TROY TECHNICAL

MATERIALS INFORMATICS

WEEKLY REPORT

October 31 - November 6, 2026 | Issue 2026-W44

Closed-loop learning from data quality to experimentally validated material performance

14	10
ANALYZED ARTICLES	PRIORITY THEMES

Issued 2026-11-06 | English edition | fixed approved cover artwork



Materials Informatics: the boundary moved from isolated claims to qualification evidence

14 English articles were reviewed independently from the Japanese edition. Ten themes are retained for management decisions.

SIGNAL 01 | DATA CAPTURE

NIMS Semiconductor Materials Co-Creation Hub: Sub-1nm Roadmap

The National Institute for Materials Science (NIMS) has established the "Semiconductor Materials Research Co-Creation Hub" to develop innovative materials across three time horizons.

SIGNAL 02 | MODELING

TabPFN and NSGA-II: Optimising CIR Powder Coating Curing

Researchers have developed an AI framework combining TabPFN and NSGA-II to optimise catalytic infrared (CIR) curing for thermosetting powder coatings. The system reduced curing times by 47-77% compared to hot-air curing while improving mechanical properties.

SIGNAL 03 | CANDIDATE DESIGN

AI-Driven Alloy Design: Recycling Scrap Metal via "Dirty Alloys

A German-Chinese research team has developed an AI-driven workflow to create "dirty alloys" that utilize scrap metal contaminants as alloying elements rather than removing them.

SIGNAL 04 | EXPERIMENT

WAAM Aluminum Strength: ML Framework for ER5356 Optimization

Researchers have developed a machine learning framework that predicts tensile strength, elongation, flexural strength, and hardness for ER5356 aluminum alloy parts produced via Wire Arc Additive Manufacturing (WAAM).

DECISION

Focus this week's management attention on closed-loop learning from data quality to experimentally validated material performance. Move only when the linked evidence can be reproduced under your own operating conditions.

THREE MANAGEMENT MOVES

1. Buyers: select high-value decisions where data lineage and experimental feedback can be measured.
2. Suppliers: provide machine-readable composition, process, test conditions, uncertainty and failure data.
3. Executives: track dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EVIDENCE DISCIPLINE

FACT states what the collected English source reports. BUSINESS READ and ACTION are editorial interpretations. UNKNOWN lists information that the source file does not establish. A linked article is not treated as independent confirmation of every claim.

Five numbers or evidence anchors that require conditions

1nm A10	SOURCE-BOUND CONDITION The initiative targets the transition to sub-1nm generations and future computing architectures to address the power consumption demands of AI.
77% A14	SOURCE-BOUND CONDITION The system reduced curing times by 47-77% compared to hot-air curing while improving mechanical properties.
15.2% A01	SOURCE-BOUND CONDITION Using ductile cast iron, the team achieved a 15.2% increase in tensile strength and a 73.2% increase in elongation at break compared to previous recycled materials.
1.18% A04	SOURCE-BOUND CONDITION The model's predictions for a confirmation build were within 1.18% to 4.61% of measured values, demonstrating a method to reduce physical testing in metal AM.
16 w A12	SOURCE-BOUND CONDITION The system can produce 300 new compositions in approximately 16 weeks, potentially shrinking material development timelines from decades to just a few years.

HOW TO USE THESE NUMBERS

Each value is shown with the condition stated in the collected English article. Do not compare values across different test methods, device sizes, operating temperatures or commercial stages without normalizing those conditions.

Where the value chain moved

Each stage combines one leading theme and one supporting theme. The report treats handoffs as evidence transfers, not decorative arrows.

1

Data capture

P01/P06

The National Institute for Materials Science (NIMS) has established the "Semiconductor Materials Research Co-Creation Hub" to.

2

Modeling

P02/P07

Researchers have developed an AI framework combining TabPFN and NSGA-II to optimise catalytic infrared (CIR) curing for.

3

Candidate design

P03/P08

A German-Chinese research team has developed an AI-driven workflow to create "dirty alloys" that utilize scrap metal.

4

Experiment

P04/P09

Researchers have developed a machine learning framework that predicts tensile strength, elongation, flexural strength, and.

5

Scale & governance

P05/P10

Researchers have implemented a physics-informed Bayesian optimization (BO) framework to automate quantitative high-resolution.

EVIDENCE REQUIRED AT EACH HANDOFF

Data capture to Modeling	Transfer test conditions, acceptance criteria, failure data, owner and decision date. Recheck dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.
Modeling to Candidate design	Transfer test conditions, acceptance criteria, failure data, owner and decision date. Recheck dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.
Candidate design to Experiment	Transfer test conditions, acceptance criteria, failure data, owner and decision date. Recheck dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.
Experiment to Scale & governance	Transfer test conditions, acceptance criteria, failure data, owner and decision date. Recheck dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

COMMON CONTROL POINT

No theme moves to a commercial commitment until a named owner has reproduced the relevant evidence and documented dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

Priority map: maturity and next decision locus



P01	NIMS Semiconductor Materials Co-Creation Hub: Sub-1nm Roadmap Tech / process | cue: no system/business cue
P02	TabPFN and NSGA-II: Optimising CIR Powder Coating Curing System / adoption | cue: system
P03	AI-Driven Alloy Design: Recycling Scrap Metal via "Dirty Alloys Tech / process | cue: no system/business cue
P04	WAAM Aluminum Strength: ML Framework for ER5356 Optimization Tech / process | cue: no system/business cue
P05	Physics-informed Bayesian optimization: HRTEM quantification efficiency System / adoption | cue: system
P06	MEMo AI: Predicting Mixture Properties via Molecular Interaction Business / rules | cue: NIST
P07	Radical AI: Autonomous Labs for Alloy Discovery and Supply Chain Business / rules | cue: Supply Chain
P08	AutoDNA: AI-native lab for autonomous biomolecular operations System / adoption | cue: system
P09	Mat2Vec-*: Hybrid Element Representations for Materials Prediction Tech / process | cue: no system/business cue
P10	Hydrogen-1.0: Deep Principle's AI model for materials discovery System / adoption | cue: integration

REPRODUCIBLE POSITIONING RULE

Horizontal position uses five discrete stages: Research, Prototype, Joint evaluation, Product adoption and Scale. The vertical bands classify the next decision locus: Tech / process, System / adoption, or Business / rules (including supply systems). Article-title cues take precedence; the overview is used only when the title is silent. These are categories, not impact ranks. Bubble diameter reflects the editorial score.

FACT is source-bound. BUSINESS READ, ACTION and UNKNOWN are explicit editorial layers.

P01 NIMS Semiconductor Materials Co-Creation Hub: Sub-1nm Roadmap

A10 | Data capture | Research

2026-11-02

FACT

The National Institute for Materials Science (NIMS) has established the "Semiconductor Materials Research Co-Creation Hub" to develop innovative materials across three time horizons. The initiative targets the transition to sub-1nm generations and future computing architectures to address the power consumption demands of AI.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P01.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 21/25 | MATURITY 1/5 | DECISION LOCUS: TECH / PROCESS

P02 TabPFN and NSGA-II: Optimising CIR Powder Coating Curing

A14 | Modeling | Joint evaluation

2026-11-04

FACT

Researchers have developed an AI framework combining TabPFN and NSGA-II to optimise catalytic infrared (CIR) curing for thermosetting powder coatings. The system reduced curing times by 47-77% compared to hot-air curing while improving mechanical properties. This provides a practical digital tool for industrial process control where predictive models were previously lacking.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P02.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 20/25 | MATURITY 3/5 | DECISION LOCUS: SYSTEM / ADOPTION

FACT is source-bound. BUSINESS READ, ACTION and UNKNOWN are explicit editorial layers.

P03 AI-Driven Alloy Design: Recycling Scrap Metal via "Dirty Alloys

A01 | Candidate design | Product adoption

2026-11-05

FACT

A German-Chinese research team has developed an AI-driven workflow to create "dirty alloys" that utilize scrap metal contaminants as alloying elements rather than removing them. Using ductile cast iron, the team achieved a 15.2% increase in tensile strength and a 73.2% increase in elongation at break compared to previous recycled materials. This approach reduces production costs by approximately 8% and minimizes the need for energy-intensive primary metals.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P03.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 4/5 | DECISION LOCUS: TECH / PROCESS

P04 WAAM Aluminum Strength: ML Framework for ER5356 Optimization

A04 | Experiment | Pilot

2026-11-06

FACT

Researchers have developed a machine learning framework that predicts tensile strength, elongation, flexural strength, and hardness for ER5356 aluminum alloy parts produced via Wire Arc Additive Manufacturing (WAAM). The model's predictions for a confirmation build were within 1.18% to 4.61% of measured values, demonstrating a method to reduce physical testing in metal AM.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P04.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 2/5 | DECISION LOCUS: TECH / PROCESS

FACT is source-bound. BUSINESS READ, ACTION and UNKNOWN are explicit editorial layers.

