TROY TECHNICAL

MATERIALS INFORMATICS
WEEKLY REPORT

November 8 - November 14, 2026 | Issue 2026-W45

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

12	10
ANALYZED ARTICLES	PRIORITY THEMES

Issued 2026-11-14 | English edition | fixed approved cover artwork



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

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

SIGNAL 01 | DATA CAPTURE

Metal Recycling ML Framework: Enhancing Scrap-Based Alloys

A new machine-learning framework enables the design of high-performance alloys using 100% metal scrap by treating impurities as beneficial alloying elements.

SIGNAL 02 | MODELING

MLP Copilot: AI Agent Framework for Atomic Modeling in 2026

MLP Copilot is a multi-AI agent framework that automates the organization of evidence and validation in atomic interaction modeling.

SIGNAL 03 | CANDIDATE DESIGN

Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026)

Machine learning potentials reveal that the glass transition temperature (Tg) is the key descriptor for Li-ion diffusion in amorphous alloy anodes.

SIGNAL 04 | EXPERIMENT

High-Entropy Carbides: Finite-Temperature Disorder and Diffusion

Research on (Hf,Zr,Ta,Nb,Ti)C reveals that thermal expansion is nearly additive while elastic softening at 2000 K is mode-selective.

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.

Numbers and evidence anchors that require conditions

100%
A10

SOURCE-BOUND CONDITION
A new machine-learning framework enables the design of high-performance alloys using 100% metal scrap by treating impurities as beneficial alloying elements.

89.6%
A07

SOURCE-BOUND CONDITION
The model achieves 89.6% classification accuracy and reveals a "frustration inversion" principle that governs amorphous stability.

5.4 w
A12

SOURCE-BOUND CONDITION
OpenAI and Molecule.one integrated GPT-5.4 with the Maria experimental platform to improve yields in Chan-Lam coupling reactions, a long-standing bottleneck in pharmaceutical synthesis.

218 MW
A02

SOURCE-BOUND CONDITION
At room temperature, the armchair interface exhibits a higher ITC of 218 MW/m2•K compared to 188 MW/m2•K for the zigzag interface, providing a mechanism for controlling heat dissipation in nanoelectronic devices.

2.0%
A04

SOURCE-BOUND CONDITION
The model achieves bond-distance MAE of ~0.04 Å and coordination number errors under 2.0%, enabling full 3D geometry reconstruction including bond angles.

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

A new machine-learning framework enables the design of high-performance alloys using 100% metal scrap by treating impurities.

2

Modeling

P02/P07

MLP Copilot is a multi-AI agent framework that automates the organization of evidence and validation in atomic interaction.

3

Candidate design

P03/P08

Machine learning potentials reveal that the glass transition temperature (Tg) is the key descriptor for Li-ion diffusion in.

4

Experiment

P04/P09

Research on (Hf,Zr,Ta,Nb,Ti)C reveals that thermal expansion is nearly additive while elastic softening at 2000 K is.

5

Scale & governance

P05/P10

Researchers have developed a graph neural network approach to align inconsistent DFT energy scales, converting PBE energies.

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	Metal Recycling ML Framework: Enhancing Scrap-Based Alloys Tech / process | cue: no system/business cue
P02	MLP Copilot: AI Agent Framework for Atomic Modeling in 2026 System / adoption | cue: integrating
P03	Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026) System / adoption | cue: orders
P04	High-Entropy Carbides: Finite-Temperature Disorder and Diffusion Tech / process | cue: no system/business cue
P05	GPTFF Model: Aligning Heterogeneous DFT Datasets via GNN System / adoption | cue: integration
P06	Pd-Catalyzed Acetylene Hydrogenation: 850°C Surface Motifs Tech / process | cue: no system/business cue
P07	Glass Formation Mechanisms: ML-Driven Analysis of 78,889 Entries System / adoption | cue: integrated
P08	OpenAI and Molecule.one: Improving Chan-Lam Coupling Yields via GPT-5.4 System / adoption | cue: integrated
P09	MoSe2/MoS2 Heterostructures: Interface Orientation and ITC Specs Tech / process | cue: no system/business cue
P10	Equivariant Diffusion Models: 3D Atomic Coordination from Spectra Tech / process | cue: no system/business cue

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 Metal Recycling ML Framework: Enhancing Scrap-Based Alloys

A10 | Data capture | Product adoption

2026-11-10

FACT

A new machine-learning framework enables the design of high-performance alloys using 100% metal scrap by treating impurities as beneficial alloying elements. In tests with ductile iron, 14 of 17 designs showed superior strength-ductility trade-offs and an 8.1 percent reduction in manufacturing costs. This approach reduces reliance on primary raw materials and lowers the environmental impact of metal production.

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 20/25 | MATURITY 4/5 | DECISION LOCUS: TECH / PROCESS

P02 MLP Copilot: AI Agent Framework for Atomic Modeling in 2026

A11 | Modeling | Joint evaluation

2026-11-09

FACT

MLP Copilot is a multi-AI agent framework that automates the organization of evidence and validation in atomic interaction modeling. By integrating quantum calculations with active learning, it enabled the simulation of aluminum nanoparticle oxidation and the discovery of a "breathing mode" in oxide shells.

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 Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026)

A06 | Candidate design | Product adoption

Prior release 2026-11-07

FACT

Machine learning potentials reveal that the glass transition temperature (Tg) is the key descriptor for Li-ion diffusion in amorphous alloy anodes. The study finds that conventional Arrhenius extrapolation overestimates room-temperature diffusivity by 1-2 orders of magnitude, particularly in Li-poor phases. These results suggest that reducing Tg through alloy composition optimization can improve Li transport for fast-charging batteries.

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 20/25 | MATURITY 4/5 | DECISION LOCUS: SYSTEM / ADOPTION

P04 High-Entropy Carbides: Finite-Temperature Disorder and Diffusion

A03 | Experiment | Product adoption

2026-11-12

FACT

Research on (Hf,Zr,Ta,Nb,Ti)C reveals that thermal expansion is nearly additive while elastic softening at 2000 K is mode-selective. The study demonstrates that static barrier ensembles are insufficient to interpret carbon transport at finite concentrations due to significant MACE potential underestimates.

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 4/5 | DECISION LOCUS: TECH / PROCESS

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

P05 GPTFF Model: Aligning Heterogeneous DFT Datasets via GNN

A05 | Scale & governance | Pilot

2026-11-10

FACT

Researchers have developed a graph neural network approach to align inconsistent DFT energy scales, converting PBE energies to r2SCAN-level accuracy with a mean absolute error of 14.3 meV/atom. By resolving systematic discrepancies between exchange-correlation functionals, this method enables the integration of multi-source DFT data for high-performance materials AI models.

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 2/5 | DECISION LOCUS: SYSTEM / ADOPTION

P06 Pd-Catalyzed Acetylene Hydrogenation: 850°C Surface Motifs

A01 | Data capture | Product adoption

2026-11-13

FACT

Researchers identified Pd(100)-like 4-fold hollow sites as the key surface motifs for selective acetylene-to-ethylene hydrogenation at 850°C. The study utilized a combination of experimental screening, machine learning potential (MLP), and DFT calculations to determine that these motifs enable high ethylene productivity with low coke formation. This finding suggests a path for downstream upgrading in direct non-oxidative methane conversion (DNMC) without intermediate cooling.

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 4/5 | DECISION LOCUS: TECH / PROCESS

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

P07 Glass Formation Mechanisms: ML-Driven Analysis of 78,889 Entries

A07 | Modeling | Pilot

Prior release 2026-11-06

FACT

Researchers have developed a SHAP-integrated XGBoost machine learning framework that identifies universal and system-specific mechanisms for glass formation across covalent, ionic, and metallic networks. The model achieves 89.6% classification accuracy and reveals a "frustration inversion" principle that governs amorphous stability. This provides a data-driven foundation for the design of functional glasses across different bonding characters.

