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CASE STUDY · MARLUC SYNOPSIS

Google DeepMind GNoME and the Berkeley Lab A-Lab

IMPLEMENTED 2023 ONWARDS · SCIENCE AND RESEARCH · UK · BAND E · PARTLY PROVED

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In 2023 Google DeepMind published a deep-learning model that predicted 2.2 million stable crystal structures, and Berkeley Lab published an autonomous lab that reported making new compounds. Outside chemists disputed the novelty and identification claims, and in January 2026 Nature corrected the lab paper.

ABOUT THIS SYNOPSIS

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NOTICE WORDING LAST UPDATED 16 NOVEMBER 2026

AT A GLANCE

No measurable effect: tested, no effect.

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: Deep-learning model predicting crystal stability (GNoME), with an AI-guided robotic synthesis lab (A-Lab).

Implemented: 2023 onwards. Grade: band E, No measurable effect, Partly proved.

Headline result, as reported: 2.2 million predicted crystal structures and an autonomous lab, by the developers' account; novelty claims disputed and the lab paper corrected in 2026

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

Google DeepMind. AI research group (Google DeepMind, London) and a US national laboratory (Lawrence Berkeley National Laboratory, with the University of California, Berkeley). The Materials Project is the open database the model was built on. Staff numbers: Not reported. Canvas block: 6. Data and technology. Also 4. Operations and process.

Business challenge

The challenge. The GNoME paper says discovery of inorganic crystals has been bottlenecked by expensive trial-and-error approaches. It reports building on 48,000 stable crystals already identified.

How it was addressed. DeepMind trained graph networks at scale to predict which crystal structures are stable and reports 2.2 million structures below the current convex hull, 381,000 of them on the updated hull. Stable discoveries were to be made available for screening. The Berkeley Lab paper reported an autonomous laboratory, using AI and robotics, that made new compounds from predicted targets. After outside concerns, Nature published a correction to that paper in January 2026. [1] [2] [3] [4] [5]

Who implemented it

In-house (In-house): Google DeepMind: Developed GNoME and co-authored the A-Lab paper.
Lawrence Berkeley National Laboratory (University or research lab): Authors of the A-Lab paper, with researchers from the University of California, Berkeley.
The Materials Project is named in the GNoME paper as the database the model was trained on and compared against.

Technology (SEAM pillar E)

SEAM types: T5 Custom / fine-tuned models, T8 Predictive / ML models. Deployment: Not reported. Vendors and products: GNoME (graph networks for materials exploration), A-Lab.

Where it was built in: GNoME predicts which inorganic crystal structures are stable; the stable predictions were released for researchers to screen. The A-Lab at Lawrence Berkeley National Laboratory is a robotic laboratory that attempts to make predicted compounds and identifies them from diffraction patterns.

What changed

Before: about 48,000 stable crystals known, by the paper's account. After, by DeepMind's account: 381,000 newly predicted stable entries released for researchers to screen. Change in laboratory practice or any product: Not reported. [1] [2] [3] [4] [5]

What it cost

Not reported

What it saved

Not reported. The paper reports that the efficiency of materials discovery improved by an order of magnitude; no time or cost saving in practice is reported. [1] [2] [3] [4] [5]

Governance and control

Scientific review rather than operating controls: Nature's correction says the re-analysis of the A-Lab diffraction data was peer-reviewed after publication. Accountable owner and other controls: Not reported.

S2 · Accountable owner · Not reported
Not reported.

A1 · Safe use · Not reported
Not reported.

A2 · Human in the loop · Not reported
Not reported.

A3 · Monitoring and assurance · Evidenced
Nature's correction notice says the authors manually re-analysed the diffraction patterns and that the re-analysis was peer-reviewed after publication; outside chemists also published critiques of both papers. [2] [3] [4]

A4 · Vendor AI · Not reported
Not reported.

A5 · Agent controls · Not reported
Not reported.

A6 · Standards and regulation · Not reported
Not reported.

What worked, what did not, what is unproven

WORKED

– The GNoME paper reports that 736 of the stable structures have been independently realised in experiments.