P05 Physics-informed Bayesian optimization: HRTEM quantification efficiency

A08 | Scale & governance | Product adoption

2026-11-04

FACT

Researchers have implemented a physics-informed Bayesian optimization (BO) framework to automate quantitative high-resolution transmission electron microscopy (HRTEM). Using a BaTiO 3 single crystal, the system determined a 3D crystal structure from a single image with a three- to four-order-of-magnitude improvement in time efficiency. This advancement enables faster, automated analysis of larger sample volumes and potential in-situ applications.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P05.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 4/5 | DECISION LOCUS: SYSTEM / ADOPTION

P06 MEMo AI: Predicting Mixture Properties via Molecular Interaction

A11 | Data capture | Pilot

2026-11-05

FACT

Professor Jun-young Jung's research team at Kookmin University developed MEMo, an AI model that predicts the properties of chemical mixtures by learning intermolecular interactions. Validated against 860,000 data points from NIST, the model outperforms existing methods in predicting density, sound speed, vapor pressure, refractive index, and surface tension.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P06.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 2/5 | DECISION LOCUS: BUSINESS / RULES

FACT is source-bound. BUSINESS READ, ACTION and UNKNOWN are explicit editorial layers.

P07 Radical AI: Autonomous Labs for Alloy Discovery and Supply Chain

A12 | Modeling | Research

2026-10-30

FACT

Radical AI uses an AI-driven autonomous laboratory platform to develop advanced alloys that reduce dependence on supply-constrained critical minerals. The system can produce 300 new compositions in approximately 16 weeks, potentially shrinking material development timelines from decades to just a few years.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P07.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 1/5 | DECISION LOCUS: BUSINESS / RULES

P08 AutoDNA: AI-native lab for autonomous biomolecular operations

A09 | Candidate design | Pilot

2026-11-05

FACT

Researchers from Shanghai Jiao Tong University have developed AutoDNA, an AI-native autonomous laboratory capable of designing and executing DNA-related molecular biology experiments. The system coordinates over 20 instruments to perform thousands of steps with minimal human intervention, bridging the gap between AI-driven experimental design and physical "wet lab" execution.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P08.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 2/5 | DECISION LOCUS: SYSTEM / ADOPTION

FACT is source-bound. BUSINESS READ, ACTION and UNKNOWN are explicit editorial layers.

P09 Mat2Vec-*: Hybrid Element Representations for Materials Prediction

A06 | Experiment | Research

2026-10-30

FACT

Researchers have developed Mat2Vec-*, a transferable supervised chemical prior that hybridizes handcrafted descriptors and learned embeddings. By distilling supervised element geometry into reusable tables, the method improves performance across MatBench composition tasks and reduces errors in structure-based predictors.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P09.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 1/5 | DECISION LOCUS: TECH / PROCESS

P10 Hydrogen-1.0: Deep Principle's AI model for materials discovery

A03 | Scale & governance | Pilot

2026-11-06

FACT

Deep Principle has released Hydrogen-1.0, an open-weight scientific model designed to automate experimental planning and materials discovery. The model outperforms GPT-6-Astra and Kimi-K3 in specific transition metal complex design and scientific computing tasks. This integration of AI with laboratory workflows aims to reduce the number of attempts required to find materials with desired properties.

WHY IT MATTERS

The decision relevance is closed-loop learning from data quality to experimentally validated material performance. The signal should be tested at the application and operating-system level, not accepted from a headline alone.

BUSINESS READ

For operating companies, compare the reported change with current qualification, sourcing and product-roadmap assumptions. For suppliers, provide machine-readable composition, process, test conditions, uncertainty and failure data.

ACTION

Within 30 days, select high-value decisions where data lineage and experimental feedback can be measured; record the evidence and owner against P10.

UNKNOWN

Still unproven or incompletely stated: dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.

EDITORIAL SCORE 19/25 | MATURITY 2/5 | DECISION LOCUS: SYSTEM / ADOPTION

Playbook and 0-5 year roadmap

STAKEHOLDER	NOW | 0-30 DAYS	NEXT | 1-12 MONTHS	LATER | 1-5 YEARS
Operating companies	select high-value decisions where data lineage and experimental feedback can be measured	Run production-like qualification with explicit acceptance and stop criteria.	Build a portfolio and architecture that can absorb technology and supplier changes.
Materials, equipment and technology suppliers	provide machine-readable composition, process, test conditions, uncertainty and failure data	Create shared reliability, process-window and failure-analysis data with customers.	Standardize interfaces, traceability, lifecycle support and recovery services.
Trading, investment and legal teams	Map dataset bias, reproducibility, IP, model transfer, experiment cost and adoption.	Contract for capacity, quality, change notice, liability, alternatives and exit.	Diversify regional, technical and customer concentration risk.

ROADMAP

NOW | 0-30 DAYS
Evidence ledger
Owner: Strategy + quality
Deliverable: claim, source, condition, owner

NOW | 0-30 DAYS
Risk screen
Owner: Procurement + legal
Deliverable: unknowns, alternatives, stop

NEXT | 1-12 MONTHS
Joint qualification
Owner: R&D + supplier
Deliverable: process window and failure data

NEXT | 1-12 MONTHS
Commercial gate
Owner: Business + finance
Deliverable: unit economics and capacity

LATER | 1-5 YEARS
Platform strategy
Owner: Executive team
Deliverable: portfolio and interface roadmap

LATER | 1-5 YEARS
Service layer
Owner: Operations + channel
Deliverable: monitoring, maintenance and recovery

GO / NO-GO GATES

GATE	OWNER	REQUIRED EVIDENCE	NO-GO CONDITION
G1 Evidence	**Quality**	Source, test conditions and reproducibility	No traceable evidence
G2 Integration	**R&D**	Interface, process window and failure analysis	Cannot meet system conditions
G3 Commercial	**Business**	Capacity, total cost, contract and alternatives	Economics or supply cannot be supported
G4 Lifecycle	**Operations**	Monitoring, maintenance, change notice and exit	No accountable operating plan

ANALYZED ARTICLES | ITEMS 01-14

Every title and URL is displayed in full. URLs wrap without shortening and remain clickable. A verified-reference label means the translated HTML did not retain its original source URL.

ID	FULL ARTICLE TITLE	FULL SOURCE / VERIFIED REFERENCE URL - CLICKABLE
A01	AI-Driven Alloy Design: Recycling Scrap Metal via "Dirty Alloys	https://www.heise.de/en/news/Researchers-use-AI-to-make-alloys-from-scrap-metal-11512823.html
A02	Asahi Kasei Smart Laboratory: AI-Driven Pymel Material Roadmap	https://monoist.itmedia.co.jp/mn/articles/2611/06/news014.html
A03	Hydrogen-1.0: Deep Principle's AI model for materials discovery	https://finance.yahoo.com/technology/ai/articles/deep-principle-introduces-hydrogen-1-073500519.html
A04	WAAM Aluminum Strength: ML Framework for ER5356 Optimization	https://3dprintingindustry.com/news/machine-learning-predicts-wire-arc-3d-printed-aluminum-strength-256249/
A05	Thermoelectric ML Framework: Physical Consistency and ZT Screening	https://doi.org/10.1371/journal.pone.0360053
A06	Mat2Vec-*: Hybrid Element Representations for Materials Prediction	https://doi.org/10.1038/s42004-026-02246-6
A07	OptiMat Alloys: LLM-powered FAIR database for multi-principal element alloys	https://www.nature.com/articles/s41524-026-02377-3
A08	Physics-informed Bayesian optimization: HRTEM quantification efficiency	https://www.nature.com/articles/s41524-026-02364-8
A09	AutoDNA: AI-native lab for autonomous biomolecular operations	https://news.qq.com/rain/a/20261105A06PUP00
A10	NIMS Semiconductor Materials Co-Creation Hub: Sub-1nm Roadmap	https://newswitch.jp/p/50680
A11	MEMo AI: Predicting Mixture Properties via Molecular Interaction	https://www.dailysmart.co.kr/news/articleView.html?idxno=132087
A12	Radical AI: Autonomous Labs for Alloy Discovery and Supply Chain	https://www.mining.com/radical-ai-uses-autonomous-labs-to-accelerate-alloy-discovery/
A13	MXenes: Machine Learning Discovery of Rare Earth 2D Materials	https://www.chemistryworld.com/news/dozens-of-unknown-mxenes-found-buried-in-materials-databases/4024445.article
A14	TabPFN and NSGA-II: Optimising CIR Powder Coating Curing	https://www.european-coatings.com/news/coatings-technologies/ai-framework-optimises-infrared-curing-of-powder-coatings/

MaterialsInformatics — Selected Articles

Date: 2026-11-08

Articles: 14

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#01 AI-Driven Alloy Design: Recycling Scrap Metal via "Dirty Alloys

Published November 05, 2026 heise online Germany



OVERVIEW

A German-Chinese research team has developed an AI-driven workflow to create "dirty alloys" that utilize scrap metal contaminants as alloying elements rather than removing them. Using ductile cast iron, the team achieved a 15.2% increase in tensile strength and a 73.2% increase in elongation at break compared to previous recycled materials. This approach reduces production costs by approximately 8% and minimizes the need for energy-intensive primary metals.