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 2/5 | DECISION LOCUS: SYSTEM / ADOPTION

P08 OpenAI and Molecule.one: Improving Chan-Lam Coupling Yields via GPT-5.4

A12 | Candidate design | Pilot

2026-11-12

FACT

OpenAI and Molecule.one integrated GPT-5.4 with the Maria experimental platform to improve yields in Chan-Lam coupling reactions, a long-standing bottleneck in pharmaceutical synthesis. The semi-autonomous system executed over 10,000 experiments in three months, demonstrating that AI-driven hypothesis generation and automated validation can significantly accelerate drug discovery.

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 MoSe2/MoS2 Heterostructures: Interface Orientation and ITC Specs

A02 | Experiment | Pilot

2026-11-10

FACT

Researchers have demonstrated that interfacial thermal conductance (ITC) in lateral MoSe2/MoS2 heterostructures is tunable via interface orientation. At room temperature, the armchair interface exhibits a higher ITC of 218 MW/m2•K compared to 188 MW/m2•K for the zigzag interface, providing a mechanism for controlling heat dissipation in nanoelectronic devices.

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 2/5 | DECISION LOCUS: TECH / PROCESS

P10 Equivariant Diffusion Models: 3D Atomic Coordination from Spectra

A04 | Scale & governance | Pilot

2026-11-12

FACT

Researchers have developed an equivariant diffusion model that reconstructs 3D atomic coordinates directly from near-edge spectra (ELNES/XANES). The model achieves bond-distance MAE of ~0.04 Å and coordination number errors under 2.0%, enabling full 3D geometry reconstruction including bond angles.

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: TECH / PROCESS

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 01-12

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	Pd-Catalyzed Acetylene Hydrogenation: 850°C Surface Motifs	https://doi.org/10.21203/rs.3.rs-11376353/v1
A02	MoSe2/MoS2 Heterostructures: Interface Orientation and ITC Specs	https://doi.org/10.1088/1361-648x/aec07d
A03	High-Entropy Carbides: Finite-Temperature Disorder and Diffusion	https://doi.org/10.1088/1361-648x/aec1af
A04	Equivariant Diffusion Models: 3D Atomic Coordination from Spectra	https://www.nature.com/articles/s41524-026-02384-4
A05	GPTFF Model: Aligning Heterogeneous DFT Datasets via GNN	https://www.nature.com/articles/s41524-026-02366-6
A06	Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026)	https://www.nature.com/articles/s41524-026-02383-5
A07	Glass Formation Mechanisms: ML-Driven Analysis of 78,889 Entries	https://www.nature.com/articles/s41524-026-02385-3
A08	Self-Building Labs: AI-Driven Digital Twins for Chemistry Experiments	https://finance.sina.cn/tech/2026-11-08/detail-inixyrxk4290415.d.html?vt=4
A09	WorldParticle: Unified AI Model for Multi-Physics Simulation	https://bioengineer.org/unified-ai-model-accurately-simulates-diverse-physical-phenomena-from-sand-to-proteins/
A10	Metal Recycling ML Framework: Enhancing Scrap-Based Alloys	https://www.mpg.de/27038557/turning-scrap-impurities-into-enhanced-alloys?c=2249
A11	MLP Copilot: AI Agent Framework for Atomic Modeling in 2026	https://www.sflorg.com/2026/11/cosc11092601.html
A12	OpenAI and Molecule.one: Improving Chan-Lam Coupling Yields via GPT-5.4	https://news.yahoo.co.jp/articles/497f70451ca7ac00516046d5c810f102340faec8

MaterialsInformatics — Selected Articles

Date: 2026-11-15

Articles: 12

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#04 Equivariant Diffusion Models: 3D Atomic Coordination from Spectra

#05 GPTFF Model: Aligning Heterogeneous DFT Datasets via GNN

#06 Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026)

#07 Glass Formation Mechanisms: ML-Driven Analysis of 78,889 Entries

#08 Self-Building Labs: AI-Driven Digital Twins for Chemistry Experiments

#09 WorldParticle: Unified AI Model for Multi-Physics Simulation

#10 Metal Recycling ML Framework: Enhancing Scrap-Based Alloys

#11 MLP Copilot: AI Agent Framework for Atomic Modeling in 2026

#12 OpenAI and Molecule.one: Improving Chan-Lam Coupling Yields via GPT-5.4

#01 Pd-Catalyzed Acetylene Hydrogenation: 850°C Surface Motifs

Published November 13, 2026　Research Square（プレプリント）



OVERVIEW

Researchers identified Pd(100)-like 4-fold hollow sites as the key surface motifs for selective acetylene-to-ethylene hydrogenation at 850°C. The study utilized a combination of experimental screening, machine learning potential (MLP), and DFT calculations to determine that these motifs enable high ethylene productivity with low coke formation. This finding suggests a path for downstream upgrading in direct non-oxidative methane conversion (DNMC) without intermediate cooling.

IN DEPTH

Key Findings

Pd catalysts supported on cristobalite demonstrated the highest hydrocarbon formation rate of approximately 3.0 × 10^3 μmol-C g cat^{-1} h^{-1} at 850°C. The process exhibited high ethylene productivity, negligible deactivation, and low coke formation. Through MLP screening of 31 Pd surfaces, the study determined that Pd(100)-like 4-fold hollow sites bind acetylene substantially more strongly than Pd(111)-like 3-fold sites.

Technical Details

DFT calculations incorporating high temperature entropy corrections confirmed that acetylene adsorption is favorable on Pd(100) and several high-index surfaces exposing 4-fold motifs at 1123 K, while adsorption on Pd(111) was unfavorable. The research also evaluated the impact of tensile strain, finding that strains up to 2.0% had only a minor effect on performance.

On Pd(100)-2.0%, the sequential hydrogenation steps to C_2H_3* and C_2H_4* required activation free energies of 1.03 eV and 1.02 eV, respectively. These barriers were lower than those of competing dehydrogenation and C–C coupling pathways, ensuring selectivity toward ethylene.

Background & Context

The research addresses the challenge of selective acetylene hydrogenation at temperatures relevant to direct non-oxidative methane conversion (DNMC). By achieving hydrogenation at these high temperatures, the need for intermediate cooling and reheating during downstream upgrading is eliminated.

