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CASE STUDY · MARLUC SYNOPSIS

Microsoft MatterGen: generative AI for materials design

IMPLEMENTED 2024–2025 · SCIENCE AND RESEARCH · UK · BAND E · PARTLY PROVED

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Microsoft Research published MatterGen, a generative model that proposes new crystal structures to meet set properties, in Nature in January 2025 and released it openly. As a proof of concept, a Shenzhen lab made one of four selected designs, TaCr2O6, and measured its stiffness within 20% of the target. An independent analysis argues that this compound was already known since 1972 and was in the model's training data. No change in how organisations find materials is reported.

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Facts and figures are as reported by the sources listed below, which may be incomplete, self-reported or out of date.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.

The impact band, proof marker and SEAM view are MarLuc's opinion. The organisation is not a MarLuc client and has not reviewed or endorsed this synopsis. Names and trademarks belong to their owners.

NOTICE WORDING LAST UPDATED 16 NOVEMBER 2026

AT A GLANCE

No measurable effect: no results reported.

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 used: Generative AI: a diffusion model (MatterGen) that proposes crystal structures for target properties, with Microsoft's MatterSim model used in stability checks.

Implemented: 2024–2025. Grade: band E, No measurable effect, Partly proved.

Headline result, as reported: Nature paper on Microsoft's MatterGen reported one AI-designed material made in the lab within 20% of its target stiffness; an independent crystallographer argues the compound was already known and in the training data

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 Research AI for Science, with the Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences. Microsoft Research AI for Science, a research group with teams in Cambridge (UK), Berlin, Amsterdam, Redmond, Shanghai and Beijing; the corresponding authors are in Cambridge, UK. Lab work was done with the Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences. Staff numbers: Not reported. Canvas block: 6. Data and technology. Also 4. Operations and process.

Business challenge

The challenge. Per Microsoft, finding a new material for a target use is like finding a needle in a haystack, and computational screening is limited to lists of known candidates. The paper says earlier generative models had a low success rate in proposing stable crystals or could meet only a few property constraints.

How it was addressed. Microsoft built MatterGen, a diffusion model trained on 608,000 stable materials from the Materials Project and Alexandria databases, which can be fine-tuned to generate structures with set chemistry, symmetry or properties. For a lab test, it generated 8,192 candidates for each of four stiffness targets, filtered them to 75, and experts chose four to make. Synthesis worked for one, TaCr2O6, made in a disordered form. Microsoft released the code and data under the MIT licence and offers the model in Microsoft Foundry. [1] [2] [3] [4] [5]

Who implemented it

In-house (In-house): Built, trained, evaluated and released MatterGen, with teams in Cambridge (UK), Berlin, Amsterdam, Redmond and China..
Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences (University or research lab): Prof. Li Wenjie's team synthesised the TaCr2O6 sample with Microsoft..
The critique is by Mikkel Juelsholt, who declares no conflict of interest; it is not a Microsoft partner.

Technology (SEAM pillar E)

SEAM types: T5 Custom / fine-tuned models, T6 Open-source / locally hosted models.
Deployment: Not reported. Vendors and products: Microsoft, MatterGen, MatterSim, Microsoft Foundry.

Where it was built in: A research model built by Microsoft Research AI for Science, released as open source and offered in the Microsoft Foundry model catalogue. For the proof of concept, candidates were filtered with MatterSim and DFT calculations and the chosen designs were made at the Shenzhen Institute of Advanced Technology.

What changed

Before: computational searches screened lists of known or enumerated structures. After: an openly licensed model that proposes structures for set properties is available to researchers. No organisation is reported, in the sources opened, to have found or used a new material through it. [1] [2] [3] [4] [5]

What it cost

Not reported

What it saved

Not reported [1] [2] [3] [4] [5]

Governance and control

Nature peer review, an open code and data release, and a disclosed pending patent application by seven Microsoft authors. Experts chose the synthesis candidates. Microsoft's own pages still describe TaCr2O6 as a novel material after the independent critique. Accountable owner and AI controls: Not reported.

S2 · Accountable owner · Claimed
The Nature paper names Ryota Tomioka and Tian Xie of Microsoft Research AI for Science as corresponding authors. [1]

A1 · Safe use · Not reported
No safe-use rules for the released model are described in the sources opened.