IN DEPTH

Key Findings

Researchers have successfully utilized machine learning to develop alloys from scrap metal that are insensitive to composition variations and benefit from the presence of contaminants. In tests using ductile cast iron (nodular cast iron), 14 out of 17 AI-generated alloy variants showed superior properties. Specifically, tensile strength increased by up to 15.2% and elongation at break rose by as much as 73.2% compared to earlier recycled materials. Additionally, production costs were approximately 8% lower than conventional processes that mix scrap with primary iron.

Technical Details

The development process employs a multi-stage AI workflow:

- **Candidate Generation:** An algorithm generates new alloy candidates by varying parameters within set limits, including chemical composition, heat treatment temperature, and duration.
- **Property Prediction:** Artificial neural networks predict the tensile strength and elongation at break for each candidate to find an optimal balance between strength and ductility.
- **Verification:** A second model, trained on a larger dataset of material properties and compositions, validates the selected candidates.
- **Iterative Optimization:** Experimental results from the most promising materials are fed back into the database to refine the prediction model for subsequent rounds.

Background & Context

Conventional metal production accounts for 10% of global energy consumption and roughly 8% of all greenhouse gas emissions. While recycling scrap metal can reduce environmental impact by up to 95%, contaminants typically lower the quality of new alloys. Traditionally, these contaminants are diluted by adding primary metals, which increases CO_2 emissions and energy requirements.

Significance & Outlook

By treating contaminants as opportunities rather than obstacles, this method enhances the environmental benefits of recycling. The research was a collaboration between the Max Planck Institute for Sustainable Materials, Shanghai Jiao Tong University, City University of Hong Kong, East China University of Science and Technology, and Central South University. The findings were published in *Science Advances*. The team now plans to extend this AI-assisted methodology to other materials, including recycled aluminum, copper alloys, and steels.

Source: https://www.heise.de/en/news/Researchers-use-AI-to-make-alloys-from-scrap-metal-11512823.html

Collected: November 07, 2026 | Automated Research System (AI)

#02 Asahi Kasei Smart Laboratory: AI-Driven Pymel Material Roadmap

Published November 06, 2026 MONOist Japan



OVERVIEW

Asahi Kasei is establishing a "Smart Laboratory" in Fuji City, Shizuoka, to automate the development of Pymel photosensitive insulating materials for semiconductors. The platform integrates AI and automation to increase the number of development experiments by approximately four times, accelerating the discovery of materials that meet complex next-generation performance requirements.

IN DEPTH

Key Findings

Asahi Kasei announced on November 5, 2026, the establishment of a "Smart Laboratory" platform designed to autonomously execute the entire material development process. Scheduled to begin operations in January 2027, the facility focuses on the development of Pymel, a photosensitive insulating material for semiconductors. By automating the blending of multiple raw materials and the subsequent processing and performance evaluation stages, the company expects to increase the volume of development experiments—defined as the number of compositions evaluated over a specific period—by approximately four times compared to conventional methods.

Technical Details

The Smart Laboratory functions as a single autonomous experimental system that manages a closed loop of material design, experimentation, evaluation, and learning. The system automates the following sequence:

- Experimental planning and scheduling.
- Raw material blending and sample preparation.
- Processing and evaluation based on semiconductor package manufacturing processes.
- Data feedback for learning and analysis to propose the next set of compositions and conditions.

This autonomous cycle is integrated with a data infrastructure that leverages Materials Informatics (MI). By combining vast amounts of existing Pymel experimental data with public data, simulation, and theoretical science, the system identifies new compositions that may have been overlooked by traditional human-led research.

Background and Context

The demand for interlayer insulating films is growing at an average annual rate of approximately 8%, a trend expected to continue until around 2030. However, the rise of generative AI has increased the technical difficulty of advanced semiconductors, requiring materials to balance multiple high-level performance metrics, such as fine processing, shape stability, high reliability, and high resolution. Asahi Kasei has positioned its electronics business as a "priority growth" sector within its "Medium-Term Management Plan 2027 ～Trailblaze Together～."

Significance and Outlook

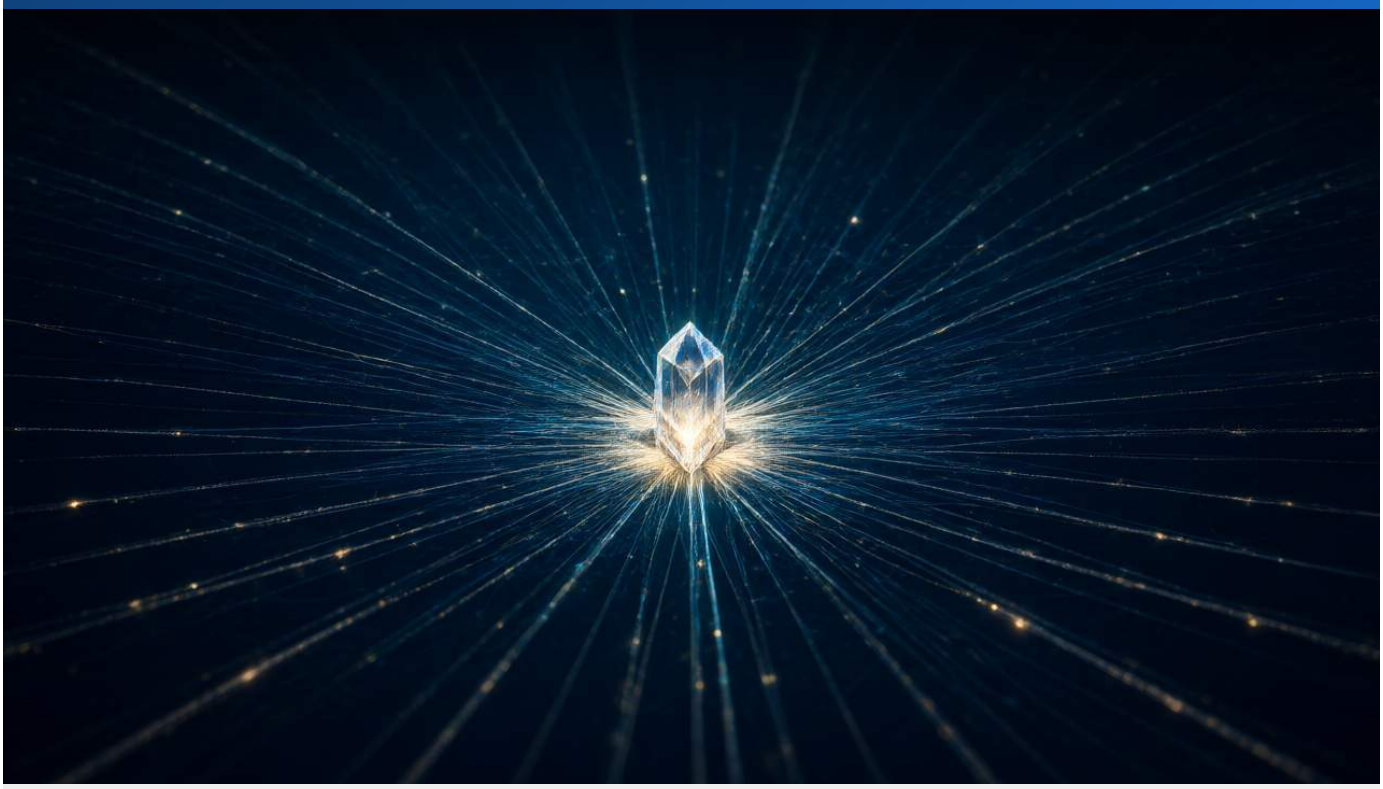
The transition to an AI-driven autonomous system allows Asahi Kasei to move beyond researcher experience to explore a wider range of possibilities more efficiently. The company intends to accumulate technical expertise from the Pymel project to expand this autonomous experimental approach to other electronic materials and, eventually, other material domains.

Source: https://monoist.itmedia.co.jp/mn/articles/2611/06/news014.html

Collected: November 07, 2026 | Automated Research System (AI)

#03 Hydrogen-1.0: Deep Principle's AI model for materials discovery

Published November 06, 2026 Yahoo Finance（PR Newswire） USA



OVERVIEW

Deep Principle has released Hydrogen-1.0, an open-weight scientific model designed to automate experimental planning and materials discovery. The model outperforms GPT-6-Astra and Kimi-K3 in specific transition metal complex design and scientific computing tasks. This integration of AI with laboratory workflows aims to reduce the number of attempts required to find materials with desired properties.

IN DEPTH

Key Findings

Hydrogen-1.0 demonstrates superior performance in iterative materials discovery compared to other large language models. In a transition metal complex design evaluation seeking a larger HOMO–LUMO gap, Hydrogen-1.0 achieved a mean best-so-far gap of 4.318 eV by the fifth round, surpassing GPT-6-Astra (3.689 eV) and Kimi-K3 (3.353 eV). Additionally, in internal scientific computing and one-step forward reaction prediction, Hydrogen-1.0 outperformed GPT-6-Astra across all thinking settings, leading by 5.13 and 4.76 percentage points against Astra's maximum thinking setting.