Significance & Outlook

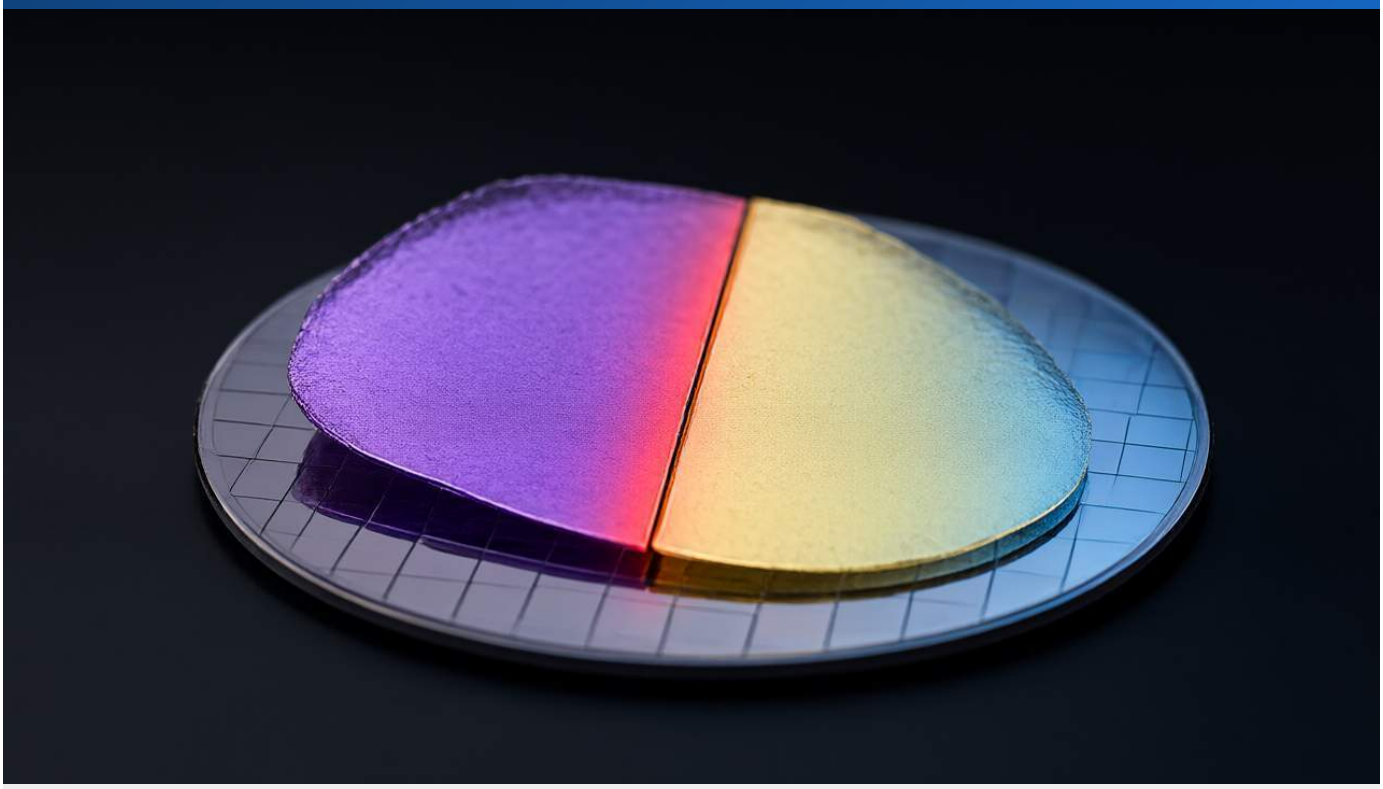
The integration of experimental catalyst screening with MLP-assisted surface analysis and DFT calculations allowed for the precise identification of the Pd(100)-like 4-fold ensembles as the active sites. This methodology demonstrates a viable framework for identifying specific surface motifs responsible for high-temperature chemical conversions, potentially streamlining the development of catalysts for high-temperature industrial processes.

Source: https://doi.org/10.21203/rs.3.rs-11376353/v1

Collected: November 15, 2026 | Automated Research System (AI)

#02 $MoSe_2/MoS_2$ Heterostructures: Interface Orientation and ITC Specs

Published November 10, 2026 Journal of Physics: Condensed Matter イラン



OVERVIEW

Researchers have demonstrated that interfacial thermal conductance (ITC) in lateral $MoSe_2/MoS_2$ heterostructures is tunable via interface orientation. At room temperature, the armchair interface exhibits a higher ITC of 218 MW/m²•K compared to 188 MW/m²•K for the zigzag interface, providing a mechanism for controlling heat dissipation in nanoelectronic devices.

IN DEPTH

Key Findings

The study identifies that the orientation of the interface in lateral $MoSe_2/MoS_2$ heterostructures significantly impacts thermal transport. At room temperature, the armchair interface achieves an interfacial thermal conductance (ITC) of 218 MW/m²•K, while the zigzag interface shows a lower value of 188 MW/m²•K. Both orientations exhibit an increase in ITC as temperature rises.

Technical Details

To analyze these properties, the researchers employed a deep learning interatomic potential (DLP) trained using the DeePMD-kit on density functional theory (DFT) data. This DLP was paired with non-equilibrium molecular dynamics (NEMD) simulations. The reliability of the trained potential was verified through its close match with DFT energies, forces, and phonon dispersion relations.

The difference in thermal performance was attributed to the vibrational density of states. Analysis revealed that the armchair interface possesses greater phonon spectral overlap, which drives its superior thermal transport capabilities compared to the zigzag orientation.

Background & Context

Managing heat flow across interfaces in lateral 2D transition-metal dichalcogenide (TMD) heterostructures is a critical challenge for the development of next-generation optoelectronic and nanoelectronic devices. Efficient heat dissipation is essential to maintain device stability and performance at the nanoscale.

Significance & Outlook

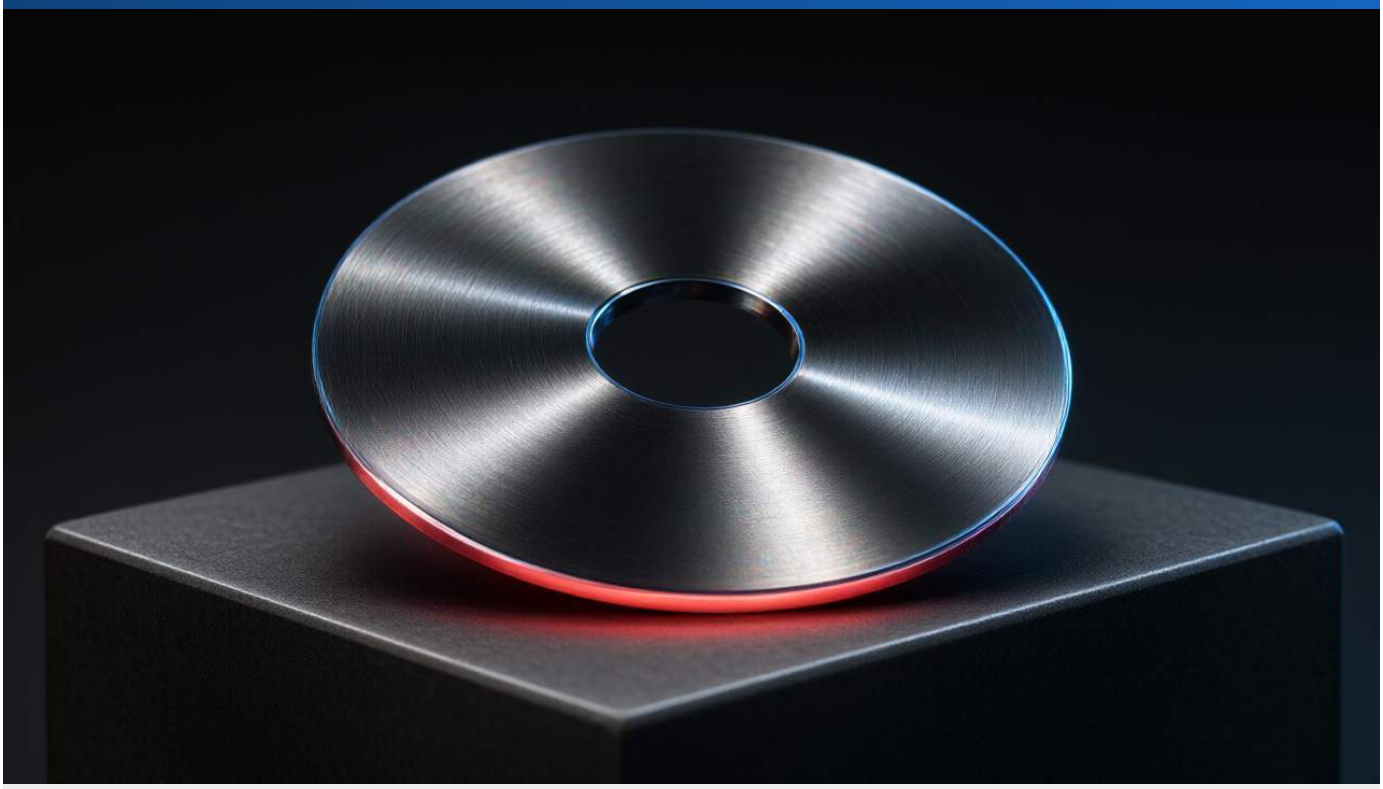
These results establish a machine-learning framework for studying heat transport in lateral TMD heterostructures. By identifying interface orientation as an effective means of controlling heat dissipation, the study provides a practical pathway for engineering the thermal properties of junctions in 2D material-based electronics.

