

Norges miljø- og biovitenskapelige universitet



# Digital passports and digital twins for battery manufacturing:

The projects DigiPass and BatCAT (starting from 2024)

**Martin Thomas Horsch** 

28<sup>th</sup> September 2023 MatInfo seminar

Fakultet for realfag og teknologi

Forskergruppe materialteori og -informatikk



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# The challenge





Horizon Europe ID 101137725



Horizon Europe ID 101138510

MatInfo-seminar

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# **Explainable artificial intelligence**

**Epistemic opacity** (Humphreys, 2011): A "process is **epistemically opaque** relative to a cognitive agent *X* at time *t* [... if ...] *X* does not know at *t* all of the epistemically relevant elements"

**European AI Act proposal:** "To address the **opacity** that may make certain AI systems incomprehensible to or too complex for natural persons, a certain degree of transparency should be required for high-risk AI systems.<sup>1</sup> Users should be able to interpret the system output and use it appropriately. High-risk AI systems should therefore be accompanied by **relevant documentation**".

**Tendency:** Data must become explainable-AI-ready (XAIR). Making data trustworthy through explanations will increasingly become a **legal requirement**.

<sup>1</sup>Systems with "high risk" include all "safety components" related to "water, gas, heating, and electricity." MatInfo seminar 28<sup>th</sup> September 2023 3









# Explainable artificial intelligence

**Epistemic opacity** (Humphreys, 2011): A "process is **epistemically opaque** relative to a cognitive agent *X* at time *t* [... if ...] *X* does not know at *t* all of the **epistemically relevant elements**"

**European Al Act proposal:** "To address the **opacity** that may make certain Al systems incomprehensible to or too complex for natural persons, a certain degree of transparency should be required for high-risk Al systems.<sup>1</sup> Users should be able to interpret the system output and use it appropriately. High-risk Al systems should therefore be accompanied by **relevant documentation**".

**Tendency:** Data must become explainable-AI-ready (XAIR). Beginning with the EC's **Battery Regulation**, **digital product passports** (DPPs) will be mandatory first for batteries, later textiles, electronics, and more and more products.

<sup>1</sup>Systems with "high risk" include all "safety components" related to "water, gas, heating, and electricity." MatInfo seminar 28<sup>th</sup> September 2023 4





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# BatCAT and DigiPass





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## **BatCAT key objectives**

|     |                            | WP lead | IFPEN                         | POLITO     | RPTU                     | UKRI      | ITWM              | CPI           | GCL                | NMBU       |
|-----|----------------------------|---------|-------------------------------|------------|--------------------------|-----------|-------------------|---------------|--------------------|------------|
|     |                            |         | WP1                           | WP2        | WP3                      | WP4       | WP5               | WP6           | WP7                | WP8        |
|     |                            |         | characterization              | simulation | interoperability         | knowledge | digital twin      | demonstration | exploitation       | management |
|     |                            |         |                               |            |                          |           |                   |               |                    |            |
| КО1 | experiments and sensorics  |         |                               |            |                          |           |                   |               |                    |            |
| KO2 | multiphysics modelling     |         |                               |            |                          |           |                   |               |                    |            |
| КОЗ | technical interoperability |         |                               |            |                          |           |                   |               |                    |            |
| KO4 | integrated data space      |         |                               |            |                          |           |                   |               |                    |            |
| KO5 | digital twin platform      |         |                               |            |                          |           |                   |               |                    |            |
| KO6 | pilot and transferability  |         |                               |            |                          |           |                   |               |                    |            |
| КО7 | long-term exploitation     |         |                               |            |                          |           |                   |               |                    |            |
|     |                            |         |                               |            |                          |           |                   |               |                    |            |
|     |                            |         |                               |            |                          |           |                   |               |                    |            |
|     |                            |         | main responsible work package |            | substantial contribution |           | some contribution |               | minor contribution |            |

KO1: In situ measurements and characterization, targeting cell manufacturing and behaviour.
KO2: Multiscale and multiphysics modelling, targeting scalability and computational efficiency.
KO3: Technical interoperability and linking of models, data, and processes.
KO4: Knowledge base for a federated, integrated, and semantically enriched data space.

**KO5:** Interpretable industrial decision support system and Industry 5.0 real-time environment.

**KO6:** Demonstrate the developments in a pilot production line and verify transferability.

**KO7:** Create the preconditions for a long-term exploitation of the project outcomes.

### BatCAT architecture



### **BatCAT focus areas**



### **BatCAT consortium**



### **DigiPass consortium**



### **DigiPass key objectives and work plan**





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# NMBU's role





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### **NMBU-led work packages and deliverables**

<u>D10</u>: Ontology evaluation and common metadata framework (M12)

### <u>WP7</u>: Semantic interoperability and data spaces (M19-36)

Demonstrate the metadata framework for materials research; align it with EMMO, OCES, and data spaces.



<u>D4.2</u>: Report on data stewardship and good practice (M21)



<u>D7.3</u>: Report on citizens' role, societal, and gender dimensions (M36)

#### WP8: Technical management (M1-42)

NMBU leads the technical management work package since it is the partner coordinating BatCAT. <u>D8.1</u>: Consortial handbook (M3) <u>D8.2</u>: Data management plan (M6)

### NMBU-led work packages, deliverables, and tasks

#### <u>T6.1</u>: Critical evaluation of pre-existing ontologies (M4-12)

Assess EMMO aligned ontologies (and others) and suggest improvements, delivering a critical analysis.