Technical Details

Built via post-training of GLM-5.3, Hydrogen-1.0 utilizes chemistry, materials science, and life sciences data, including agent trajectories from Deep Principle's laboratories. The training process employs supervised fine-tuning for reasoning and experimental protocols, while reinforcement learning incorporates feedback from research outcomes. The model is capable of:

- **Experiment Design:** Converting research goals into JSON protocols. In a 12-vial Suzuki coupling example, the model detected and corrected an aspiration error during a virtual rehearsal.
- **Simulation Workflow:** Writing Python to build a polyethylene melt and running GROMACS, including the ability to repair topology errors.
- **Pathway Exploration:** Generating 27 molecular structures via 30 reactions in an Ireland–Claisen rearrangement network to identify bottlenecks.

Background & Context

The model is accessible via open-weight downloads on Hugging Face and ModelScope, an API on NeuroSpark, or through Mira, Deep Principle's AI Scientist. Development involved collaborations with UniPat and Mind Lab on data and training pipelines, and NeuroSpark on infrastructure. In benchmark evaluations, Hydrogen-1.0 outperforms GPT-6-Astra on FrontierScience-Research and improves upon GLM-5.3 on GPQA Diamond.

Significance & Outlook

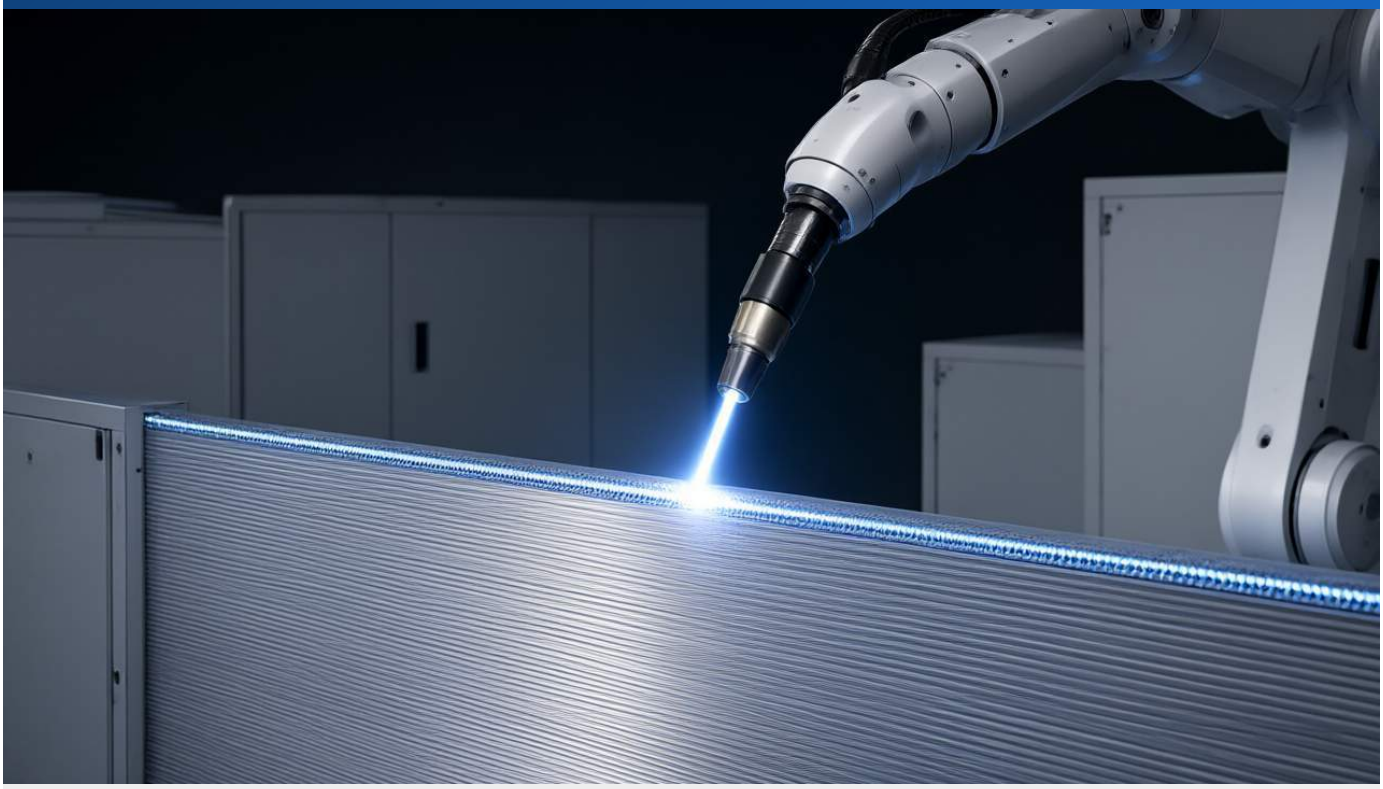
By training on complete discovery trajectories—connecting desired properties to synthesis and evaluation—Hydrogen-1.0 enables researchers to prioritize investigations more effectively. Deep Principle intends to extend this learning across different material families so that experience from one campaign improves subsequent discovery efforts.

Source: https://finance.yahoo.com/technology/ai/articles/deep-principle-introduces-hydrogen-1-073500519.html

Collected: November 07, 2026 | Automated Research System (AI)

#04 WAAM Aluminum Strength: ML Framework for ER5356 Optimization

Published November 06, 2026 3D Printing Industry USA



OVERVIEW

Researchers have developed a machine learning framework that predicts tensile strength, elongation, flexural strength, and hardness for ER5356 aluminum alloy parts produced via Wire Arc Additive Manufacturing (WAAM). The model's predictions for a confirmation build were within 1.18% to 4.61% of measured values, demonstrating a method to reduce physical testing in metal AM.

IN DEPTH

Key Findings

A new machine learning framework can simultaneously predict four mechanical properties of aluminum WAAM parts: tensile strength, elongation, flexural strength, and hardness. In a confirmation build using optimized settings, the model predicted a tensile strength of 295.20 MPa and 40.10% elongation; the actual measured values were 288.90 MPa and 38.25%, respectively. While the predicted strength gain was not fully realized, the elongation result was 2.53 percentage points higher than the best previous run.

Technical Details

The study utilized a Fronius iWave 500i AC/DC welding unit with an ABB IRB 1520ID robotic arm operating in cold metal transfer (CMT) mode. Researchers used a Taguchi L27 design plus three center-point runs to create 30 builds on a fixed circular path, varying four parameters:

- Wire feed speed: 7.5 to 9.5 m/min
- Travel speed: 6 to 10 mm/s
- Interpass temperature: 80 to 160°C
- Shielding gas flow: 12 to 18 L/min

The team employed a stacked ML model called PG-MOSR. In five-fold cross-validation, R^2 values were 0.7799 for tensile strength, 0.8299 for elongation, 0.8142 for flexural strength, and 0.8599 for hardness. A version trained on raw settings performed even better, with R^2 values between 0.8779 and 0.8885.

Background & Context

Most previous WAAM research focused on single responses, such as bead geometry or surface roughness. This study differs by predicting multiple mechanical properties for circular-path ER5356 deposits. For comparison, other frameworks have targeted Ti-6Al-4V via laser powder bed fusion (LPBF) or Al-Si-Mg parts using microstructural and void data to reduce physical testing.

Significance & Outlook

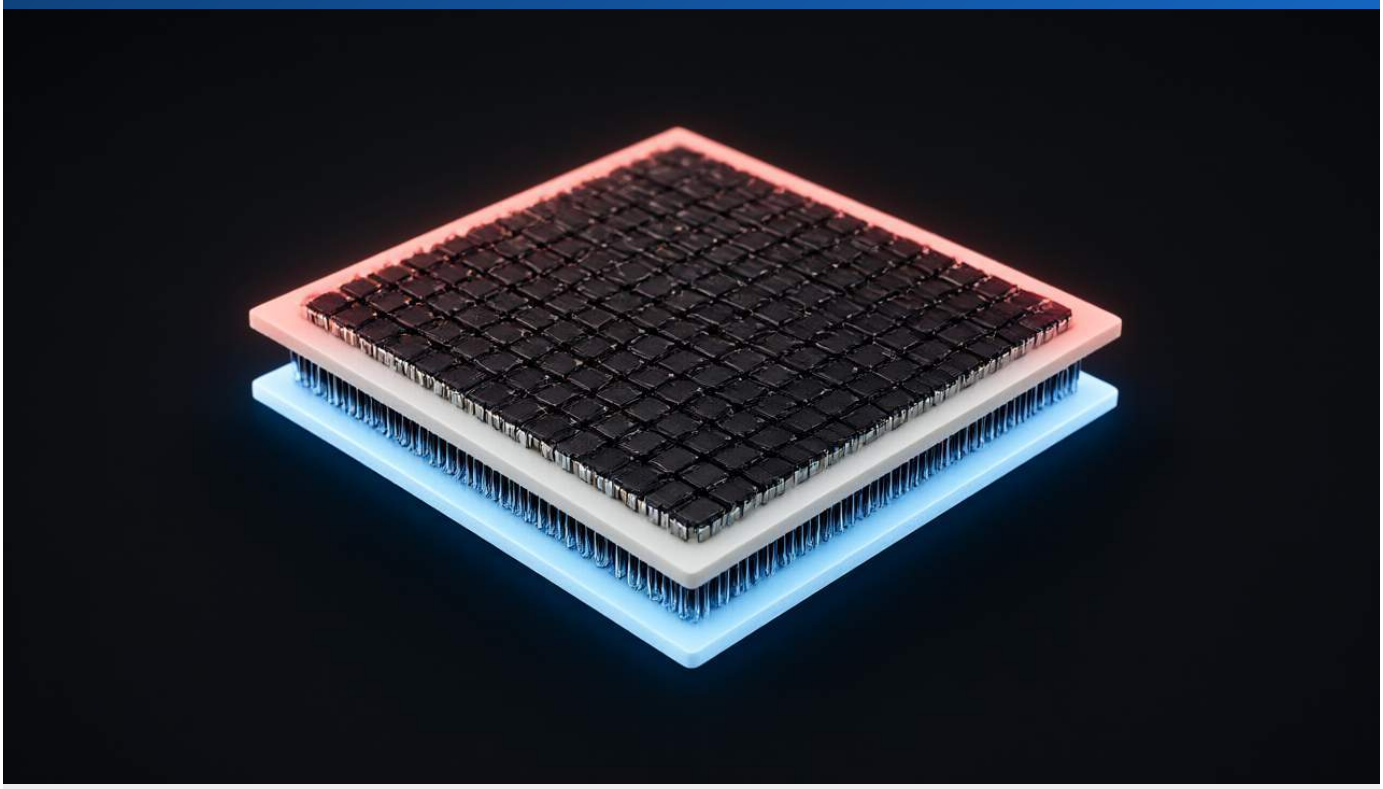
The framework allows for the screening of thousands of parameter combinations—50,000 in this study—to identify optimal settings. However, the researchers note that fracture surfaces showed clustered pores, which may explain why some strengths fell short of predictions. Future work is expected to incorporate CT-based porosity measurement, in-situ thermal monitoring, and larger datasets to improve reproducibility and validation.