Source: https://doi.org/10.1088/1361-648x/aec07d

Collected: November 15, 2026 | Automated Research System (AI)

#03 High-Entropy Carbides: Finite-Temperature Disorder and Diffusion

Published November 12, 2026 Journal of Physics: Condensed Matter トルコ



OVERVIEW

Research on (Hf,Zr,Ta,Nb,Ti)C reveals that thermal expansion is nearly additive while elastic softening at 2000 K is mode-selective. The study demonstrates that static barrier ensembles are insufficient to interpret carbon transport at finite concentrations due to significant MACE potential underestimates.

IN DEPTH

Key Findings

The study identifies that thermal expansion across nineteen compositions is nearly additive, with values ranging from 5.4–6.7 × 10−6 K−1, falling within ±5% of the binary rule of mixtures. Elastic softening observed at 2000 K is mode-selective, with C11 decreasing by 18–37% and C44 decreasing by 3–7%. Additionally, nominal two-phase melting estimates rise by approximately 1000 K along a composition path moving from group-IV-rich to group-V-rich.

Technical Details

The researchers utilized the unmodified MACE-MP-0 potential to examine chemical disorder in rocksalt (Hf,Zr,Ta,Nb,Ti)C. The following deviations were noted regarding the potential's transferability:

- Binary optical phonons are 4–16 meV softer than density-functional perturbation theory.
- Multicomponent lattice parameters exceed density functional theory (DFT) values by 0.14–0.31%.
- Binary melting estimates deviate from experimental data by −21% to +35%.

Regarding carbon transport, twenty static single-vacancy migration paths showed a mean barrier of 2.53 ± 0.40 eV. However, at 12.5% carbon vacancies, fitted MD Arrhenius barriers were 1.36–1.54 eV, which is below the sampled ensemble minimum of 1.89 eV. A matched DFT comparison revealed that the MACE barrier underestimate is 1.22 eV.

Background & Context

Chemical disorder in high-entropy carbides creates heterogeneous local environments. These environments affect activated carbon transport and collective thermomechanical responses differently. The study specifically tests the limits of the MACE-MP-0 potential in capturing these complex interactions compared to DFT and experimental benchmarks.

Significance & Outlook

The results establish that while expansion is near-additive, the collective response of the material is highly mode-selective. Furthermore, the discrepancy between static barrier ensembles and MD Arrhenius barriers indicates that static ensembles alone cannot determine the interpretation of finite-concentration carbon transport, as they fail to distinguish local-environment effects from factors such as vacancy concentration, correlated motion, or limited diffusion statistics.

Source: https://doi.org/10.1088/1361-648x/aec1af

Collected: November 15, 2026 | Automated Research System (AI)

#04 Equivariant Diffusion Models: 3D Atomic Coordination from Spectra

Published November 12, 2026 npj Computational Materials Japan



OVERVIEW

Researchers have developed an equivariant diffusion model that reconstructs 3D atomic coordinates directly from near-edge spectra (ELNES/XANES). The model achieves bond-distance MAE of ~0.04 Å and coordination number errors under 2.0%, enabling full 3D geometry reconstruction including bond angles.

IN DEPTH

Key Findings

The developed equivariant diffusion model enables the generative inverse estimation of site-specific 3D atomic structures from near-edge spectra. When trained on Si–O crystals, the model demonstrates radial accuracy comparable to Extended X-ray Absorption Fine Structure (EXAFS), with a bond-distance mean absolute error (MAE) of ~0.04 Å. Notably, the model provides superior coordination number precision, with errors remaining below 2.0%, compared to approximately 20% for EXAFS.

Technical Details

Unlike conventional 1D radial distribution analysis, this generative approach reconstructs full 3D geometries, including bond angles. The model was trained exclusively on crystalline lattices but demonstrated composition-dependent transferability to amorphous systems. To validate the feasibility of the approach with experimental data, the researchers applied the model to experimental O K-edge spectra from stishovite, cristobalite, and α-quartz.

Background & Context

Extracting 3D atomic coordinates from spectroscopic data has historically been a challenging inverse problem. Traditional methods often rely on template matching, which is limited to retrieving structures from predefined reference libraries. This new approach moves beyond template matching by allowing the exploration of candidate 3D structures within a learned structural space.

Significance & Outlook

This research represents a step toward the automated and quantitative inference of 3D local structures from spectroscopic data. By overcoming the limitations of 1D analysis and predefined templates, the model provides a more flexible and precise method for determining atomic coordination. The study was supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), the Japan Science and Technology Agency (JST), and the New Energy and Industrial Technology Development Organization (NEDO), with contributions from the University of Tokyo and Mitsubishi Chemical Corporation.

Source: https://www.nature.com/articles/s41524-026-02384-4

Collected: November 15, 2026 | Automated Research System (AI)

#05 GPTFF Model: Aligning Heterogeneous DFT Datasets via GNN

Published November 10, 2026 npj Computational Materials China



OVERVIEW

Researchers have developed a graph neural network approach to align inconsistent DFT energy scales, converting PBE energies to r²SCAN-level accuracy with a mean absolute error of 14.3 meV/atom. By resolving systematic discrepancies between exchange-correlation functionals, this method enables the integration of multi-source DFT data for high-performance materials AI models.

IN DEPTH

Key Findings

The GPTFF model architecture successfully converts conventional PBE energies to r²SCAN-level accuracy, achieving a mean absolute error of 14.3 meV/atom. This performance surpasses the 18.2 meV/atom achieved by CHGNet. The approach allows for the upgrade of massive legacy PBE datasets to high-precision r²SCAN standards, facilitating more reliable predictions of reaction thermodynamics, battery voltage profiles, and phase stability.

Technical Details

The researchers utilized graph-based transfer learning to resolve data silo barriers. The model was trained using 380,190 structurally paired PBE–r²SCAN entries sourced from the MatPES database. By employing a structure-aware graph neural network, the system predicts cross-functional energy residuals to align inconsistent DFT energy scales.

Background and Context

Heterogeneous density functional theory (DFT) calculations, specifically plane-wave implementations, often introduce systematic formation energy errors. These errors range from tens to hundreds of meV/atom and are caused by variations in:

- Exchange-correlation functionals
- Kinetic energy cutoffs
- Pseudopotentials
- Dispersion corrections

As evidence, the MatPES dataset shows that identical structures can have an average energy discrepancy of 107 meV/atom between PBE and r²SCAN calculations. These method-dependent discrepancies have historically hindered the integration of multi-source DFT data, limiting the quality and scale of datasets available for training robust materials AI models.

