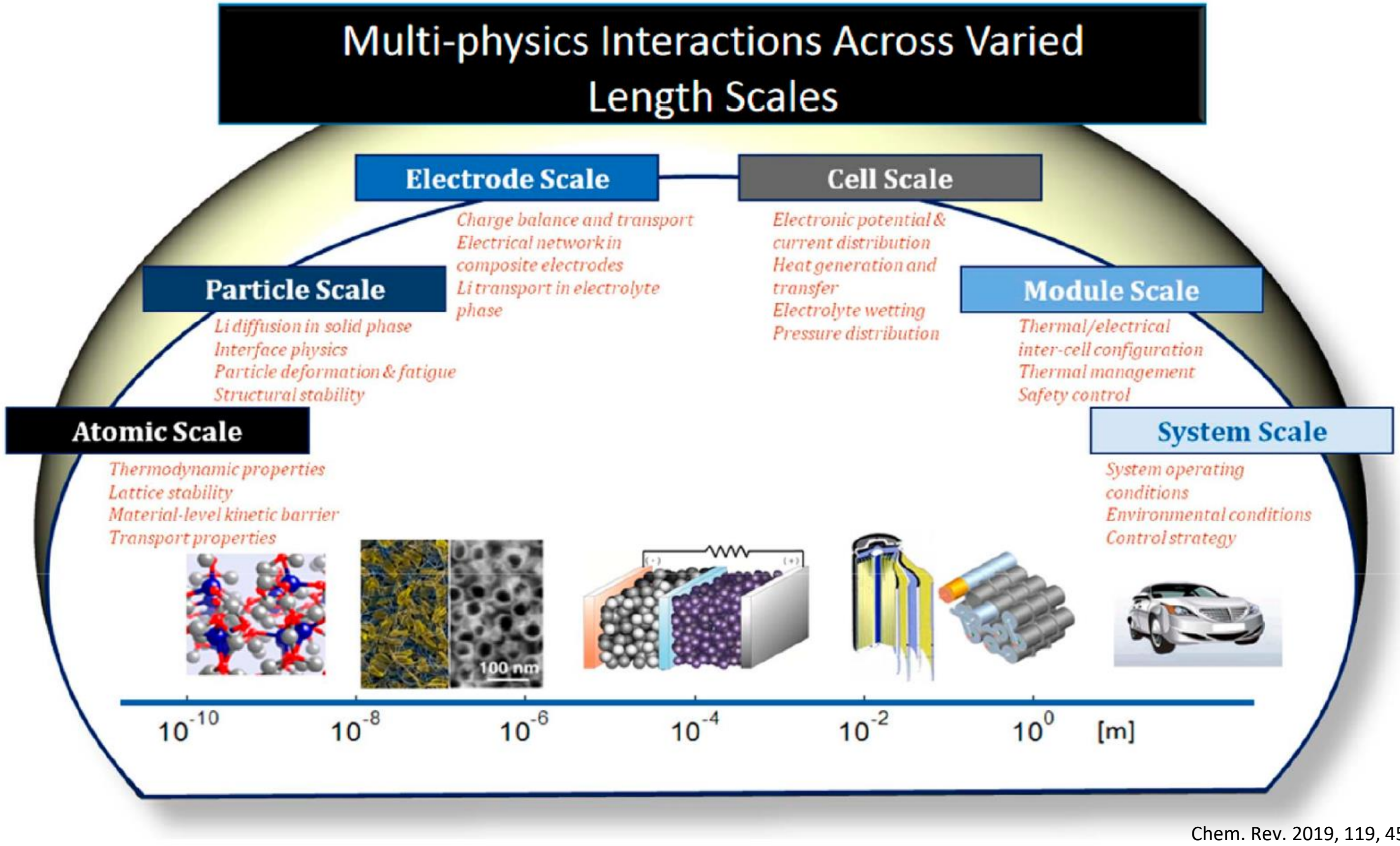


Multi-domain battery pack model

J. C. Wurzenberger … T. Katrašnik, SAE paper 2021-01-0757, 2020-01-0857

Why scale bridging?

- Because all relevant phenomena are not yet fully understood.
- Because transfer (bridging) across the scales is not yet (fully) mastered.
- …



Chem. Rev. 2019, 119, 4569–4627

Figure 61. Length scale dependent physics impacting battery modeling. Reproduced with permission from ref 9. Copyright 2016 Elsevier Ltd.