Source: https://3dprintingindustry.com/news/machine-learning-predicts-wire-arc-3d-printed-aluminum-strength-256249/

Collected: November 07, 2026 | Automated Research System (AI)

#05 Thermoelectric ML Framework: Physical Consistency and ZT Screening

Published November 02, 2026　PLOS ONE（Dongguan University of Technology）



OVERVIEW

A physics-guided machine learning framework has been developed to screen thermoelectric materials by independently predicting transport properties rather than direct ZT regression. By integrating uncertainty propagation and material-wise validation, the approach reduces target leakage and provides more physically consistent performance estimations.

IN DEPTH

Key Findings

The developed machine learning (ML) framework demonstrates a robust strategy for thermoelectric materials screening by prioritizing physical consistency over apparent predictive accuracy. Unlike direct regression models that predict the figure of merit (ZT), this framework independently predicts the Seebeck coefficient, electrical conductivity, and thermal conductivity. While this method shows lower apparent accuracy than direct ZT models, it provides improved interpretability and eliminates target leakage caused by the mathematical derivation of ZT from multiple transport properties.

Technical Details

The framework utilizes several specific methodologies to ensure reliability:

- **Material-wise Validation:** To prevent material-level information leakage, exact chemical formulas are kept exclusively in either the training or held-out test subsets, rather than distributing measurements from the same material across both.
- **Uncertainty Quantification:** Predictive uncertainty is quantified using ensemble learning. This uncertainty is then propagated into the thermoelectric performance evaluation and uncertainty-aware Lower Confidence Bound (LCB) screening.
- **Data Source:** The models were evaluated using experimental data from the ESTM database.

Background & Context

Thermoelectric materials convert heat into electricity via the Seebeck effect, making them valuable for waste heat recovery and localized cooling. However, discovery is hindered by the interdependence of the Seebeck coefficient (S), electrical conductivity (σ), and thermal conductivity (κ), where improving one often negatively impacts another. Historically, this has required resource-intensive experimental iteration. While supervised learning models like random forests and deep neural networks have been applied to accelerate this process, many suffer from overly optimistic performance due to hidden statistical correlations in the datasets.

Significance & Outlook

By integrating physical consistency and uncertainty propagation, this framework offers a more realistic approach to identifying candidate materials. The transition from direct ZT prediction to a structured, property-based evaluation allows researchers to avoid the pitfalls of target leakage and provides a more reliable roadmap for data-driven thermoelectric materials discovery.

Source: https://doi.org/10.1371/journal.pone.0360053

Collected: November 07, 2026 | Automated Research System (AI)

#06 Mat2Vec-*: Hybrid Element Representations for Materials Prediction

Published October 30, 2026 Communications Chemistry（Beijing Information Science and Technology University） China



OVERVIEW

Researchers have developed Mat2Vec-*, a transferable supervised chemical prior that hybridizes handcrafted descriptors and learned embeddings. By distilling supervised element geometry into reusable tables, the method improves performance across MatBench composition tasks and reduces errors in structure-based predictors.

IN DEPTH

Key Findings

The study introduces Mat2Vec-*, a compact and transferable element representation that combines handcrafted descriptors with supervised embeddings. Testing across eight structure-based MatBench regression tasks involved 2,240 models utilizing controlled CGCNN and MEGNet benchmarks. The results demonstrate that Mat2Vec-* can replace or augment corpus-derived Mat2Vec in composition-only models like CrabNet, improving performance across all four MatBench composition tasks. Additionally, Mat2Vec-* features reduce errors for several modern structure-based predictors on the Matbench Discovery WBM benchmark via lightweight residual correction.

Technical Details

The methodology is based on the observation that handcrafted and supervised representations encode complementary chemical information. The researchers identified rotation-invariant cosine-distance relations from top-performing models to reconstruct the Mat2Vec-* tables. This approach treats element representations as an embedding layer similar to token embeddings in natural language processing (NLP), mapping discrete elemental identities into continuous vector spaces to support interaction modeling in crystal graph networks and formula-based models.

Background & Context

Materials informatics typically relies on three types of element representations:

- **Mat2Vec:** Unsupervised representations learned from materials corpora based on co-occurrence statistics.
- **Handcrafted descriptors:** Interpretable features encoding prior chemical and physical knowledge.
- **Learnable embeddings:** End-to-end optimized vectors that are task-dependent but often lack interpretability and transferability.

Previously, these three methods were treated as mutually exclusive. However, the researchers noted that models like CrabNet successfully fuse different information channels (such as stoichiometry and elemental identity) through simple additive fusion,

suggesting that domain-knowledge descriptors and supervised embeddings may occupy separable subspaces.

Significance & Outlook

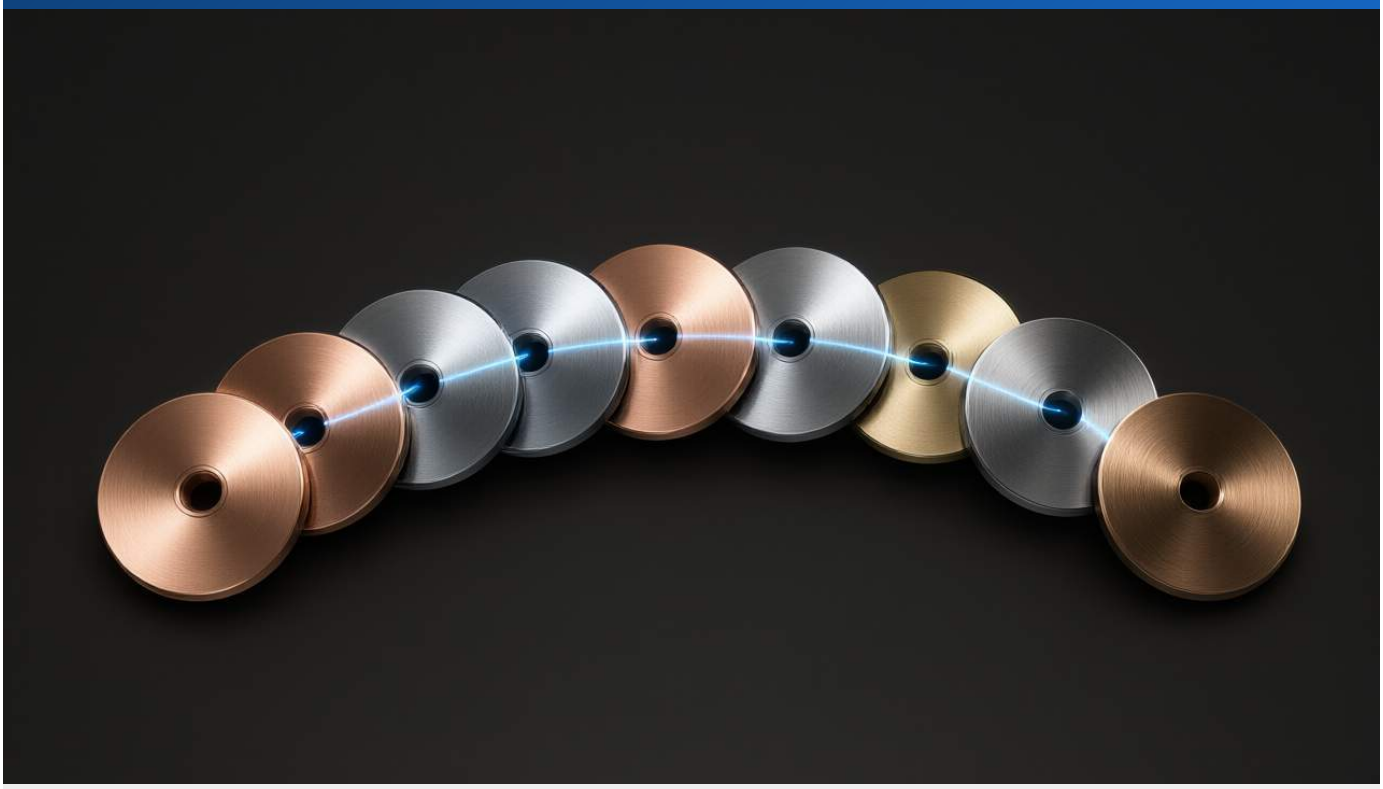
By establishing Mat2Vec-* as a reusable chemical prior, this work bridges the gap between data-driven embeddings and domain-knowledge descriptors. This hybrid approach allows materials prediction models to utilize supervised chemical geometry without requiring full retraining for every new task, enhancing the efficiency of surrogate modeling in the physical sciences.