Significance and Outlook

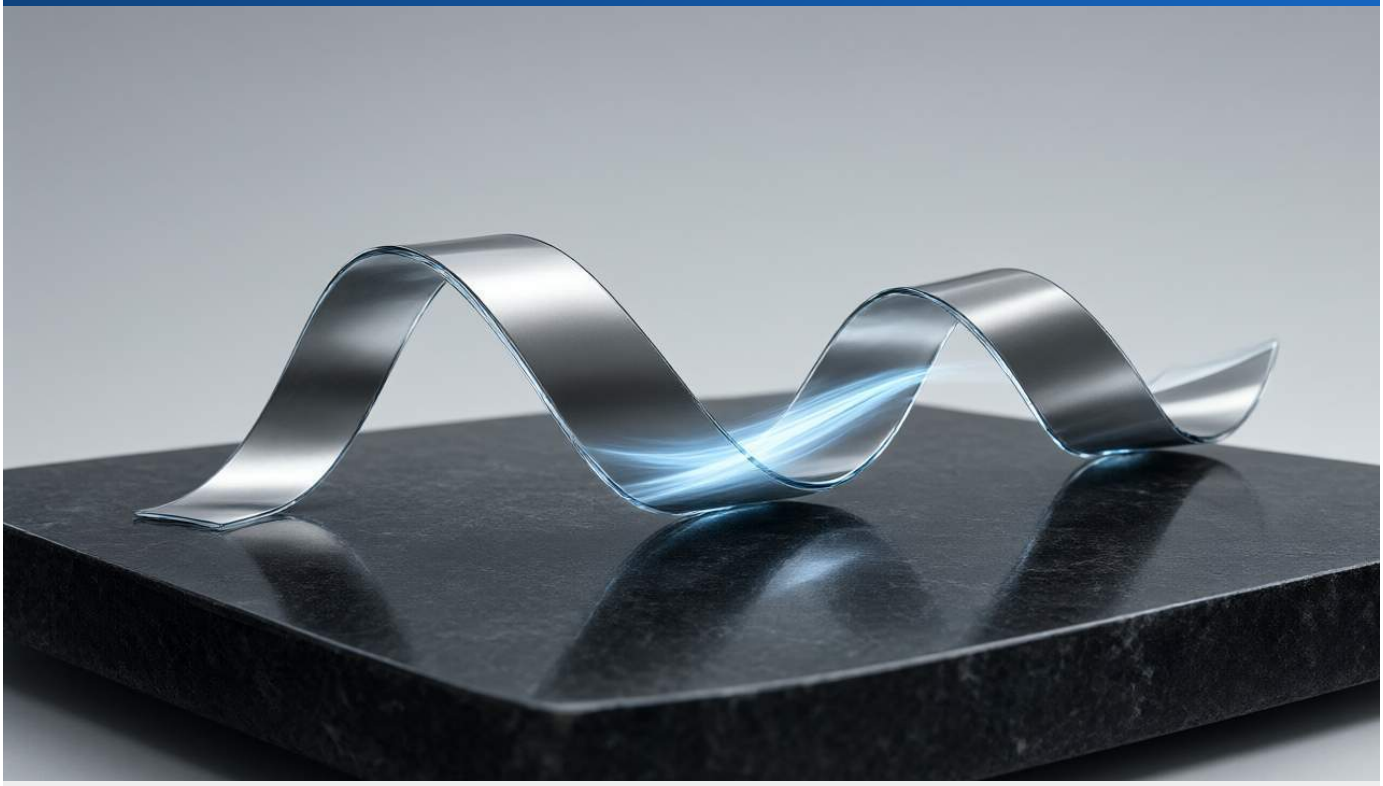
This versatile alignment approach removes a fundamental barrier to data integration in materials science. By enabling the combination of diverse DFT datasets, the method supports the development of high-performance materials foundation models. The research was supported by the National Key R&D Program of China, the Chinese Academy of Sciences, and the National Natural Science Foundation of China.

Source: https://www.nature.com/articles/s41524-026-02366-6

Collected: November 15, 2026 | Automated Research System (AI)

#06 Amorphous Alloy Anodes: Li-ion Diffusion and Tg Impact (2026)

Published November 07, 2026 npj Computational Materials China



OVERVIEW

Machine learning potentials reveal that the glass transition temperature (Tg) is the key descriptor for Li-ion diffusion in amorphous alloy anodes. The study finds that conventional Arrhenius extrapolation overestimates room-temperature diffusivity by 1–2 orders of magnitude, particularly in Li-poor phases. These results suggest that reducing Tg through alloy composition optimization can improve Li transport for fast-charging batteries.

IN DEPTH

Key Findings

The primary discovery is that the glass transition temperature (Tg) governs the transition between liquid-like and glass-like diffusion dynamics in Li–Si/Ge/Sn/Pb systems. Above Tg, systems exhibit rapid Li motion and structural rearrangement. Below Tg, Li motion becomes localized with slow structural relaxation. Furthermore, the research demonstrates that standard Arrhenius extrapolation from high-temperature data is inaccurate, overestimating room-temperature Li diffusivity (D Li) by 1–2 orders of magnitude in Li-poor phases.

Technical Details

Researchers utilized high-precision machine-learning potentials to investigate the Li-ion diffusion mechanisms. The study employed three dynamical analyses to characterize the behavior of different phases:

- **Li-poor phases:** Exhibit stronger Li localization and slower relaxation.
- **Li-rich phases:** Exhibit broader displacements and faster relaxation.

The simulations confirm that D Li increases in correlation with both temperature and Li content, mirroring experimental trends. The data supports a gradual transition from cage-confined, localized motion to more active and extended displacements as the system crosses the Tg threshold.

Background & Context

Developing batteries with improved cycling stability and rate performance requires a deep understanding of Li diffusion in amorphous alloy anodes. However, the complex structural evolution of amorphous phases has historically made the atomic diffusion mechanism unclear. This study addresses this gap by establishing a clear relationship between composition, local structure, and diffusion.

Significance & Outlook

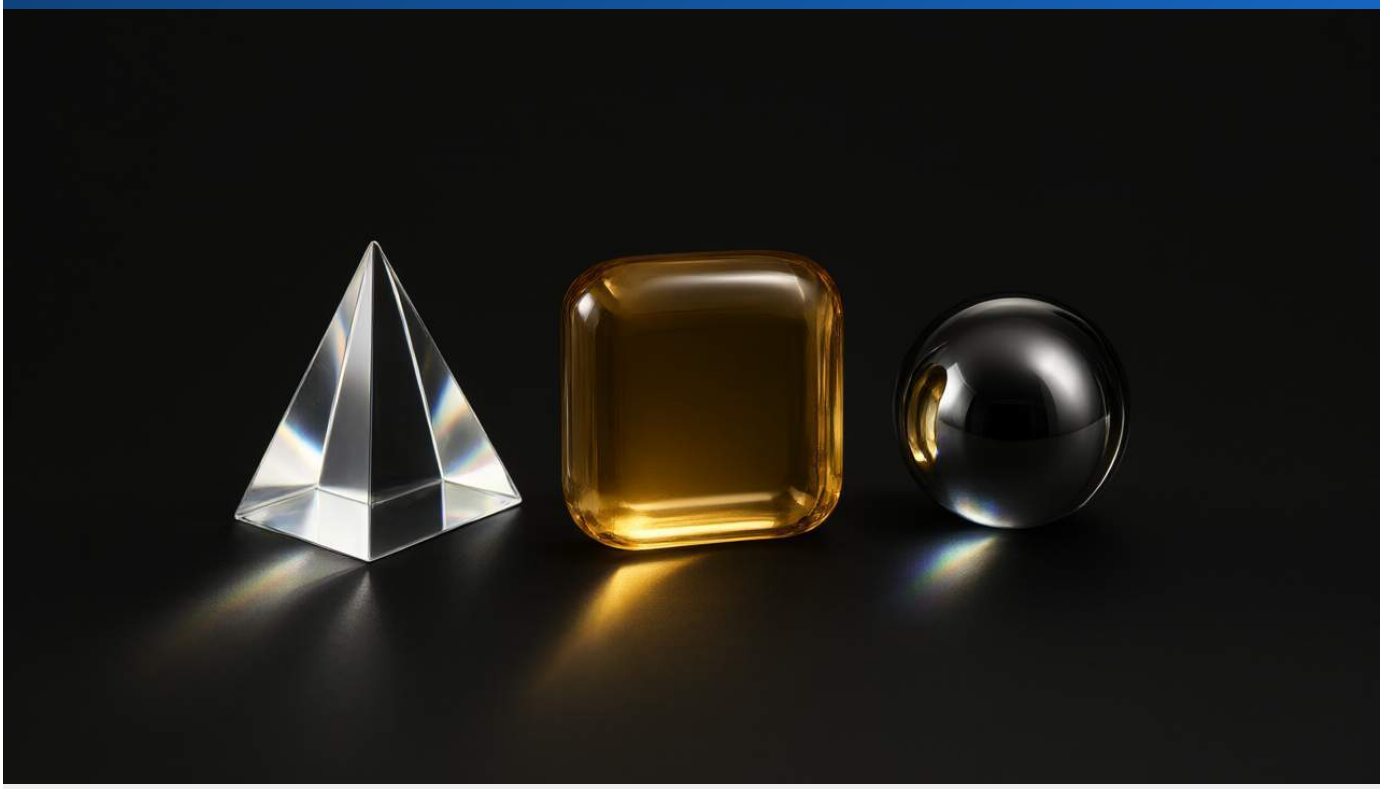
By identifying Tg as the critical descriptor for diffusion behavior, this work provides a theoretical framework for the design of next-generation battery anodes. The findings indicate that optimizing the alloy composition specifically to reduce the glass transition temperature may enhance Li transport, offering a pathway toward the development of faster-charging battery technologies.