Modelling - Emerging approaches and Future research needs (selected examples)

Electronic/atomistic models → **Mesoscopic models** → **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models

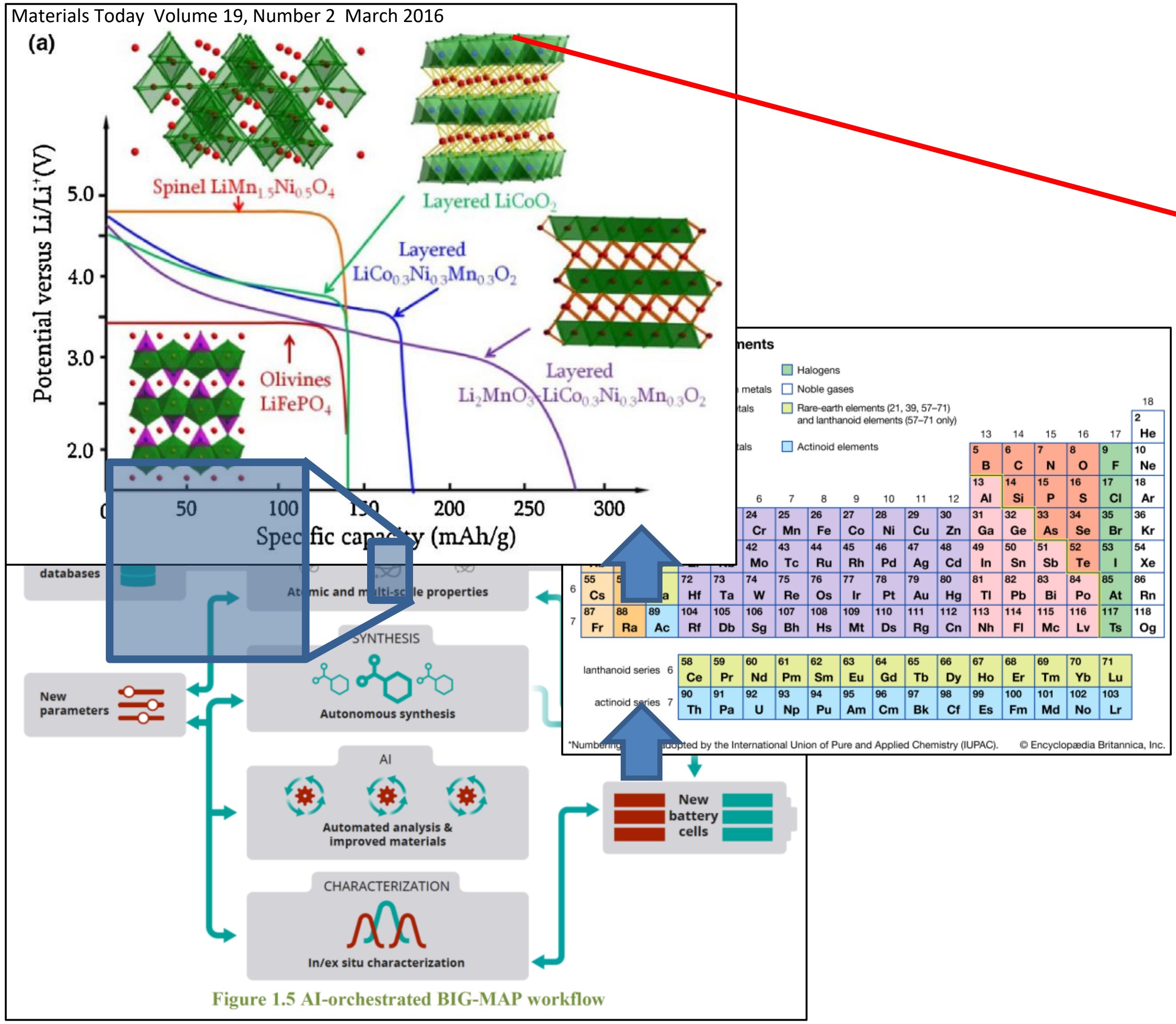
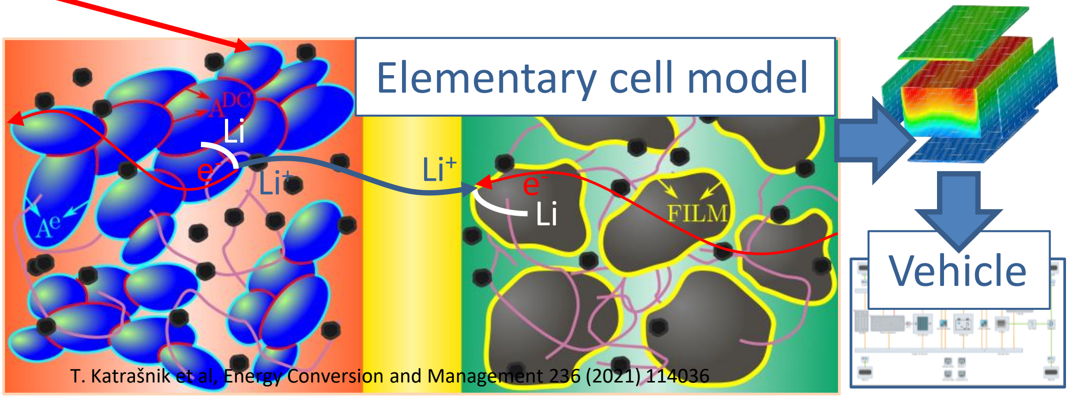