Source: https://doi.org/10.1038/s42004-026-02246-6

Collected: November 07, 2026 | Automated Research System (AI)

#07 OptiMat Alloys: LLM-powered FAIR database for multi-principal element alloys

Published November 04, 2026 npj Computational Materials（Empa） Switzerland



OVERVIEW

OptiMat Alloys is a conversational agent that enables on-demand computation and automatic persistence of multi-principal element alloy data into a FAIR-aligned living database. By integrating foundational machine learning interatomic potentials with a natural-language interface, it removes the need for programming expertise in computational alloy screening.

IN DEPTH

Key Findings

OptiMat Alloys introduces a large language model (LLM)-powered conversational agent designed for the exploration of multi-principal element alloys. Unlike existing FAIR materials repositories that only provide pre-computed entries, this system utilizes LLM-based workflow orchestration to perform calculations on demand. These results are automatically persisted in a local database with full provenance, creating a "living database" that eliminates the need for a separate deposition step.

Technical Details

The system is built on several technical pillars to ensure accessibility and reliability:

- **Low-Barrier Accessibility:** The agent is accessible via a web interface, allowing users to conduct research without programming expertise.
- **Built-in Uncertainty Quantification:** The system reports uncertainty through cross-potential and cross-configuration validation.
- **Broad Material Coverage:** It couples natural-language interaction with foundational machine learning interatomic potentials that cover nearly the entire periodic table.
- **FAIR Alignment:** The automated persistence of calculations ensures that records are provenance-rich and aligned with FAIR (Findable, Accessible, Interoperable, and Reusable) data principles.

Background & Context

Traditional materials repositories are often perpetually incomplete because they cannot adapt to new questions on demand. This research was conducted by authors from Empa (Swiss Federal Laboratories for Materials Science and Technology) and the National Centre for Computational Design and Discovery of Novel Materials MARVEL. The project received computing resources from the Swiss National Supercomputing Centre (CSCS) and funding from NCCR MARVEL via the Swiss National Science Foundation (grant number 205602).

Significance & Outlook

By combining domain knowledge with on-demand computation, OptiMat Alloys brings computational alloy screening within reach of any materials scientist. The integration of LLMs allows for targeted exploration guided by the user's specific expertise, potentially accelerating the discovery and validation of multi-principal element alloys.

Source: https://www.nature.com/articles/s41524-026-02377-3

Collected: November 07, 2026 | Automated Research System (AI)

#08 Physics-informed Bayesian optimization: HRTEM quantification efficiency

Published November 04, 2026　npj Computational Materials（TU Darmstadt・Forschungszentrum Jülich）　Germany



OVERVIEW

Researchers have implemented a physics-informed Bayesian optimization (BO) framework to automate quantitative high-resolution transmission electron microscopy (HRTEM). Using a BaTiO 3 single crystal, the system determined a 3D crystal structure from a single image with a three- to four-order-of-magnitude improvement in time efficiency. This advancement enables faster, automated analysis of larger sample volumes and potential in-situ applications.

IN DEPTH

Key Findings

The implementation of a physics-informed Bayesian optimization (BO) framework has significantly reduced the time required for quantitative high-resolution transmission electron microscopy (HRTEM). In a model system using a BaTiO 3 single crystal containing heavy, medium, and light elements, the framework determined the three-dimensional crystal structure from a single HRTEM image. This process achieved a time efficiency improvement of three to four orders of magnitude compared to conventional methods.

Technical Details

The framework utilizes a stepwise strategy and a probabilistic engine to refine high-dimensional parameter spaces. The quantification process involves a physics-informed model where parameters are categorized into two groups:

- **Imaging-related parameters:** These include image spread σ and residual aberrations of the imaging lens system, such as defocus C 1, twofold astigmatism A 1, threefold astigmatism A 2, axial coma B 2, spherical aberration C 3, fourfold astigmatism A 3, and star aberration S 3.
- **Structure parameters:** These include atomic positions, atomic occupancies, and the electron absorption factor AF.

The system compares simulated images with experimental images using criteria such as image contrast (standard deviation of intensity distribution), image similarity (normalized cross-correlation coefficient or structural similarity index metric), and goodness of fit (χ 2 statistic or R-factor).

Background & Context

HRTEM allows for the direct atomic resolution observation of crystal lattices, defects, and interfaces. However, essential structural information is often distorted by imaging imperfections, residual aberrations, sample orientation misalignment, and noise, including magnetic Johnson noise. While model-based iterative image simulation has been used for quantification, the high number of parameters typically makes the process time-consuming and dependent on experienced users, limiting its application to small sample areas.

Significance & Outlook

By moving toward full automation, this BO framework overcomes the limitations of user-supervised iterative approaches. This capability opens new avenues for the analysis of larger sample volumes and provides a promising pathway for in-situ applications, such as observing phase transformations and catalysis processes in real-time.

Source: https://www.nature.com/articles/s41524-026-02364-8

Collected: November 07, 2026 | Automated Research System (AI)

#09 AutoDNA: AI-native lab for autonomous biomolecular operations

Published November 05, 2026 腾讯新闻（生物世界） China



OVERVIEW

Researchers from Shanghai Jiao Tong University have developed AutoDNA, an AI-native autonomous laboratory capable of designing and executing DNA-related molecular biology experiments. The system coordinates over 20 instruments to perform thousands of steps with minimal human intervention, bridging the gap between AI-driven experimental design and physical "wet lab" execution.

IN DEPTH

Key Findings

A research team including Hai-bo Chen, Chun-hai Fan, Fei Wang, Zhao-guo Wang, Ming-yu Wu, and Jia-bin Wang from the Jiashan Xiangfu Laboratory has developed AutoDNA, an AI-native autonomous biomolecular experimental platform. The system can translate natural language requirements into executable experimental workflows, autonomously coordinating more than 20 types of instruments. In a representative DNA data storage and retrieval experiment, AutoDNA executed 11,382 steps over approximately eight days to encode and read a specific phrase into DNA sequences, requiring human intervention only for hardware maintenance and the replenishment of reagents and 108 pipette tips.

Technical Details

Unlike traditional automation that adds AI to existing systems, AutoDNA utilizes a multi-agent architecture designed from the ground up to be AI-native. This architecture enables a closed-loop "design-experiment-optimization" workflow. The platform integrates common nucleic acid experimental instruments and uses robotic arms for sample transport. The system is capable of performing core operations including nucleic acid synthesis, amplification, transcription, and sequencing, and can autonomously adjust protocols based on experimental feedback.

Background & Context

While AI is commonly used for "dry lab" tasks such as data analysis and prediction, "wet lab" operations involving biological materials typically require significant manual labor and precision. Professor Hai-bo Chen noted that creating a "self-driving lab" for molecular biology is particularly challenging due to the complexity of workflows and the high precision required for coordinating multiple instruments. AutoDNA aims to move beyond systems where AI only handles a single segment of a process, instead managing the entire lifecycle of an experiment.