Source: https://www.nature.com/articles/s41524-026-02383-5

Collected: November 15, 2026 | Automated Research System (AI)

#07 Glass Formation Mechanisms: ML-Driven Analysis of 78,889 Entries

Published November 06, 2026 npj Computational Materials China



OVERVIEW

Researchers have developed a SHAP-integrated XGBoost machine learning framework that identifies universal and system-specific mechanisms for glass formation across covalent, ionic, and metallic networks. The model achieves 89.6% classification accuracy and reveals a "frustration inversion" principle that governs amorphous stability. This provides a data-driven foundation for the design of functional glasses across different bonding characters.

IN DEPTH

Key Findings

The study establishes a unified physicochemical framework for glass formation by analyzing a success-bias-free dataset of 78,889 compositional entries. The resulting XGBoost framework attained 89.6% classification accuracy on the all-glass dataset and demonstrated robust generalization when applied to higher-dimensional spaces and extrapolative elemental substitutions.

Technical Details

The researchers encoded compositions as elemental-property matrices using the Magpie database. By applying Shapley analysis to both all-glass and system-specific models, the study determined that four glass families share the same set of frustration mechanisms, though the relative weights of these mechanisms redistribute based on bonding character.

A critical discovery is the "frustration inversion" effect, characterized by a bounded, non-monotonic dependence of governing descriptors. This principle indicates that compositional heterogeneity stabilizes the amorphous state only up to a family-specific threshold; this threshold narrows as network rigidity decreases, providing quantitative bounds on the confusion principle. Additionally, the analysis identified BCC-polymorph-referenced elemental descriptors as compositional-level predictors that encode structural preferences toward vitrification.

Background & Context

Existing models for glass formation have historically been limited because they were largely confined to a single glass family or biased toward compositions that had already been successfully vitrified. This research bridges that gap by utilizing a comprehensive dataset drawn from glass-forming region maps to eliminate success bias.

Significance & Outlook

By uncovering the universal mechanisms of amorphous stability across covalent, ionic, and metallic systems, this work provides a cross-system foundation for materials science. The integration of machine learning and SHAP analysis offers a scalable, data-driven route to the design of functional glasses, moving beyond trial-and-error compositional searches.

Source: https://www.nature.com/articles/s41524-026-02385-3

Collected: November 15, 2026 | Automated Research System (AI)

#08 Self-Building Labs: AI-Driven Digital Twins for Chemistry Experiments

Published November 08, 2026 新浪科技（DeepTech深科技） China



OVERVIEW

A research team from the University of Toronto and partners has developed "Self-Building Labs" (SBL), a system where AI autonomously identifies capability gaps and constructs digital twins to execute physical chemistry experiments. By coordinating robotic agents and simulation, the system can expand its own operational boundaries without requiring manual engineering for every new device.

IN DEPTH

Key Findings

The SBL system enables AI to move beyond executing pre-defined workflows to autonomously expanding laboratory capabilities. In a primary validation experiment, the system synthesized cadmium sulfide quantum dots (CdS QDs), coordinating a liquid handling robot, a robotic arm, and optical detection equipment. The AI generated and verified a Python program consisting of 236 operation instructions to manage reagent preparation, liquid transfer, and measurement.

Technical Details

The architecture relies on a digital twin created via NVIDIA Isaac Sim, which maps the physical lab using photos, CAD models, and camera data to minimize discrepancies between virtual and real environments. Three specialized agents manage the process:

- **Scientific Agent:** Translates abstract research goals into concrete experimental steps based on literature and domain knowledge.
- **Twin Agent:** Converts scientific plans into device-specific instructions and develops new operational skills within the digital twin.
- **Safety Agent:** Simulates potential hazards, such as equipment collisions or reagent spills, to establish safety rules.

To handle high-precision tasks, such as HPLC plate loading requiring sub-millimeter accuracy, the system integrates vision, depth information, and force/torque sensor feedback to correct simulation errors in real-time.

Background & Context

Traditional Self-Driving Labs (SDL) are limited by the equipment and interfaces installed at the time of construction; adding new tools typically requires professional engineers to write new code. SBL aims to integrate the definition and expansion of these boundaries into the automation loop. The team, including researchers from the Vector Institute, Acceleration Consortium, CIFAR, and NVIDIA, previously developed computational agents like El Agente for quantum chemistry and MLIP simulations.

