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CASE STUDY · MARLUC SYNOPSIS

Microsoft and PNNL: AI-screened solid electrolyte for batteries

IMPLEMENTED 2023–2024 · SCIENCE AND RESEARCH · US · BAND D · PARTLY PROVED

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Microsoft used AI models and about 1,000 cloud virtual machines to screen 32.6 million candidate materials for solid battery electrolytes, ending with 23 candidates. PNNL chemists chose and made a sodium-lithium-yttrium chloride from the list and measured its conductivity. Microsoft says PNNL built a working battery with it. The material was still being optimised in 2024 and no later results on it were found; the two organisations now work together on Microsoft's agentic Discovery platform.

ABOUT THIS SYNOPSIS

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Facts and figures are as reported by the sources listed below, which may be incomplete, self-reported or out of date. Check the original source before relying on any figure.

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NOTICE WORDING LAST UPDATED 16 NOVEMBER 2026

AT A GLANCE

Frontier case: AI used for a scientific, medical or engineering breakthrough. The transformation is potential and unproven; MarLuc grades what has changed in practice so far.

AI and automation used: Machine-learning models built on the M3GNet framework, combined with physics-based simulation on Microsoft's Azure Quantum Elements cloud platform, used to screen candidate battery electrolytes.

Implemented: 2023–2024. Grade: band D, Task support, Partly proved.

Headline result, as reported: AI models and cloud computing narrowed 32.6 million candidate materials to 23 in under 80 hours; PNNL made and tested a new sodium-lithium solid electrolyte, which it said in 2024 still needed optimisation to compete with published benchmarks

1 · The case

The facts, as reported by the 5 sources listed at the end. Where a source is silent, the field says "Not reported".

Organisation

Microsoft (Azure Quantum) and Pacific Northwest National Laboratory (PNNL). Microsoft's Azure Quantum team working with the US Department of Energy's Pacific Northwest National Laboratory in Richland, Washington. Staff numbers for the teams involved: Not reported. Canvas block: 6. Data and technology. Also 4. Operations and process.

Business challenge

The challenge. Per the paper, large-scale computational searches for new materials are limited by computing resources, and examples carried through to experimental validation remain scarce. Microsoft says lithium is scarce and expensive and that solid-state batteries are assumed to be safer than liquid ones.

How it was addressed. Microsoft generated 32,598,079 candidate materials by substituting elements into known crystal structures. AI models filtered them for stability and battery-relevant properties, DFT calculations re-checked the AI predictions, and AI-accelerated simulations estimated ion movement, leaving 23 candidates. PNNL chose four rare-earth halides to make, synthesised a series of sodium-lithium-yttrium chlorides (NaxLi3-xYCl6) and measured their structure and conductivity. Microsoft says PNNL then built a working all-solid-state battery tested at room temperature and about 80 °C. [1] [2] [3] [4] [5]

Who implemented it

Microsoft (Azure Quantum) (Model or cloud provider): Built the AI models and ran the cloud screening on Azure Quantum Elements..
Pacific Northwest National Laboratory (University or research lab): Set screening criteria, chose candidates, and synthesised and tested the electrolyte..
PNNL is a US Department of Energy national laboratory. The battery prototype is reported by Microsoft; the paper opened reports structure and conductivity measurements only.

Technology (SEAM pillar E)

SEAM types: T5 Custom / fine-tuned models, T8 Predictive / ML models. Deployment: Vendor SaaS. Vendors and products: Microsoft, Azure Quantum Elements, M3GNet, Microsoft Discovery.

Where it was built in: Screening ran on Microsoft's Azure cloud (about 1,000 virtual machines), with AI models filtering for stability and battery-relevant properties and density functional theory (DFT) calculations re-checking the AI predictions. PNNL scientists added screening criteria, chose candidates and carried out synthesis and testing in the lab.

What changed

Before: per PNNL, a similar discovery process had taken several years. In this project: AI did most of the screening in under 80 hours, and the project went from start to a working battery in under nine months, by the organisations' account. Since then: the collaboration has moved to Microsoft Discovery, which PNNL describes as connected to its laboratory automation. The electrolyte has not been reported in use. [1] [2] [3] [4] [5]

What it cost

Not reported. The screening used about 1,000 cloud virtual machines for under 80 hours, per the paper.

What it saved

Time: screening under 80 hours and the whole project under nine months, by Microsoft's and PNNL's account, against several years for similar processes, per PNNL. Lithium: about 70% less than existing lithium-ion batteries, by Microsoft's account. Cost saving: Not reported. [1] [2] [3] [4] [5]

Governance and control

The AI output passed through DFT re-checks, expert selection and lab tests before any claim about the material. The results come from the two organisations, one of which sells the platform; no independent replication is reported. Accountable owner and AI-specific controls: Not reported.

S2 · Accountable owner · Claimed
The paper names Vijayakumar Murugesan (PNNL) and Matthias Troyer (Microsoft) as corresponding authors; no other accountable owner is reported. [2]

A1 · Safe use · Not reported
No AI-specific safe-use rules are described in the sources opened.

A2 · Human in the loop · Claimed
Per Microsoft, PNNL expertise added screening parameters that narrowed the final candidates, and the paper says the team chose four halides for experimental validation. [2] [3]

A3 · Monitoring and assurance · Claimed
Microsoft says DFT calculations re-computed AI-predicted properties because the AI models have a non-zero prediction error; lab measurements then tested the chosen material. [2] [3]

A4 · Vendor AI · Claimed
Microsoft supplied the platform and models and is also co-author of the results, so the vendor reported on its own product; Microsoft called the project a proof point for Azure Quantum Elements. [2] [3]

A5 · Agent controls · Not reported
No agents were used in the 2024 work; the 2026 PNNL work on Microsoft Discovery uses AI agents, and controls for them are not reported. [5]

A6 · Standards and regulation · Not reported
Laboratory research with no regulatory decision involved; a journal version of the paper is linked from the arXiv record. [1]

What worked, what did not, what is unproven

WORKED

– The pipeline screened 32,598,079 candidates down to 23 in under 80 hours on about 1,000 cloud virtual machines; 18 of the 23 had compositions not previously reported.