Figure 1.5 AI-orchestrated BIG-MAP workflow

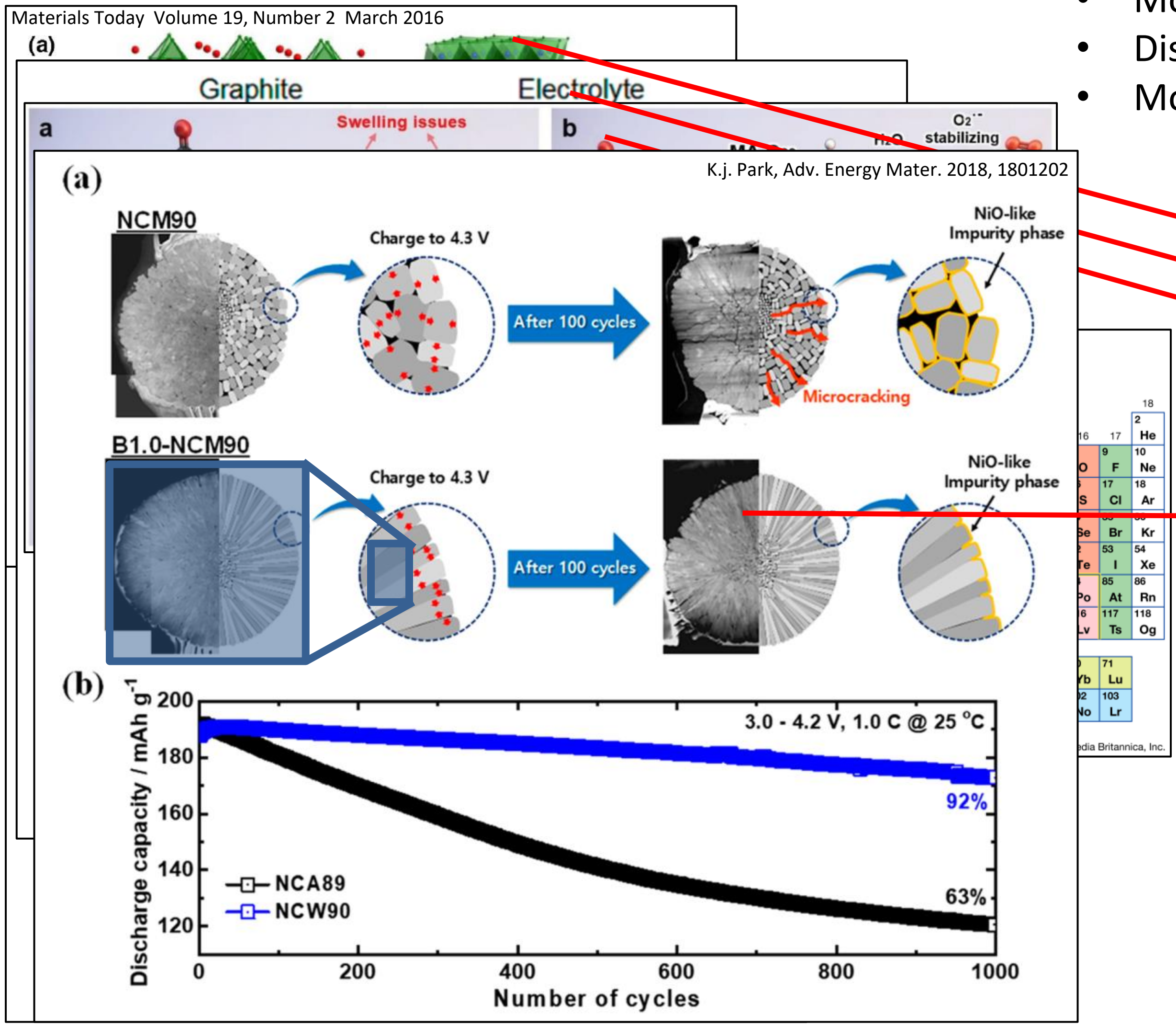


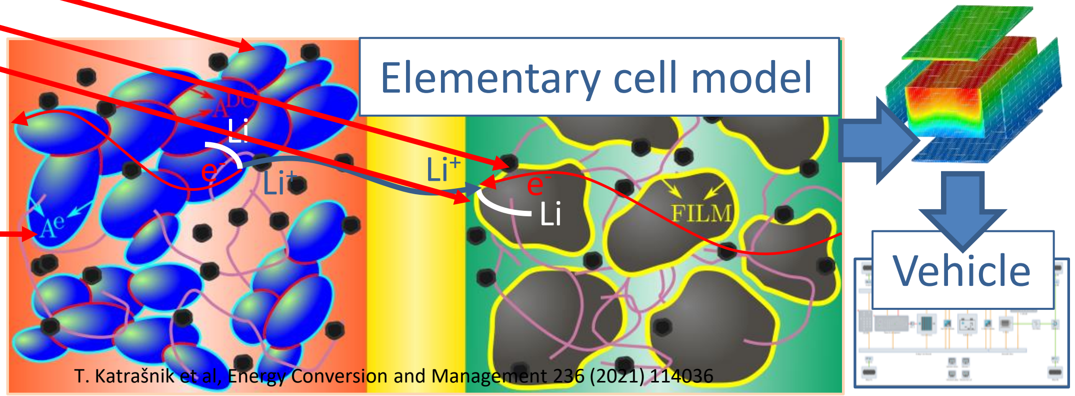
Modelling - Emerging approaches and Future research needs (selected examples)