Significance & Outlook

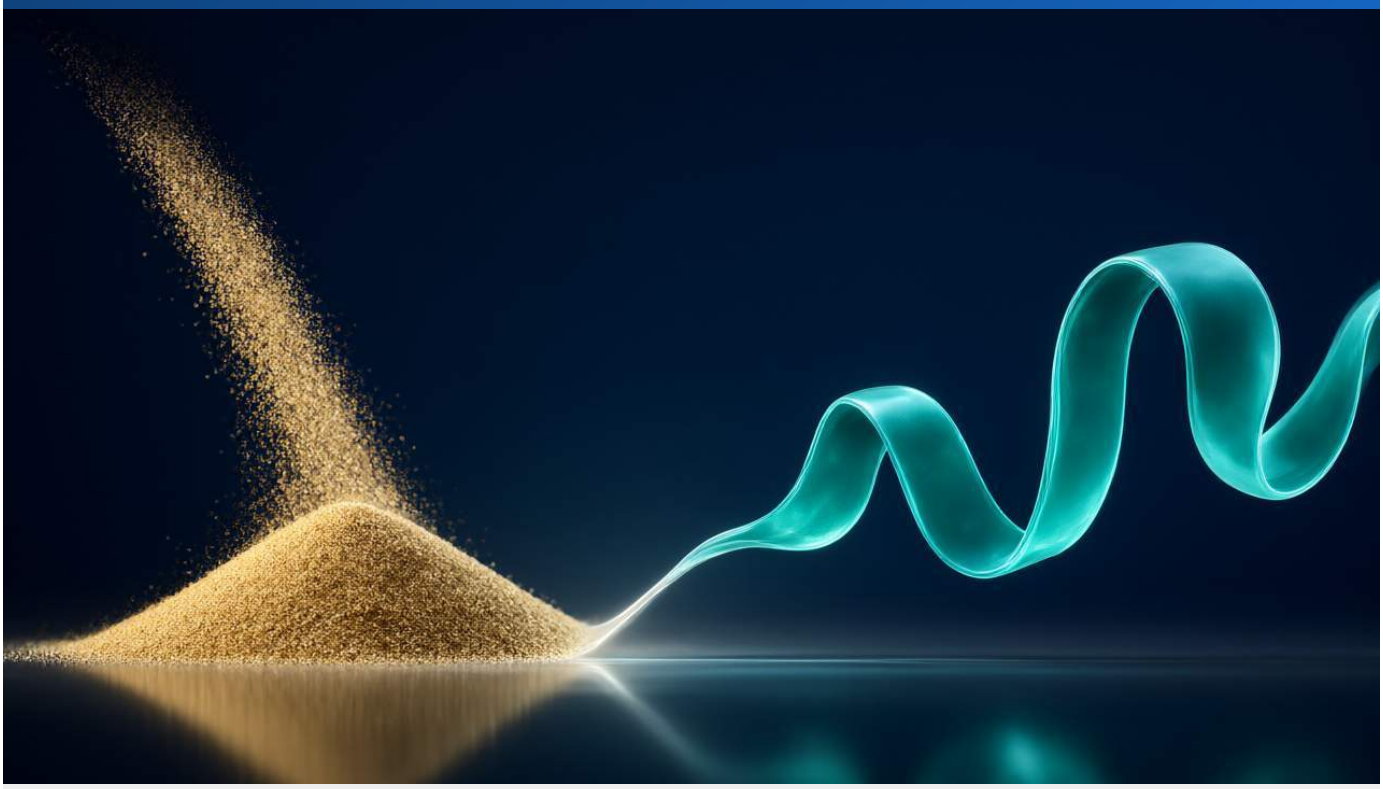
The researchers envision "vertical expansion," where robots move between different labs or floors in a building to schedule resources. Future goals include AI designing custom experimental equipment via 3D printing. While AI handles the execution, human scientists remain essential to provide "boundary conditions," defining risk parameters and efficiency constraints to guide the AI's search space.

Source: https://finance.sina.cn/tech/2026-11-08/detail-inixyrxk4290415.d.html?vt=4

Collected: November 15, 2026 | Automated Research System (AI)

#09 WorldParticle: Unified AI Model for Multi-Physics Simulation

Published November 14, 2026 BIOENGINEER.ORG USA



OVERVIEW

Researchers from MIT and the University of British Columbia have developed WorldParticle, a deep-learning system that simulates diverse physical phenomena from sand to proteins within a single architecture. The model outperforms conventional numerical methods in accuracy and simulates protein structural changes approximately 100 times faster than traditional solvers.

IN DEPTH

Key Findings

WorldParticle provides a unified framework for modeling varied physical processes, eliminating the need for the separate, specialized simulators traditionally used by engineers. In comparative tests across six distinct physical phenomena—including granular materials, deformable solids, and protein structures—the system demonstrated higher accuracy than conventional numerical simulation methods. Notably, WorldParticle correctly simulated the collapse of granular objects into stable piles, whereas some baseline methods left particles unnaturally suspended in mid-air.

Technical Details

The system utilizes a Lagrangian representation, breaking complex objects into thousands or millions of three-dimensional particles. Inspired by the architecture of ChatGPT, the neural network predicts the spatial movement and physical state of these particles in one-second increments rather than predicting sequential words. To maintain physical fidelity across diverse environments, the model employs a specific workflow:

- **Force Isolation:** External forces are separated from the internal physical system prior to each simulation step to isolate impulse forces.
- **Reintegration:** External forces are reintegrated after establishing preliminary particle states to adjust positional predictions.
- **Particle Merging:** To overcome computational bottlenecks associated with millions of points, a merging technique compresses particles while retaining fine-grained movement details.

Background & Context

Conventional computational approaches rely on hand-coded numerical solvers tailored to specific regimes, such as dedicated solvers for fluid mechanics or separate formulas for protein folding. This creates a fragmented patchwork of tools. WorldParticle overcomes this by learning to solve governing equations in general, taking three-dimensional coordinates and physical properties as inputs to predict subsequent frames.

Significance & Outlook

By unifying multiple physical regimes, WorldParticle enables the simulation of complex multi-physics interactions, such as oil exerting pressure on an elastic valve or soft robotic manipulators interacting with soil and sand. The research, co-led by Minghao Guo and Peter Yichen Chen, will be presented at the ACM SIGGRAPH Conference and Exhibition in Asia. Future development aims to expand the model's capabilities to include soft robotic manipulation.

Source: https://bioengineer.org/unified-ai-model-accurately-simulates-diverse-physical-phenomena-from-sand-to-proteins/

Collected: November 15, 2026 | Automated Research System (AI)

#10 Metal Recycling ML Framework: Enhancing Scrap-Based Alloys

Published November 10, 2026 Max-Planck-Gesellschaft Germany



OVERVIEW

A new machine-learning framework enables the design of high-performance alloys using 100% metal scrap by treating impurities as beneficial alloying elements. In tests with ductile iron, 14 of 17 designs showed superior strength-ductility trade-offs and an 8.1 percent reduction in manufacturing costs. This approach reduces reliance on primary raw materials and lowers the environmental impact of metal production.

IN DEPTH

Key Findings

Researchers have developed a machine-learning strategy that transforms impurities in metal scrap into advantages, creating "dirty alloys" with enhanced mechanical properties. Using ductile iron as a model material, the team identified 14 new alloys that outperformed existing recycled-iron datasets. Specifically, tensile strength increased by up to 15.2 percent at comparable elongation, or elongation at fracture increased by up to 73.2 percent at comparable tensile strength. Additionally, production costs were 8.1 percent lower than conventional methods that blend scrap with virgin iron.

Technical Details

The ML framework links alloy composition and processing conditions directly to performance, bypassing heavy reliance on microstructural features. The process utilizes a tree-search algorithm to generate candidates by varying composition and parameters such as temperature and time. Neural-network models then predict tensile strength and elongation to optimize the strength-ductility trade-off. A second model, trained on a larger composition-property dataset, screens these candidates before physical manufacturing and testing. Experimental results are fed back into the database to iteratively refine the predictive model.

Background and Context

Global metal production reaches approximately two billion tonnes annually, with primary raw materials contributing an estimated 40 percent of industrial greenhouse gas emissions and 10 percent of global energy consumption. While recycling reduces this impact, variations in scrap composition typically compromise mechanical properties. The conventional industry response is to dilute impurities with virgin materials, which increases energy consumption and CO2 emissions.