Significance & Outlook

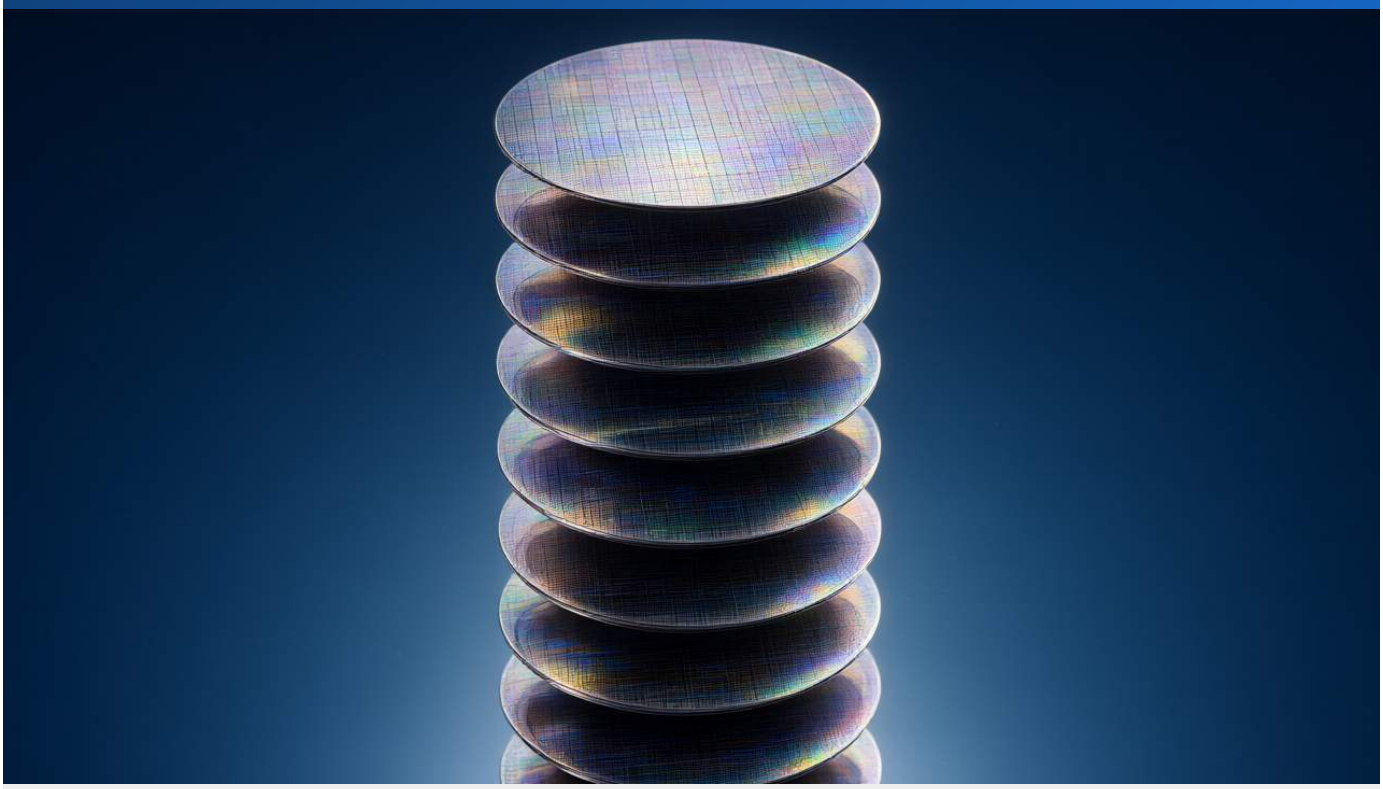
The team validated AutoDNA across four applications: nucleic acid detection, enzymatic DNA synthesis optimization, DNA data storage and reading, and tumor-related mutation detection. The research, published in Nature on November 4, 2026, provides a blueprint for "Science as a Service," potentially accelerating biological discovery in fields such as synthetic biology and information storage.

Source: https://news.qq.com/rain/a/20261105A06PUP00

Collected: November 07, 2026 | Automated Research System (AI)

#10 NIMS Semiconductor Materials Co-Creation Hub: Sub-1nm Roadmap

Published November 02, 2026　ニュースイッチ（日刊工業新聞）　Japan



OVERVIEW

The National Institute for Materials Science (NIMS) has established the "Semiconductor Materials Research Co-Creation Hub" to develop innovative materials across three time horizons. The initiative targets the transition to sub-1nm generations and future computing architectures to address the power consumption demands of AI.

IN DEPTH

Key Findings

NIMS launched the Semiconductor Materials Research Co-Creation Hub in August to integrate fragmented research efforts and create a cross-disciplinary approach to semiconductor materials. The hub operates across three distinct timelines: immediate challenges for the "beyond 2nm" generation, mid-term development of silicon-surpassing materials, and long-term exploration of materials for post-2035 applications.

Technical Details

The hub's research is divided into specific technical milestones:

- **Short-term (Goal 2030):** Collaborating with the Leading-edge Semiconductor Technology Center (LSTC), NIMS focuses on gate stack and interconnect materials. In partnership with the University of Tokyo and the National Institute of Advanced Industrial Science and Technology (AIST), researchers developed a technique to finely adjust threshold voltage by introducing new materials into the dipole layer of gate insulating films.
- **Mid-term:** Under a project by the Japan Science and Technology Agency (JST) for next-generation edge AI semiconductors, NIMS is exploring 2D semiconductors, such as molybdenum disulfide, and oxide semiconductors. NIMS has established approximately 120 processes to build a manufacturing base for complementary field-effect transistors (CFET). Specifically, researchers including Yoshiki Sakuma achieved uniform single-crystal film growth on 2-inch wafers using metal-organic chemical vapor deposition (MOCVD) for sub-1nm mass production. Additionally, Naoyuki Harada developed palladium-cobalt oxide thin films for fine interconnects.
- **Long-term (Post-2035):** A priority project launched in 2025 focuses on 3D structures, hetero-junctions, brain-inspired computing, and next-generation computing to redefine semiconductor operating principles.

Background and Significance

The acceleration of this roadmap is driven by the explosive growth of AI and the resulting increase in power consumption. NIMS asserts that materials must be identified now to ensure mass production is viable in ten years. By leveraging its expertise in metals, structural materials, organic materials, and computational science, NIMS intends to apply a materials-first approach—determining the material before developing the process and device structure—to enable ultra-low power AI semiconductors.

Source: https://newswitch.jp/p/50680

Collected: November 07, 2026 | Automated Research System (AI)

#11 MEMo AI: Predicting Mixture Properties via Molecular Interaction

Published November 05, 2026 스마트경제 South Korea



OVERVIEW

Professor Jun-young Jung's research team at Kookmin University developed MEMo, an AI model that predicts the properties of chemical mixtures by learning intermolecular interactions. Validated against 860,000 data points from NIST, the model outperforms existing methods in predicting density, sound speed, vapor pressure, refractive index, and surface tension.

IN DEPTH

Key Findings

The MEMo (Mixture Embedding via Mole Fraction) AI model demonstrates superior predictive accuracy for chemical mixture properties compared to existing representative methods. In a validation study using over 860,000 experimental data points from the U.S. National Institute of Standards and Technology (NIST), MEMo showed significantly higher accuracy in four out of five key properties: density, sound speed, vapor pressure, refractive index, and surface tension. The performance gap was particularly pronounced in mixtures with strong intermolecular interactions, such as ionic liquids and salt solutions, as well as mixtures containing molecules not previously encountered during the AI's training phase.

Technical Details

Unlike conventional AI models that analyze individual molecular characteristics and calculate a simple weighted average based on mixing ratios, MEMo integrates "which molecule is mixed and in what proportion" from the initial stage. The architecture consists of a front-end that identifies the inherent characteristics of each molecule and a back-end where different molecules exchange information to learn real-time interactions. This allows the AI to recognize the same molecule differently depending on its mixing partner and ratio, capturing non-linear changes in properties that traditional averaging methods miss.

Background and Context

Chemical products, ranging from industrial solvents and battery electrolytes to cosmetics, are typically complex mixtures. Because properties change non-linearly based on mixing ratios, verifying every possible combination through physical experimentation is practically impossible. The research, conducted by Professor Jun-young Jung along with integrated MS/PhD student Ji-hwan Kim and undergraduate researcher Chan-jung Kim, was published in the SCI-level journal *Chemical Engineering Journal* (Impact Factor 13.2, JCR Q1) under the title "Encoding composition-dependent intermolecular interactions into learned molecular representations."

Significance and Outlook

MEMo offers high versatility, as a single model can process everything from pure substances to complex mixtures of two or three components. To support a transparent academic ecosystem, the research team has released the evaluation data and model code. This technology is expected to reduce the time and cost of research and development in fields such as battery electrolyte design, eco-friendly solvent development, and carbon dioxide capture materials.

Source: https://www.dailysmart.co.kr/news/articleView.html?idxno=132087

Collected: November 07, 2026 | Automated Research System (AI)

#12 Radical AI: Autonomous Labs for Alloy Discovery and Supply Chain

Published October 30, 2026 MINING.COM USA



OVERVIEW

Radical AI uses an AI-driven autonomous laboratory platform to develop advanced alloys that reduce dependence on supply-constrained critical minerals. The system can produce 300 new compositions in approximately 16 weeks, potentially shrinking material development timelines from decades to just a few years.

IN DEPTH

Key Findings

Radical AI has demonstrated an alloy discovery process capable of producing 300 new compositions in approximately 16 weeks. Based in New York and backed by RTX and Nvidia, the company utilizes a self-driving laboratory platform that integrates AI and robotics to design, manufacture, and test materials. This approach allows manufacturers to exclude specific elements—such as those vulnerable to geopolitical tensions or export restrictions—while maintaining required material properties.

Technical Details

The company employs an "active learning loop" to accelerate iterative discovery. The process follows these steps:

- AI identifies a promising composition based on user-defined constraints.
- The autonomous lab synthesizes a physical sample weighing between 50 and 200 grams.
- The sample is analyzed for chemical composition, grain structure, and mechanical properties, including hardness, tensile strength, and high-temperature performance relevant to hypersonic applications.
- Resulting data is fed back into machine-learning models to refine subsequent experiments.