A2 · Human in the loop · Evidenced
The peer-reviewed paper says four candidates were selected for synthesis after expert inspection; the independent analysis calls for rigorous human verification of novelty. [1] [3]

A3 · Monitoring and assurance · Claimed
Microsoft describes a new structure-matching method to judge novelty allowing for disorder; the independent analysis argues it still classed a known compound from the training data as new. [2] [3]

A4 · Vendor AI · Evidenced
Nature's competing-interest statement records that seven Microsoft authors are inventors on a pending patent application for the method; the code and data are released under the MIT licence. [1] [2]

A5 · Agent controls · Not reported
No agents described.

A6 · Standards and regulation · Not reported
Research work with no regulatory decision involved; the paper passed Nature peer review. [1]

What worked, what did not, what is unproven

WORKED

– Per the paper, MatterGen structures were more than twice as likely to be new and stable as those of earlier generative models.

– The one lab-made sample had a measured bulk modulus up to 169 GPa against a 200 GPa target, within 20%, per the paper.

– The model, training data and fine-tuning data were released openly under the MIT licence.

DID NOT

– Synthesis failed for three of the four candidates chosen for the lab.

– The lab made a compositionally disordered version of the structure, not the ordered one MatterGen predicted, per the paper.

UNPROVEN

– Whether MatterGen has led to any new material that has been made and used: none reported in the sources opened.

– Whether its novelty checks reliably separate new compounds from known disordered ones; this is disputed.

– Whether generating structures beats screening once lab synthesis is the test, rather than computed stability.

Timeline

Jan 2024 MatterGen paper received by Nature [1]

Jan 2025 Nature publishes the paper; Microsoft releases the code and training data under the MIT licence [2]

Jun 2025 Independent crystallographer posts a ChemRxiv analysis arguing the synthesised compound was already known [3]

Jan 2026 Revised analysis adds a comparison with the structures in MatterGen's training data [3]

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, no results in practice reported. One laboratory proof of concept, disputed as a known compound. Claimed A: Microsoft calls MatterGen a new paradigm and expects such models to transform materials design. That is potential and unproven.

Graded E, no results reported. MatterGen is a published, openly licensed research model, and its one laboratory test produced a material that an independent crystallographer says was already known and in the training data. The sources opened report no organisation finding or using a new material through it, so nothing has yet changed in practice. Microsoft describes a new paradigm and expects such models to transform materials design; MarLuc treats that as a claimed transformation that is potential and unproven.

The SEAM view and lessons learnt

Here the AI's part can be separated cleanly, because the dispute is about the AI output itself: whether its one lab-made design was new. Peer review in a leading journal did not catch the point the independent crystallographer raised. A leadership team weighing generative design should ask how novelty will be checked against everything already known, including disordered forms, and what share of designs survive synthesis.

1. Check AI-designed materials against known compounds, including disordered forms, before calling them new.

3. Have an independent specialist review novelty claims before announcing them.

Evidence

Score 2 of 4. Partly independent: a peer-reviewed Nature paper by Microsoft and its lab partner, challenged by an independent re-analysis (ChemRxiv working paper, not peer-reviewed at posting). No independent reports of use.

Evaluation method. Self-reported research result: computational benchmarks and one laboratory synthesis in a peer-reviewed paper, with an independent re-analysis of the synthesis by a third-party crystallographer.

Sources disagree. Microsoft's blog and its Foundry Labs page describe $TaCr_2O_6$ as a novel material. The paper calls it a compositionally disordered version of the predicted structure. Juelsholt's analysis says the compound is not novel and is identical to a compound reported in 1972 that was in MatterGen's training dataset.

Status. Research model available openly and in Microsoft Foundry; no practical results reported. Microsoft response to the critique: Not reported in the sources opened.

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-mattergen-generative-materials-design

[1] Nature: A generative model for inorganic materials design (Zeni et al., January 2025)
https://www.nature.com/articles/s41586-025-08628-5

[2] Microsoft Research blog: MatterGen: A new paradigm of materials design with generative AI (January 2025)
https://www.microsoft.com/en-us/research/blog/mattergen-a-new-paradigm-of-materials-design-with-generative-ai/

[3] ChemRxiv (Cambridge Open Engage): Continued Challenges in High-Throughput Materials Predictions: MatterGen predicts compounds from the training dataset (Juelsholt, version 2, January 2026)
https://www.cambridge.org/engage/coe/article-details/694d24f36e8e74030e9067de

[4] Microsoft Foundry Labs: MatterGen
https://labs.ai.azure.com/innovations/mattergen/

[5] MIT Technology Review: AI materials discovery startups and the gap between simulation and the lab (December 2025)
https://www.technologyreview.com/2025/12/15/1129210/ai-materials-science-discovery-startups-investment/

Microsoft Research AI for Science, with the Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences website: https://www.microsoft.com/en-us/research/

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