Significance and Outlook

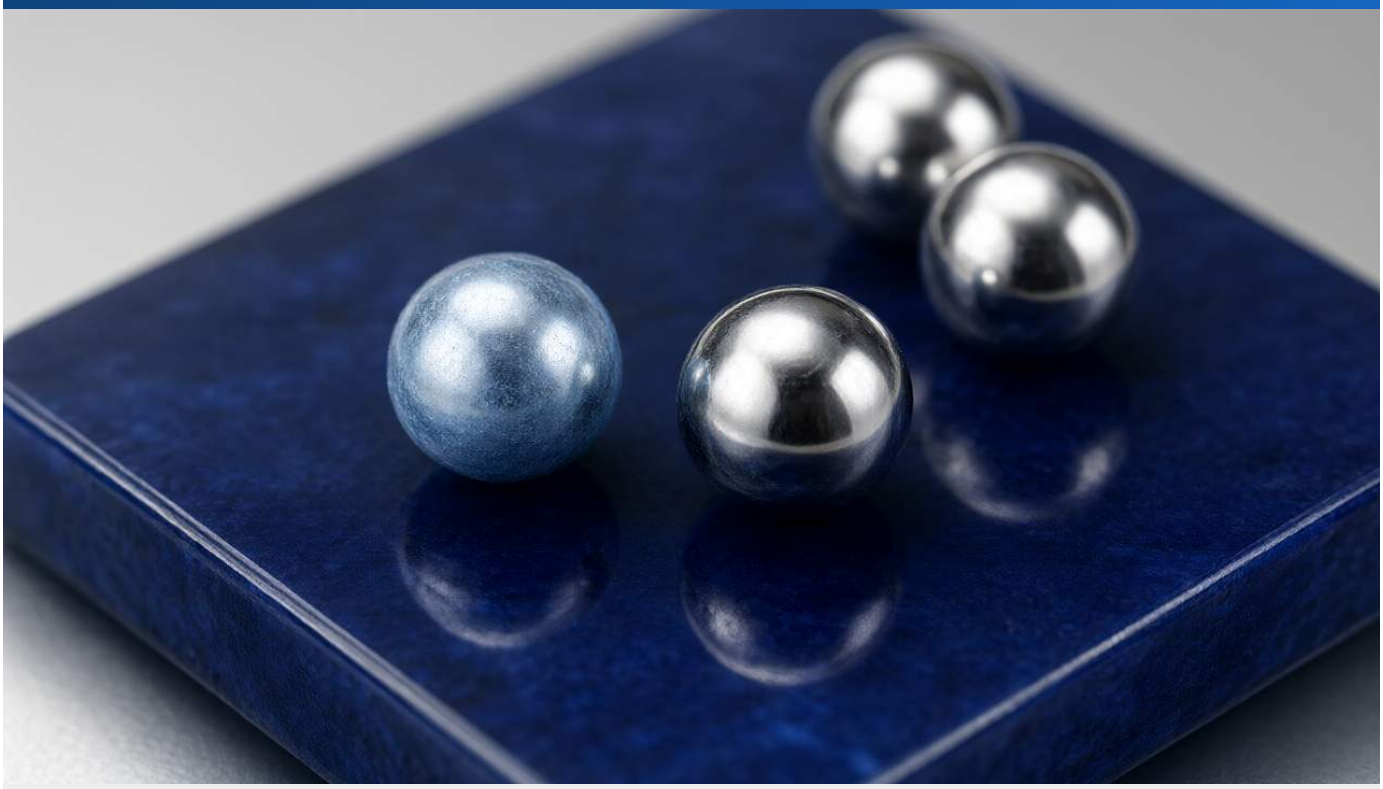
This research demonstrates that alloys made entirely from scrap can exceed the properties of those made via primary synthesis. The framework is potentially extensible to recycled aluminium, copper, and steel alloys for use in energy, transport, and industrial manufacturing. Future developments may include integrating multi-agent AI systems with automated experimental platforms to create an autonomous cycle of design, process control, and interpretation.

Source: https://www.mpg.de/27038557/turning-scrap-impurities-into-enhanced-alloys?c=2249

Collected: November 15, 2026 | Automated Research System (AI)

#11 MLP Copilot: AI Agent Framework for Atomic Modeling in 2026

Published November 09, 2026　Scientific Frontline（Tohoku University WPI-AIMR）　Japan



OVERVIEW

MLP Copilot is a multi-AI agent framework that automates the organization of evidence and validation in atomic interaction modeling. By integrating quantum calculations with active learning, it enabled the simulation of aluminum nanoparticle oxidation and the discovery of a "breathing mode" in oxide shells.

IN DEPTH

Key Findings

MLP Copilot accelerates the construction of atomic interaction models by bridging computational tools and scientific evidence under human supervision. In a demonstration focusing on aluminum nanoparticle oxidation, the framework identified two distinct behaviors of the surface oxide shell. At moderate temperatures, the shell exhibits a "breathing mode" where temporary nanoscale pathways allow oxidation while limiting material transport. At higher temperatures, the shell ruptures, exposing the aluminum core and accelerating oxidation, with outward aluminum transport serving as the dominant pathway.

Technical Details

The framework utilizes a structural workflow where AI agents organize project knowledge and retrieve evidence, while human researchers make final scientific decisions. The technical process includes:

- **Quantum Calculations:** These provide the foundational data for learning atomic energies and forces.
- **Active-Learning Iterations:** The system performed approximately 80 iterations, assembling 88,833 atomic configurations, using uncertain configurations to guide further training.
- **Validation Protocols:** Models are verified using reference results, thermodynamic properties, and independent cluster tests before full-scale simulations.
- **Simulations:** Tests conducted at 1,500 K and 2,000 K were used to observe the effects of oxide-shell changes on aluminum transport.

Background & Context

Modeling atomic interactions is traditionally computationally intensive, requiring researchers to manually track mechanisms and select calculations. MLP Copilot acts as an "auto-pilot" for materials science, automating the organization of datasets and validation planning. This approach shifts the role of AI from performing individual calculations to organizing the entire research workflow through human-agent collaboration.

Significance & Outlook

Controlling the oxide shell of aluminum nanoparticles is critical due to the immense chemical energy these particles store. Beyond this specific application, the MLP Copilot workflow is designed to be reusable across diverse materials systems. Furthermore, it establishes a basis for recursive self-improvement (RSI), where future AI agents can refine their tool use and planning based on validated outcomes assessed by researchers.

Source: https://www.sflorg.com/2026/11/cosc11092601.html

Collected: November 15, 2026 | Automated Research System (AI)

#12 OpenAI and Molecule.one: Improving Chan-Lam Coupling Yields via GPT-5.4

Published November 12, 2026　ビジネス＋IT（Yahoo!ニュース）　Japan



OVERVIEW

OpenAI and Molecule.one integrated GPT-5.4 with the Maria experimental platform to improve yields in Chan-Lam coupling reactions, a long-standing bottleneck in pharmaceutical synthesis. The semi-autonomous system executed over 10,000 experiments in three months, demonstrating that AI-driven hypothesis generation and automated validation can significantly accelerate drug discovery.

IN DEPTH

Key Findings

The integration of GPT-5.4 and the Maria platform successfully increased the average yield of Chan-Lam coupling reactions from 16.6% to 25.2%. Specifically, the proportion of reactions achieving yields over 30% rose from 15.6% to 37.5%. Human verification in flask environments confirmed yield improvements in 11 out of 14 substrate pairs, with 8 pairs showing more than double the yield compared to control conditions without additives.

Technical Details

The project targeted the formation of carbon-nitrogen bonds, specifically focusing on 1-primary sulfonamides, which historically exhibit low yields. The workflow functioned as a semi-autonomous loop:

- **Hypothesis Generation:** GPT-5.4 analyzed academic literature to identify priority substrates and automatically generated thousands of improvement proposals.
- **Human Intervention:** Human chemists screened the AI's proposals and applied minor corrections, such as excluding specific solvents.
- **Automated Execution:** The Maria platform, consisting of specialized models and an automated laboratory, executed 10,080 microliter-scale reactions across two cycles.

The AI identified that adding TEMPO, a mild oxidant, improved the reaction. This was validated across 88% of tested boronic acids and 83% of sulfonamides.

Background and Context

Chan-Lam coupling is critical for synthesizing various pharmaceuticals, including anticancer, antibacterial, and antihypertensive drugs. Traditionally, the low efficiency of this reaction in the early stages of drug discovery has acted as a significant bottleneck. By automating the path from literature review to data analysis, the team completed the process from project start to expert evaluation in approximately three months.

Significance and Outlook

This demonstration highlights the potential of "AI scientists" to handle physical experiments autonomously. The ability to compress long-term verification processes into a few months suggests a structural shift in process chemistry and industrial scientific research.

Source: https://news.yahoo.co.jp/articles/497f70451ca7ac00516046d5c810f102340faec8

Collected: November 15, 2026 | Automated Research System (AI)