Electronic/atomistic models → **Mesoscopic models** → **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models
- Modeling interfacial phenomena and formation of interphases
- Discovering scavengers of degradation reactions and healing additives
- Modeling synthesis process



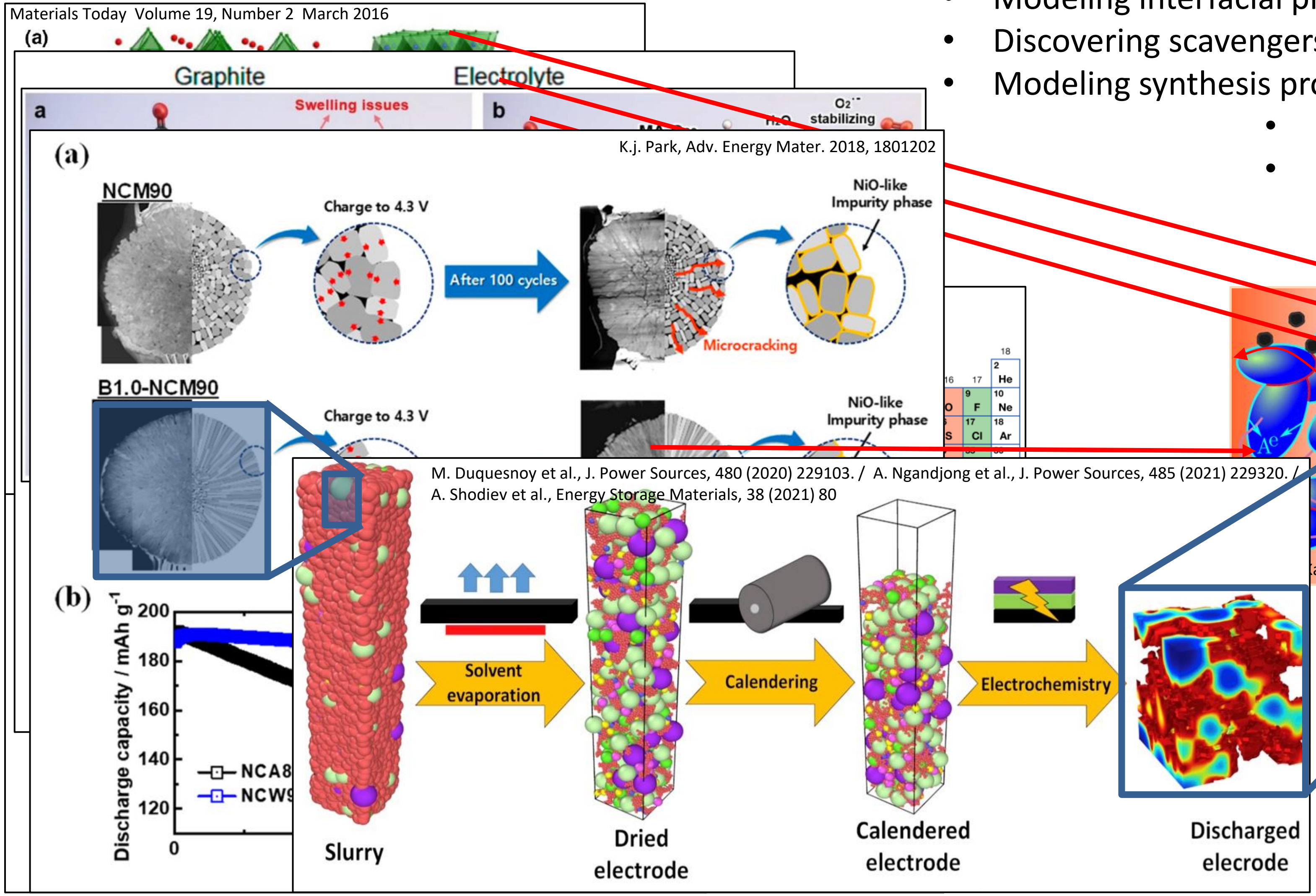


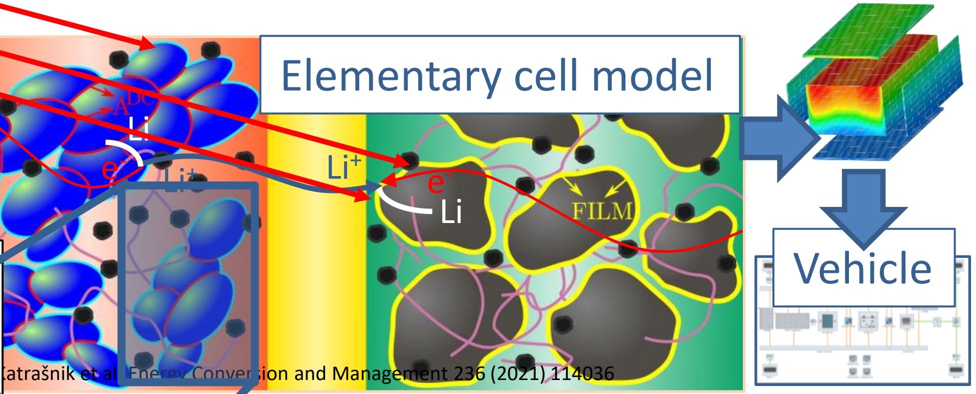
Modelling - Emerging approaches and Future research needs (selected examples)