– The paper reports a precision (hit rate) of stable predictions above 80% for structure-based models, against 1% in previous work.

– The A-Lab authors' manual re-analysis, peer-reviewed after publication, confirmed the correct conclusion in 36 of 40 reported successes, per Nature.

DID NOT

– Cheetham and Seshadri reviewed a small randomised subset of the GNoME entries and found scant evidence for compounds that combine novelty, credibility and utility.

– Leeman and colleagues examined all the A-Lab products and concluded that no new materials had been discovered; they judged two thirds of the claimed successes likely to be known compositionally disordered versions of the predicted compounds.

– Nature's correction says concerns were raised about identifying the structures from diffraction and about the novelty claims. Four compounds were inconclusive and one was removed because it was in the training data.

UNPROVEN

– Whether any of the 381,000 stable predictions is novel, makeable and useful.

– Whether the released predictions have changed how any laboratory or company chooses materials.

– Whether any A-Lab compound is new to science. Nature says novelty meant new to the prediction platform.

Timeline

Nov 2023 Nature publishes the GNoME paper and the Berkeley Lab A-Lab paper [2]

Mar 2024 Leeman and colleagues publish a critique concluding that no new materials were discovered in the A-Lab paper [4]

Apr 2024 Cheetham and Seshadri publish a perspective on the GNoME paper; DeepMind says it stands by all claims [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: E, No measurable effect. Proof: Partly proved. Level of change: Not graded.

No level assessed: band E. The sources report no change in how work is done; the potential change in materials discovery is claimed, not proved.

Graded E, claimed A. DeepMind and others describe a possible change in how new materials are found. That change is potential and unproven: the sources report no new material put to use, the novelty of the predictions and of the lab's compounds is disputed, and Nature corrected the lab paper. Band D could be argued for the released dataset, but no source we opened shows it changing how any lab works.

The SEAM view and lessons learnt

A count of AI outputs is not yet an outcome. The disputed figures here are counts of predicted or identified compounds, and the argument is about what counts as new. An organisation using AI to generate candidates needs a plain definition of success, agreed with domain experts, before it publishes totals. The correction shows the value of an outside check, including one made after publication.

1. Define what counts as new, and new to whom, before reporting discoveries.
2. Ask domain experts to sample AI output before publishing totals.
3. Correct published figures openly when outside checks change them.

Evidence

Score 3 of 4. Partly independent: peer-reviewed papers, outside critiques and a journal correction. DeepMind's account of what followed is its own.

Evaluation method. Peer-reviewed papers, published critiques and a journal correction: the November 2023 Nature GNoME paper, critiques in Chemistry of Materials and PRX Energy, and Nature's January 2026 author correction to the A-Lab paper; no independent replication of novelty or use in practice in the sources.

Sources disagree. DeepMind told The Register it stands by all claims and that hundreds of predicted materials have been independently synthesised; Cheetham and Seshadri found scant evidence of novel, credible and useful compounds in a randomised subset. For the A-Lab, Leeman and colleagues describe 43 novel materials claimed and conclude none is new. Nature's correction refers to 40 reported successes, confirms 36 and says novelty meant new to the prediction platform.

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/google-deepmind-gnome-and-a-lab

[1] Nature: Scaling deep learning for materials discovery
https://www.nature.com/articles/s41586-023-06735-9

[2] Nature: Author Correction, An autonomous laboratory for the accelerated synthesis of inorganic materials
https://www.nature.com/articles/s41586-025-09992-y

[3] Chemistry of Materials: Artificial Intelligence Driving Materials Discovery? Perspective on the Article: Scaling Deep Learning for Materials Discovery
https://pmc.ncbi.nlm.nih.gov/articles/PMC11044265/

[4] PRX Energy: Challenges in High-Throughput Inorganic Materials Prediction and Autonomous Synthesis
https://par.nsf.gov/servlets/purl/10532478

[5] The Register: Boffins deem Google DeepMind's material discoveries rather shallow
https://www.theregister.com/2024/04/11/google_deepmind_material_study/

Google DeepMind website: https://deepmind.google

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