EIC Transition Open 2026 consortium seeks industrial pilot partner in pharma or advanced materials for AI-driven molecular simulation platform

Summary

Profile type
Research & Development Request

Company's country
Luxembourg

POD reference
RDRLU20260416019

Profile status
PUBLISHED

Type of partnership
Research and development cooperation agreement

Targeted countries
- **Denmark**
- **Germany**
- **Spain**
- **Italy**
- **Sweden**
- **Netherlands**
- **France**
- **Austria**
- **Belgium**

Contact Person
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Term of validity
28 Apr 2026
28 Apr 2027

Last update
28 Apr 2026

General Information

Short summary

A Luxembourg startup, together with the University of Luxembourg and the Luxembourg National Data Service, is preparing an EIC Transition Open 2026 proposal on an AI-driven molecular simulation platform for drug discovery and advanced materials. The consortium seeks an industrial partner from another EU Member State or Associated Country to provide a real use case, validation environment, and reference data for pilot testing. A Research and development cooperation agreement is sought.

Full description

A Luxembourg-based deep-tech startup is developing an AI-accelerated molecular simulation platform for drug discovery and advanced materials. The platform is designed to make high-fidelity atomistic simulation practical in industrial R&D by automatically selecting and harmonizing suitable AI models, running simulations on scalable compute infrastructure, and returning reproducible, uncertainty-aware results.

The project is being prepared for EIC Transition Open 2026 under Horizon Europe. It builds on an ERC-funded research project. The objective is to mature these research results into a validated prototype and demonstrate their relevance in industrial R&D workflows.

The current consortium is composed of:

- The Luxembourg startup client: commercial lead and product owner; platform orchestration, model registry, API/UI, business model, and route to market.

- University: scientific R&D partner; next-generation machine-learning models and large-scale molecular simulation methods.

- Data Service: secure data layer, pseudonymization, and compliance infrastructure for sensitive industrial use cases.

The consortium is now seeking one industrial pilot partner from another EU Member State or Associated Country. The partner should bring a real use case and help validate the technology in a relevant operational environment. The primary application area is pharma/biotech, especially drug discovery workflows where molecular simulation can support compound triage, developability screening, and prioritization. However, the platform is also suitable for advanced materials, including battery materials and electrolytes, polymers, coatings, composites, and specialty formulations.

The expected contribution of the industrial partner is to:

1. define a relevant pilot use case and practical success criteria,
2. provide reference data where possible,
3. assess how simulation outputs can support real R&D decision-making,
4. and participate in validating the prototype in an industrial setting.

The project is intended to run for approximately 24–36 months and has a total expected budget of up to €2.5 million under the EIC Transition scheme.

A Research and development cooperation agreement is sought.

Advantages and innovations

The project combines three strengths:

1. cutting-edge scientific research in AI-driven molecular simulation from the University of Luxembourg,
2. product and commercialization capability through the startup client, and
3. secure data infrastructure and compliance expertise through LNDS.

The core innovation is a platform that makes quantum-level molecular simulation usable in real R&D workflows. Recent AI-based force-field models have made it possible to simulate larger and more complex systems with much higher accuracy than before, but adoption remains limited because these methods are difficult to configure, benchmark, and deploy at scale. The Luxembourg startup addresses this bottleneck by building a unified platform layer around model selection, harmonization, reproducibility, and scalable execution.

The industrial value is clear in sectors where experimental cycles are costly and slow. In pharma, the platform can support earlier and more systematic candidate prioritization. In advanced materials, it can help compare formulations, interfaces, and performance-relevant properties before expensive lab campaigns begin.

Technical specification or expertise sought

The consortium is looking for an industrial partner with internal R&D activities in either:

- Pharma / biotech, especially small-molecule drug discovery, developability screening, or formulation-related workflows; or

- Advanced materials / specialty chemicals, especially polymers, coatings, composites, battery materials, electrolytes, or related formulation problems.

The partner should be able to contribute:
1. a real industrial use case relevant to the project,
2. practical success criteria for validating the prototype,
3. reference data or benchmark information, where possible,
4. participation in pilot evaluation and exploitation discussions.

Experience with molecular modelling is welcome but not required. More important is the ability to assess whether the platform produces outputs that are relevant and useful in an actual R&D environment.

Stage of development

Under development

Sustainable Development goals

- **Goal 12: Responsible Consumption and Production**
- **Goal 9: Industry, Innovation and Infrastructure**
- **Goal 7: Affordable and Clean Energy**
- **Goal 3: Good Health and Well-being**
- **Goal 13: Climate Action**
- **Goal 17: Partnerships to achieve the Goal**

IPR Status

IPR Notes

Partner Sought

Expected role of the partner

The partner sought is an industrial pilot partner that can help validate the technology in a relevant operational environment.

Its expected role would include:

- Contributing a pilot use case from its R&D activities,
- Helping define validation metrics and practical acceptance criteria,
- Sharing reference data or benchmark information where possible,
- Evaluating whether the platform's outputs are useful for real decision-making,
- Contributing to the project's impact and exploitation plan.

The partner will not be expected to develop the core simulation technology, but rather to act as the industrial environment in which the prototype is tested and assessed. This role is important for demonstrating relevance, market pull, and concrete pathways to adoption.

Type of partnership

Research and development cooperation agreement

Type and size of the partner

- **SME 50 - 249**
- **SME 11-49**
- **SME <=10**
- **Big company**

Call Details

Framework program

Horizon Europe

Call title and identifier

EIC Transition Open

HORIZON-EIC-2026-TRANSITIONOPEN

Submission and evaluation scheme

Single-stage submission (and then interview).

Anticipated project budget

€2.5 million

Coordinator required

No

Deadline for EoI

15 Jun 2026

Deadline of the call

16 Sep 2026

Project duration in weeks

156

Web link to the call

https://eic.ec.europa.eu/eic-funding-opportunities/eic-transition_en

Project title and acronym

AETHER: AI-Enabled Trusted High-fidelity Engine for molecular R&D

Dissemination

Technology keywords

- **01003001 - Advanced Systems Architecture**
- **05001002 - Computational Chemistry and Modelling**
- **01003016 - Simulation**
- **01003003 - Artificial Intelligence (AI)**
- **01003006 - Computer Software**

Market keywords

- **05007002 - Pharmaceuticals/fine chemicals**
- **08001019 - Speciality/performance chemicals**
- **04011 - Molecular design**
- **08001009 - Speciality/performance materials: producers and fabricators**
- **03002 - Batteries**

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Sector groups involved

- **Health**
- **Energy-Intensive Industries - Materials**
- **Digital**