Electronic/atomistic models → **Mesoscopic models** → **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models
- Modeling interfacial phenomena and formation of interphases
- Discovering scavengers of degradation reactions and healing additives
- Modeling synthesis process
    - Modeling manufacturing process
    - Modeling mesoscale transport properties



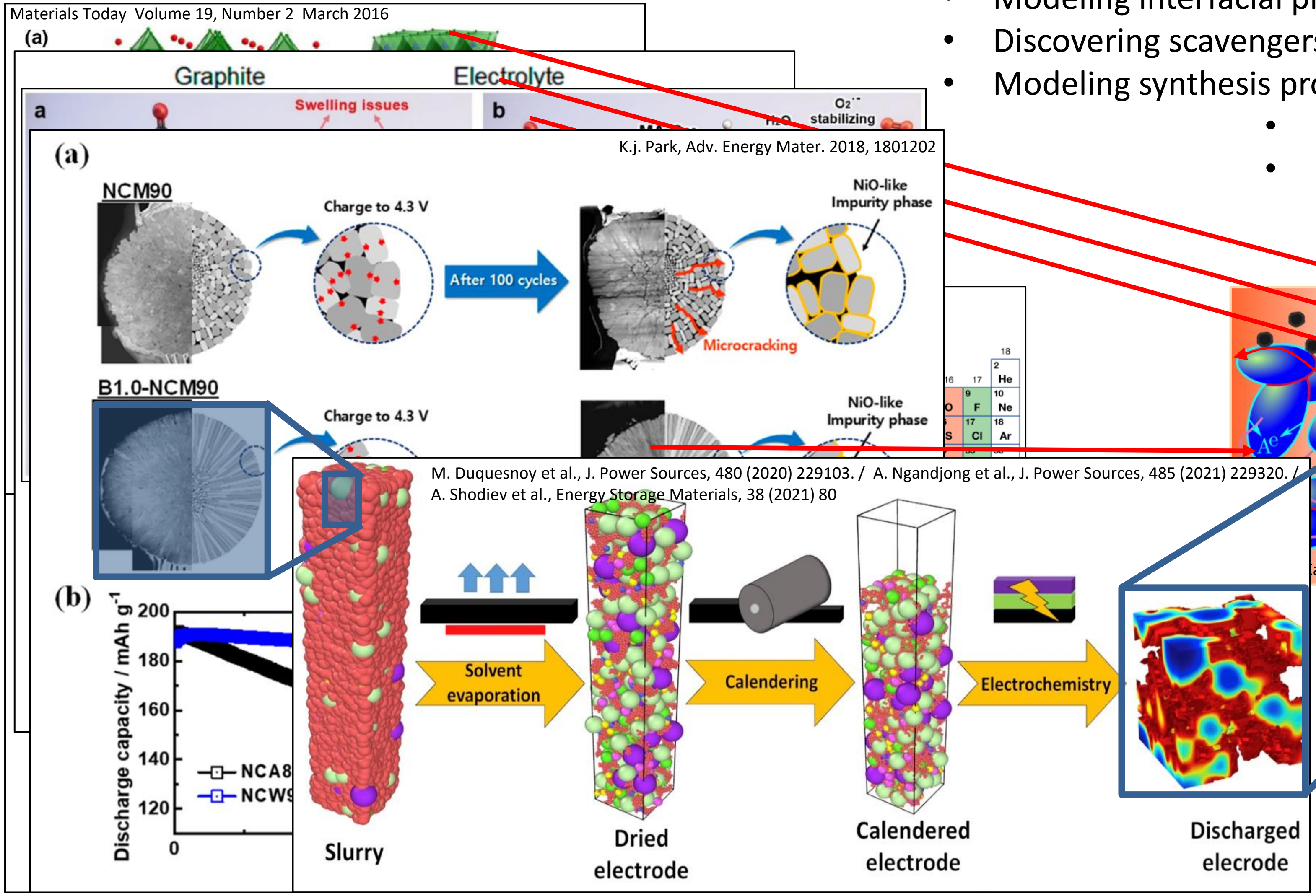


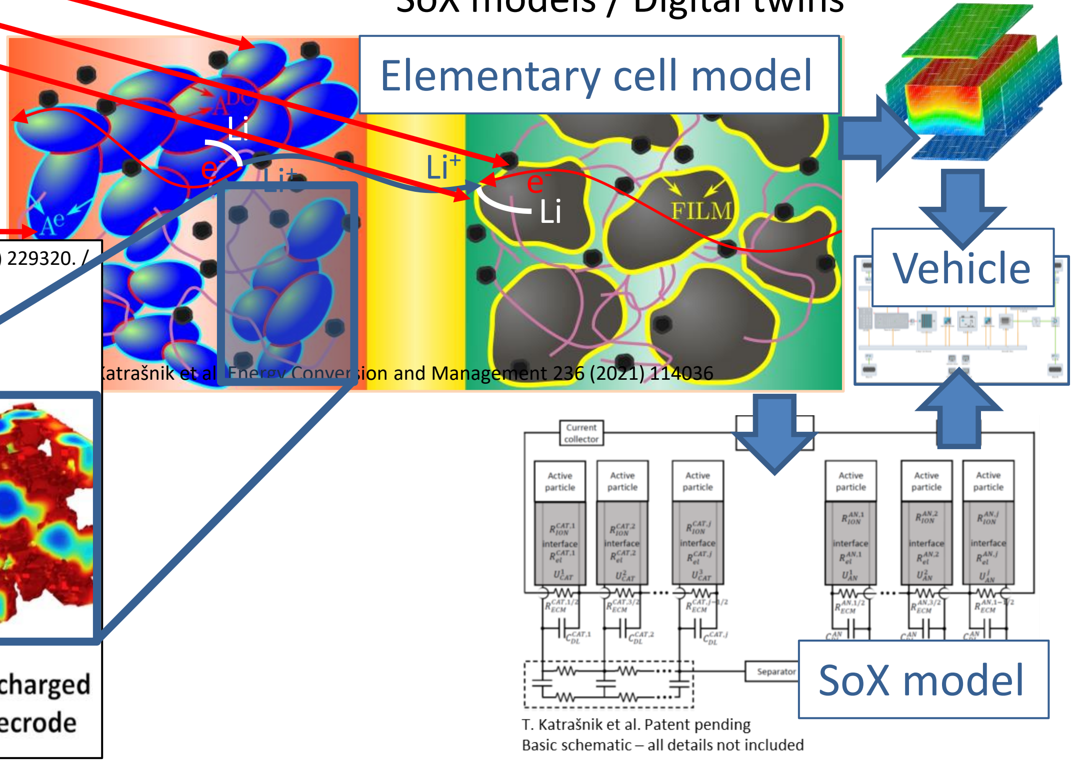
Modelling - Emerging approaches and Future research needs (selected examples)