– The synthesised Na2LiYCl6 matched the predicted structure in powder X-ray diffraction, and

– Replacing some sodium with lithium raised conductivity by more than two orders of magnitude over the parent sodium compound (2.2 × 10-6 against 6.0 × 10-8 S/cm at 100 °C).

– Microsoft reports that PNNL built a working all-solid-state battery with the material.

DID NOT

– Three of the four predicted halides PNNL tried to make (Li3YCl6 in a new structure, Li5YCl8 and Li7Y2Cl13) came out as the already known Li3YCl6 phase.

– PNNL said in January 2024 that it was still working to make the compound competitive with published benchmarks.

– Researchers cautioned that the material might not work at scale, and PNNL's chief digital officer said its significance lay less in the material than in how fast it was found.

UNPROVEN

– Whether the electrolyte can match established solid electrolytes; no later performance results were found in the sources opened.

– The battery prototype and the 70% lithium saving are Microsoft's account; the paper opened reports structure and conductivity, not a battery.

– Whether AI screening gives a better hit rate than other methods in general: one material from one search.

– Whether the agentic work on Microsoft Discovery at PNNL produces results: described only by the organisations so far.

Timeline

Jan 2024 Microsoft and PNNL post the screening and synthesis paper on arXiv [1]

Jan 2024 Microsoft announces the new electrolyte and says PNNL built a working all-solid-state battery with it [3]

Jan 2024 PNNL says the work took under nine months and that it is optimising the compound to compete with published benchmarks [4]

Jun 2026 Microsoft Discovery becomes generally available; PNNL describes the platform being connected to its laboratory automation [5]

2 · Grade and SEAM assessment

MarLuc's opinion, made on the evidence above. How cases are graded: marluc.co.uk/case-studies/how-we-rate

Level of change and impact

Claimed: A. Grade: D, Task support. Proof: Partly proved. Level of change: Task support.

Task support (Level 1, band D): AI shortened the screening step for one research team; selection, synthesis and testing stayed with lab scientists. Claimed A: Microsoft describes compressing 250 years of chemistry and materials science progress into 25. That is potential and unproven.

Graded D. AI shortened one step, the screening of candidates, for one research team, and the lab still chose, made and tested the material. No change in how PNNL or the field finds battery

The SEAM view and lessons learnt

The speed came from three things together: AI property models, cheap cloud computing at scale, and PNNL's chemistry judgement in choosing what to make. The AI's share of the screening is clear from the paper, but its value cannot be judged from one material that PNNL said still needed optimisation. A leadership team copying this should ask what share of AI-proposed candidates can actually be made and tested, and how lab results will be fed back before money is committed.

1. Report how many AI-proposed candidates could actually be made.
2. Judge an AI search by lab results, not by screening speed.
3. Keep expert selection and lab tests between AI output and investment.

Evidence

Score 2 of 4. Partly independent: a research paper by the two organisations (preprint opened; journal version linked), with the battery prototype, lithium saving and later collaboration in their own announcements, relayed by trade press. No independent replication.

Evaluation method. Self-reported research result: computational screening followed by laboratory synthesis and conductivity measurement, written up by the organisations themselves. No comparison group and no independent test.

Sources disagree. Microsoft's announcement gives 32.6 million starting candidates, about 500,000 stable materials and 18 top candidates; the paper gives 32,598,079 candidates, 589,609 predicted stable and 23 final candidates, of which 18 had new compositions. Microsoft reports a working battery; the paper opened does not.

Status. Research continuing: the electrolyte was under optimisation in 2024 with no later results found; the Microsoft and PNNL collaboration continues on Microsoft Discovery in 2026.

3 · Original sources

Read these in full. To challenge a fact or a grade, use the contact form at marluc.co.uk or the link on https://marluc.co.uk/case-studies/microsoft-pnnl-ai-screened-battery-electrolyte

[1] arXiv: Accelerating computational materials discovery with artificial intelligence and cloud high-performance computing (Chen et al., abstract page, January 2024)
https://arxiv.org/abs/2401.04070

[2] arXiv: Accelerating computational materials discovery with artificial intelligence and cloud high-performance computing (full paper, PDF)
https://arxiv.org/pdf/2401.04070

[3] Microsoft Azure blog: Unlocking a new era for scientific discovery with AI: How Microsoft's AI screened over 32 million candidates to find a better battery (January 2024)
https://azure.microsoft.com/en-us/blog/quantum/2024/01/09/unlocking-a-new-era-for-scientific-discovery-with-ai-how-microsofts-ai-screened-over-32-million-candidates-to-find-a-better-battery/

[4] Utility Dive: DOE lab, Microsoft find new battery material in AI-based energy storage research initiative (January 2024)
https://www.utilitydive.com/news/pnnl-microsoft-artificial-intelligence-research-battery/704176/

[5] Microsoft Azure blog: Announcing Microsoft Discovery general availability and Microsoft Discovery app preview (June 2026)
https://azure.microsoft.com/en-us/blog/announcing-microsoft-discovery-general-availability-and-microsoft-discovery-app-preview/

Microsoft (Azure Quantum) and Pacific Northwest National Laboratory (PNNL) website: https://www.microsoft.com

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