### <u>D10</u>: Ontology evaluation and common metadata framework (M12)

### <u>WP7</u>: Semantic interoperability and data spaces (M19-36)

Demonstrate the metadata framework for materials research; align it with EMMO, OCES, and data spaces.

#### <u>T7.1</u>: Schema for data and knowledge graph transformation (M19-27) Process and schema for documenting ontology alignments and knowledge graph mappings.

#### <u>T7.2</u>: Interoperability framework demonstration (M28-36)

The digital materials and product passport is demonstrated; focus on documentation and interoperability.

#### <u>T2.4</u>: Multiphysics modelling of redox-flow battery production (M1-18)

Study chemical and transport phenomena by QM, classical-mechanical MC/MD, and effective-circuit models.

#### <u>T4.1</u>: Knowledge infrastructure requirements analysis (M1-9)

Agile requirements analysis based on consultation with stakeholders; focus on use cases, CaosDB, and BIG-MAP.

#### T4.6: Data stewardship (M10-21)

The scientific data officer for BatCAT takes care of FAIR compliance and provision of persistent identifiers. <u>D4.2</u>: Report on data stewardship and good practice (M21)

T5.1: Cellular neural networks (M7-18) Develop a CeNN predictor that will be used for all machine-learning tasks in the project.

### <u>T7.1</u>: Battery2030+ engagement and dissemination (M1-M42)

Organize events (a hackathon, a workshop, *etc.*); take care of corporate design; connect to Battery2030+.

### <u>T7.2</u>: Citizens' role and societal and gender dimensions (M1-M36)

Conduct an agile requirements analysis, monitor societal impact, publish a memorandum (M30) and D7.3 (M36). <u>D7.3</u>: Report on citizens' role, societal, and gender dimensions (M36)

WP8: Technical management (M1-42) and all of the tasks in WP8 except one NMBU leads the technical management work package since it is the partner coordinating BatCAT. D8.1: Consortial handbook (M3) D8.2: Data management plan (M6)

### Involved\* NMBU faculty

### faculty involved\* in BatCAT



Kristian Berland (DigiPass team member)



Anne Cathrine Gjærde (PI in both projects)



Fadi Al Machot (Pl in both projects)

Martin Thomas Horsch (PI in both projects)

faculty involved\* in DigiPass



Mathijs A. Janssen (PI in BatCAT)



Thomas Martinsen (PI in BatCAT)



Kristin Tøndel (PI in BatCAT)



Jorge Mario Marchetti (BatCAT team member)



Heidi S. Nygård (BatCAT team member)



Eirik Valseth (Simula's PI in BatCAT)

Habib Ullah (BatCAT team member)

\*Planned as of now; all subject to finalization of the Consortial and Grant Agreements and everybody's actual commitment.



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# What next?





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# **Organizational membership**



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### Advanced Materials 2030 Initiative (AMI2030)

» NMBU is now listed as a member.



- » There is no organizational membership fee.
- » The relevant working group is WP1: Materials digitalization.

### Batteries European Partnership Association (BEPA)



- » Due to BatCAT, we must become organizational member.
- » Not clear what they do; and it is expensive ( $\in$  4000 / year).
- » But there is no alternative to it, and it can be arranged within the budget that we have within BatCAT.

### European Materials Modelling Council (EMMC ASBL)



- >> Used to be a very active organization, now slightly less so.
   But it is still a useful investment into networking.
  - » It will cost € 1000 per year.

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# MatInfo organizational action items

Norwegian University of Life Sciences BatCAT Battery Cell Assembly Twin

Advanced Materials 2030 Initiative (AMI2030)

Batteries European Partnership Association (BEPA)

European Materials Modelling Council (EMMC ASBL)

### **Related organizational activities:**

- Work toward the creation of a **CECAM node** in Scandinavia.
- Engage in the two new **COST actions** where we are represented.
- More intensive collaboration with **Simula**, aim at institutionalizing it.
- The ongoing COST proposal is unfortunately unrelated (medicine-only).

### **Urgent action items:**

- Look into Forskningsrådet's egenvurdering (info call on 4th October).
- Advertise and fill our open positions.

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## Positions to be created at NMBU

- Technical manager (duration: 42 months)
  - Core position for BatCAT.
  - If intelligently done, this becomes a role with high responsibility, including perspective for career devlopment and scientific work.
- Forsker (duration: 12 months; thereof, 2 PM funded through DigiPass)
  - Within BatCAT, take care of our role within work package 4.
  - Flexibility to do interesting research work additionally.
- Stipendiat (duration: 36 months + possibly teaching)
  - Start with BatCAT T2.4 (RFB modelling) and T5.1 (CeNN) until M18.
  - From there on, there is much freedom within the context of BatCAT.
- Rector's stipendiat (duration: 36 months + possibly teaching)
  - No need to be closely aligned to BatCAT.
  - We need to wait whether this really comes from the rector.
  - Strategically help us develop MatInfo into a strong research group.

We must immediately (<u>now</u>!) sit together and draft the job descriptions.

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