Electronic/atomistic models — **Mesoscopic models** — **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models
- Modeling interfacial phenomena and formation of interphases
- Discovering scavengers of degradation reactions and healing additives
- Modeling synthesis process
  - Modeling manufacturing process
  - Modeling mesoscale transport properties
    - Scaling to physiochemically consistent SoX models / Digital twins





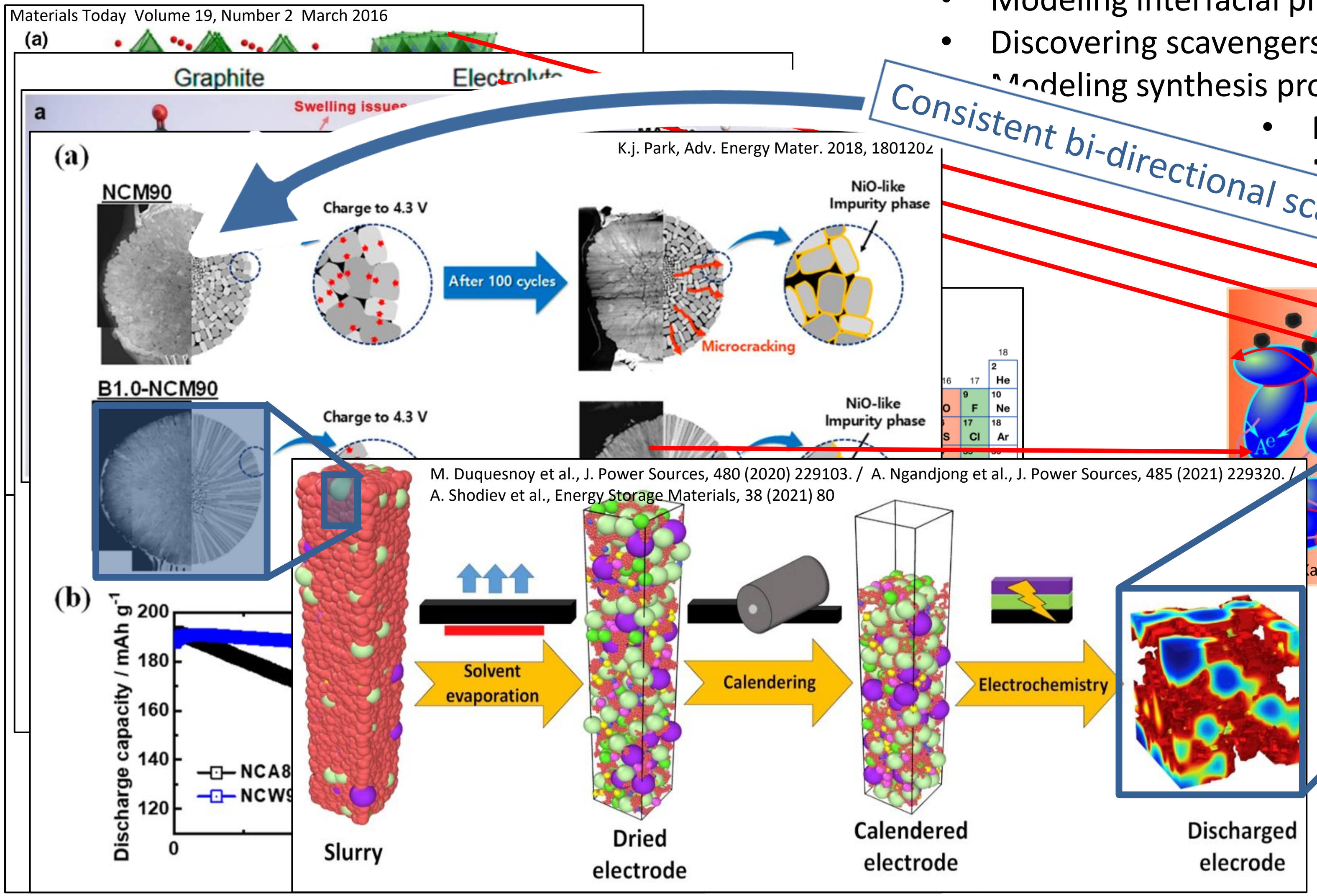
Modelling - Emerging approaches and Future research needs (selected examples)