Background & Context

Traditional material discovery is costly and slow, often taking 10 to 15 years to reach operation and costing over $100 million for a single system. Consequently, many aerospace and defense sectors rely on structural metals that are 20 to 50 years old. Radical AI operates downstream from mining and refining, focusing on the combination of existing refined metals. A primary example is the development of high-performance alloys for extreme-temperature environments that contain little to no hafnium, a strategic element heavily controlled by China's supply chain.

Significance & Outlook

The technology enables "concurrent engineering," where materials are developed specifically for the requirements of a new aircraft or engine alongside the product design itself. By reducing development timelines from 20 years to one, two, or three years, Radical AI provides a mechanism for US manufacturers to address supply chain vulnerabilities by redesigning materials around more readily available elements.

Source: https://www.mining.com/radical-ai-uses-autonomous-labs-to-accelerate-alloy-discovery/

Collected: November 07, 2026 | Automated Research System (AI)

#13 MXenes: Machine Learning Discovery of Rare Earth 2D Materials

Published November 06, 2026 Chemistry World UK



OVERVIEW

Researchers have identified dozens of previously unknown MXenes by mining existing materials databases and using machine learning to predict new candidates. The discovery of rare earth-containing MXenes introduces semiconducting and magnetic properties, enabling potential applications in spintronics and 2D field effect transistors.

IN DEPTH

Key Findings

Researchers have discovered 33 previously unknown MXenes by mining the Materials Project and the Open Quantum Materials Database. By training a machine learning algorithm on this data, the team further identified and produced 11 new rare earth-containing MXenes. These materials exhibit properties not found in conventional MXenes, specifically semiconductivity and various magnetic characteristics, such as ferromagnetism in ytterbium-containing versions and antiferromagnetism in holmium-containing versions.

Technical Details

To expand the search, the team allowed the M element to include rare earth metals alongside transition metals, and expanded the X site to include light elements like phosphorus and oxygen. The researchers synthesized seven of the identified materials, including thorium nitride oxide, using a "self-propagating high-temperature synthesis" protocol. This method produces 2D MXenes directly, eliminating the need for continuous external heating and the etching of 3D crystals, which significantly reduces energy consumption and synthesis time compared to traditional methods.

Background and Context

MXenes are layered inorganic 2D materials first developed in 2011 by Yury Gogotsi and colleagues at Drexel University. Traditionally, they consist of a transition metal (M) and carbon or nitrogen (X). While useful for supercapacitors and dry lubricants, conventional MXenes are difficult to synthesize—often requiring harsh etchants like hydrofluoric acid—and typically lack magnetism and semiconductivity.

Significance and Outlook

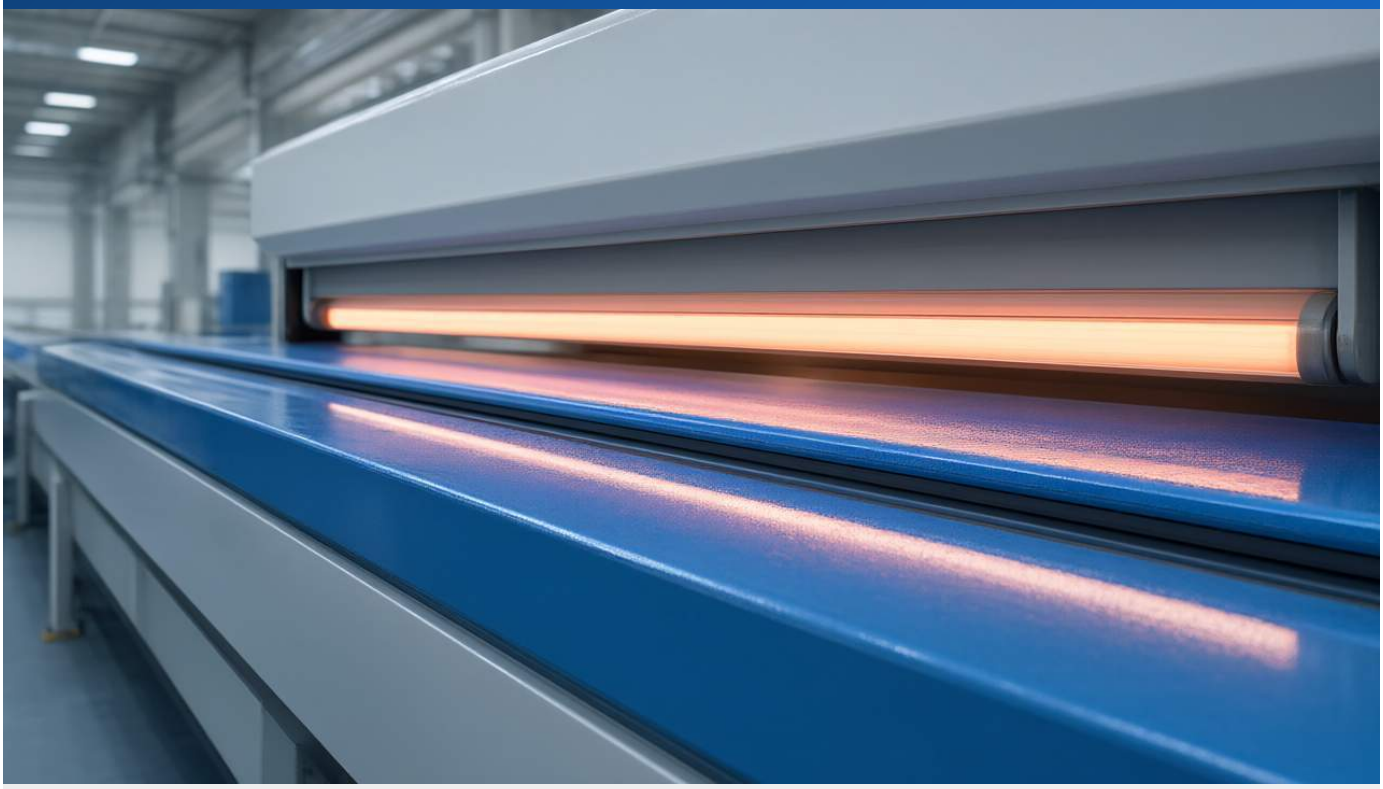
The introduction of semiconducting properties may allow MXenes to be used in 2D field effect transistors with higher carrier mobility than silicon. Additionally, the magnetic properties of rare earth-based MXenes are promising for magnetic memories and spintronics. The researchers intend to further characterize the synthesis process to expand the chemical variety and range of properties achievable in these materials. Yury Gogotsi noted that the ability to move directly from inexpensive precursors to the MXene via direct synthesis is a critical advancement.

Source: https://www.chemistryworld.com/news/dozens-of-unknown-mxenes-found-buried-in-materials-databases/4024445.article

Collected: November 07, 2026 | Automated Research System (AI)

#14 TabPFN and NSGA-II: Optimising CIR Powder Coating Curing

Published November 04, 2026 European Coatings



OVERVIEW

Researchers have developed an AI framework combining TabPFN and NSGA-II to optimise catalytic infrared (CIR) curing for thermosetting powder coatings. The system reduced curing times by 47–77% compared to hot-air curing while improving mechanical properties. This provides a practical digital tool for industrial process control where predictive models were previously lacking.

IN DEPTH

Key Findings

The integration of the Tabular Prior-data Fitted Network (TabPFN) and the Non-dominated Sorting Genetic Algorithm II (NSGA-II) has successfully optimised the quality of catalytic infrared (CIR)-cured thermosetting powder coatings. Experimental validation showed that CIR curing reduces curing time by 47–77% compared to conventional hot-air curing. While mechanical properties were improved, the study noted that high radiation intensity negatively impacts the visual appearance of the coating.

Technical Details

The researchers tested one polyester coating and two hybrid coatings using 150 experimental sets generated via Latin hypercube sampling. The framework evaluated five quality parameters: adhesion strength, hardness, impact resistance, gloss, and colour difference (ΔE). The TabPFN model, designed for small-sample learning, achieved accuracy comparable to seven baseline algorithms—including random forest, support vector machine, and artificial neural networks—but required no hyperparameter tuning and completed training in 26 seconds.

To identify optimal curing parameters, the TabPFN-NSGA-II framework was combined with the Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS), resulting in a mean relative error of 8.10% or less. Additionally, Shapley additive explanations (SHAP) analysis revealed that curing distance strongly affects single-sided heating. The analysis highlighted a trade-off: increasing radiation intensity enhances adhesion, impact resistance, and ΔE, but lowers gloss.

Background & Context

While CIR radiation curing offers high performance for thermosetting powder coatings, the industry has lacked precise process control due to a deficiency in predictive models and guidance within coating manuals. This research addresses this gap by providing a multi-objective optimisation framework suitable for engineering deployment.

Significance & Outlook

The TabPFN-NSGA-II approach offers a practical digital tool for industrial applications, allowing formulators and applicators to balance the trade-off between mechanical performance and visual appearance. This advancement contributes to the broader trend of digitalisation in coatings production, enhancing efficiency and accuracy in quality control.

Source: https://www.european-coatings.com/news/coatings-technologies/ai-framework-optimises-infrared-curing-of-powder-coatings/

Collected: November 07, 2026 | Automated Research System (AI)