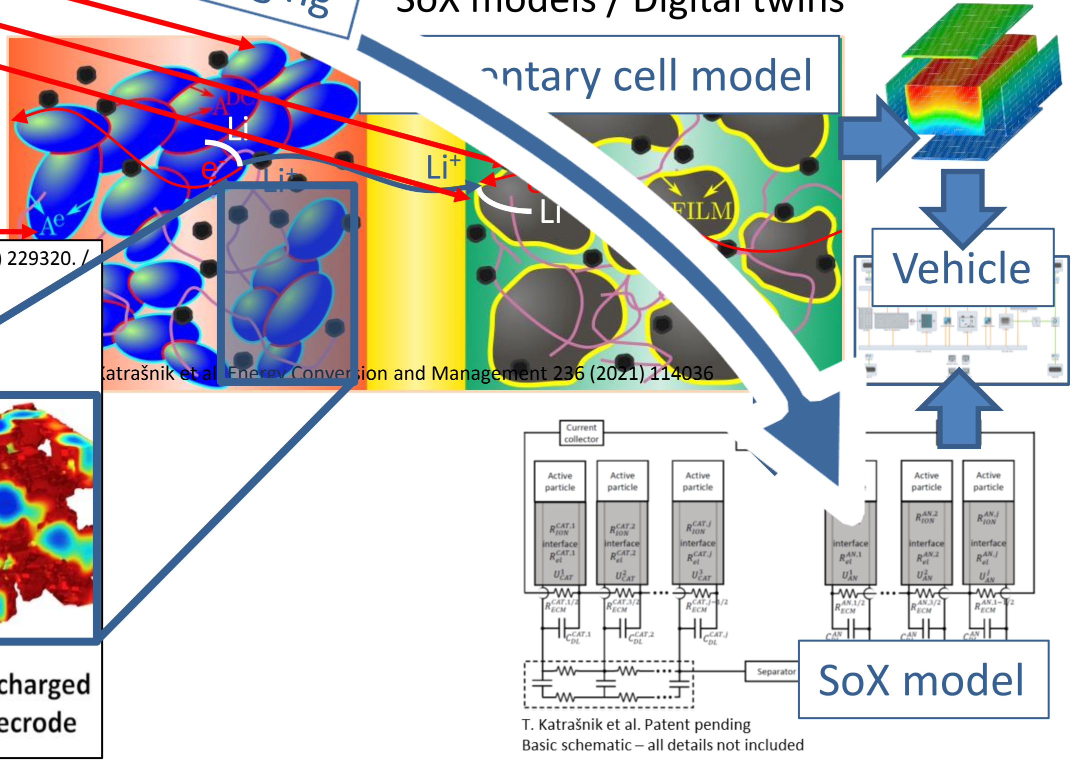
Electronic/atomistic models → **Mesoscopic models** → **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models
- Modeling interfacial phenomena and formation of interphases
- Discovering scavengers of degradation reactions and healing additives
- Modeling synthesis process
  - Modeling manufacturing process
  - Modeling mesoscale transport properties
    - Scaling to physiochemically consistent SoX models / Digital twins

Consistent bi-directional scale bridging





Modelling - Emerging approaches and Future research needs (selected examples)

Electronic/atomistic models → **Mesoscopic models** → **Continuum models**

Bridging the scales

- Predicting relevant material properties using ab-initio models
- Modeling interfacial phenomena and formation of interphases
- Discovering scavengers of degradation reactions and healing additives
- Modeling synthesis process
    - Modeling manufacturing process
    - Modeling mesoscale transport properties
        - Scaling to physiochemically consistent SoX models / Digital twins

Questions (a few examples):

Is it very likely that **innovative scale bridging methodologies and multi-scale models will enable**

- to (predictively) ***model*** from atoms to the battery pack?
- to ***mechanistically determine root-cause relations*** of battery degradation and safety critical phenomena?
- development of SoX observers in BMSs ***capable of pinpointing*** specific degradation/safety relevant phenomena and mitigate them?

Answer: **Yes.**

Message: Innovative scale bridging methodologies and multi-scale models are enablers for **higher fidelity engineering models and SoX observers of batteries** and thus provide the basis for a **paradigm shift in the battery development process** by paving the way towards **full** (a higher level of) **virtualization of the R&D process**.

Objectives

Objectives of 2Zero Partnership*

General objectives of the partnership:

- Contribute to Europe having the first carbon-neutral road transport system by 2050;
- Technology leadership supporting economic growth and safeguarding jobs, creation all over Europe;
- Ensure **European competitiveness** thanks to solutions for an integrated carbon-neutral road transport ecosystem;
- Improve the health and quality of life of EU citizens and ensure mobility for people and goods.

Specific objectives of the partnership:

- Develop zero tailpipe emission, affordable user-centric solutions (technologies and services) for road-based mobility all across Europe and accelerate their acceptance to improve air quality in urban areas and beyond;
- Develop affordable, user-friendly charging infrastructure concepts and technologies that include vehicle and grid interaction;
- Demonstrate innovative use cases for the integration of zero tailpipe emission vehicles and infrastructure concepts for the road mobility of people and goods;
- Support the development of life-cycle analysis tools and skills for the effective design, assessment and deployment of innovative concepts in products/services in a circular economy context.

Message

- **Batteries are one of the key enablers to achieve listed objectives.**
- **R&D activities in the area of battery modelling at all scales and in the area of scale bridging methodologies are needed to achieve listed objectives.**

Objectives of Batt4EU*

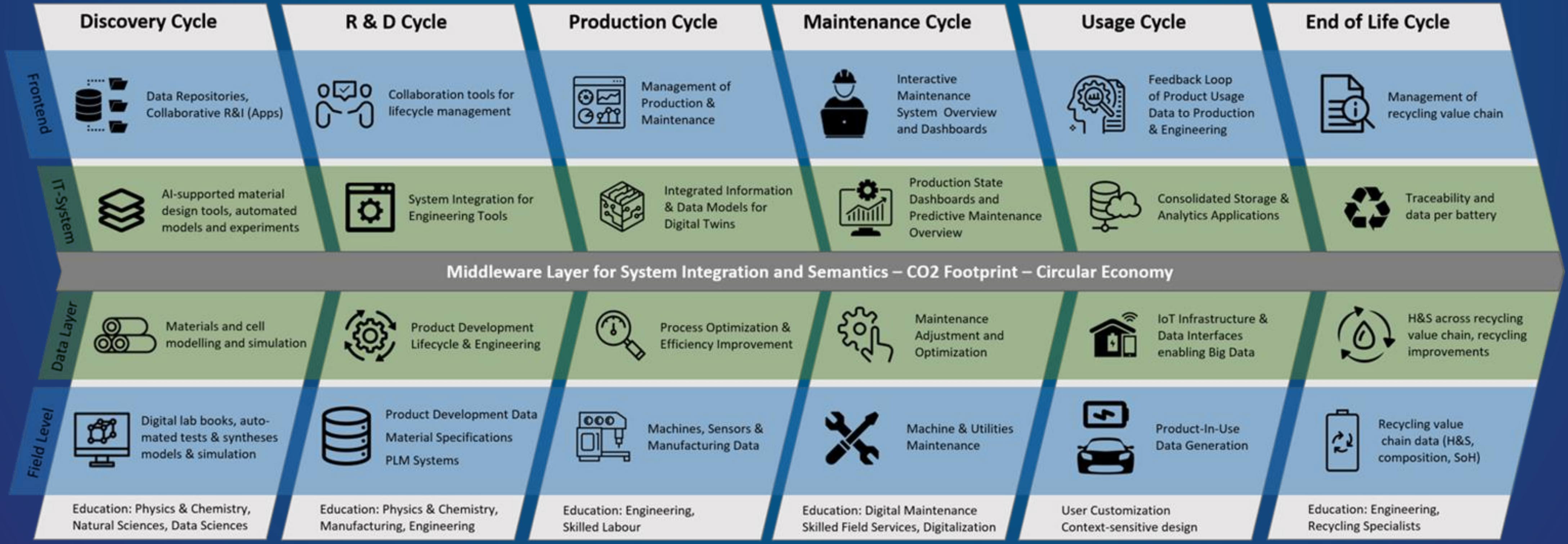
- Increase energy density
- Increase power density
- Improve cycle lifetime
- Ensure battery safety
- Implement BAT in manufacturing and recycling operations
- Improve sustainability and circularity
- Reduce battery cost

*might be subjected to changes.

Thank you for your attention

European Commission

The Batteries Europe Position Paper on Digitalization will soon be available on our website



This Workshop has been co-organised by:

BATTERIES EUROPE

ETIP SNET

EGVIA