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# AI and Advanced Materials Discovery: Accelerating Sustainable Solutions for Energy Storage and Resource Efficiency

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**Abstract**

The transition towards sustainable energy and resource-efficient industrial systems requires the development of advanced materials with improved performance, durability, affordability, and environmental compatibility. Conventional materials discovery is often constrained by lengthy experimentation cycles, high costs, complex synthesis pathways, and the enormous number of possible material compositions. Artificial Intelligence (AI), machine learning, high-throughput computation, and advanced simulation techniques are transforming this process by enabling researchers to predict material properties, identify promising compositions, optimise synthesis conditions, and accelerate experimental validation. This paper examines the convergence of AI and advanced materials discovery, with particular emphasis on energy storage and resource efficiency. A qualitative and conceptual methodology based on secondary literature is adopted to examine AI-enabled materials screening, machine-learning-assisted property prediction, generative materials design, autonomous laboratories, battery materials, hydrogen technologies, supercapacitors, catalysts, and circular-resource applications. The study proposes an integrated AI-driven materials discovery framework connecting data generation, materials databases, machine learning, computational simulation, candidate ranking, laboratory experimentation, and continuous feedback. Applications in lithium-ion, sodium-ion, solid-state and next-generation batteries demonstrate the potential of AI to accelerate the identification of materials with desirable electrochemical and structural properties. Beyond energy storage, AI can support resource efficiency through catalyst optimisation, lightweight materials, recycling technologies, corrosion-resistant materials, and low-carbon manufacturing. However, challenges remain concerning data quality, limited experimental datasets, model interpretability, generalisation, reproducibility, computational requirements, intellectual property, and the gap between predicted and experimentally achievable materials. The paper concludes that AI should be regarded not as a replacement for materials science expertise but as an enabling technology that integrates computational prediction with experimental knowledge. The combination of AI, advanced simulation, automation, and sustainable materials engineering could

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significantly reduce the time and resources required to develop technologies supporting the global transition towards sustainable energy and circular resource systems.

***Keywords:*** Artificial Intelligence, Materials Discovery, Machine Learning, Advanced Materials, Energy Storage, Batteries, Resource Efficiency, Sustainable Materials, Autonomous Laboratories, Materials Informatics.

## 1. Introduction

Modern society depends heavily on materials.

Materials determine the performance of:

- Batteries.
- Solar cells.
- Hydrogen systems.
- Electric vehicles.
- Semiconductors.
- Catalysts.
- Construction systems.
- Manufacturing equipment.

The transition towards sustainable development is therefore fundamentally a materials challenge.

For example, the expansion of renewable energy requires efficient energy-storage technologies capable of storing electricity when generation exceeds demand and releasing it when required.

Similarly, electrification of transportation requires batteries with:

- Higher energy density.
- Longer cycle life.
- Faster charging.
- Lower cost.
- Improved safety.

Developing such materials through conventional experimentation can be slow.

The number of possible combinations of:

- Elements.
- Crystal structures.
- Chemical compositions.
- Processing conditions.

is extremely large.

Artificial Intelligence offers a new approach.

Instead of experimentally testing every possible candidate, machine-learning models can identify promising materials before laboratory validation.

The emerging paradigm can therefore be represented as:

Materials Data → AI Prediction → Candidate Selection → Simulation → Experiment → Feedback

This integration is increasingly referred to as materials informatics.

**2. Materials Discovery as a Sustainability Challenge**

Traditional materials development can require:

1. Hypothesis generation.
2. Material synthesis.
3. Characterisation.
4. Property measurement.
5. Optimisation.
6. Repeated experimentation.

This process can involve substantial:

- Time.
- Energy.
- Chemicals.
- Laboratory resources.
- Financial investment.

AI can reduce the number of experimental iterations required by prioritising high-potential candidates.

The objective is therefore not simply faster discovery.

It is:

Faster discovery with fewer experimental and computational resources.

**3. Research Objectives**

This study aims to:

1. Examine the role of AI in advanced materials discovery.
2. Analyse machine-learning approaches for material-property prediction.
3. Examine applications in energy-storage materials.
4. Explore AI applications for resource efficiency.
5. Analyse autonomous and high-throughput materials research.
6. Identify technological and methodological challenges.
7. Develop an integrated AI-driven materials discovery framework.

**4. Research Methodology**

The study adopts a qualitative, conceptual, and literature-based methodology.

Research themes concerning:

- Materials informatics.
- Machine learning.
- Computational materials science.

- Battery materials.
- Catalysts.
- Energy storage.
- Materials sustainability.
- Autonomous laboratories.

are examined conceptually.
The analysis focuses on the interaction between:
**AI**
**Advanced Materials**
**Energy Systems**
**Resource Efficiency**

**5. Evolution of Materials Discovery**
Materials science has historically relied heavily on experimental approaches.
Researchers developed materials by:

- Selecting candidate compositions.
- Synthesising them.
- Measuring properties.
- Modifying compositions.
- Repeating experiments.

Computational materials science later expanded this process.
Methods such as:

- Density Functional Theory (DFT).
- Molecular dynamics.
- Monte Carlo simulations.

enabled researchers to predict material behaviour computationally.
AI introduces another layer by learning patterns from large datasets.

**6. Materials Informatics**
Materials informatics combines:
**Materials Science + Data Science + Machine Learning + Computational Modelling**
The objective is to discover relationships between:

- Composition.
- Structure.
- Processing.
- Properties.
- Performance.

A typical workflow is:

**Materials Database**
↓

**Feature Engineering**
↓
**Machine Learning**
↓
**Property Prediction**
↓
**Candidate Ranking**
↓
**Experimental Validation**

## 7. Artificial Intelligence in Materials Discovery

AI can perform several important tasks.

**Prediction**
Predicting material properties before synthesis.

**Classification**
Identifying materials according to performance categories.

**Optimisation**
Finding suitable compositions and processing conditions.

**Generation**
Proposing previously unexplored candidate materials.

**Recommendation**
Prioritising experiments.

## 8. Machine Learning Models

Different models can be applied depending on the problem.
Common approaches include:

- Linear regression.
- Random forests.
- Gradient boosting.
- Support vector machines.
- Neural networks.
- Graph neural networks.
- Gaussian processes.

The choice depends on:

- Dataset size.

- Feature complexity.
- Interpretability requirements.
- Computational resources.

**9. Materials Representation**

Machine-learning performance depends heavily on how materials are represented.

Materials can be described using:

- Elemental composition.
- Crystal structure.
- Atomic coordinates.
- Electronic structure.
- Chemical descriptors.
- Graph representations.

For crystalline materials, graph-based representations can capture relationships between atoms and bonds.

**10. Graph Neural Networks**

Graph neural networks are particularly relevant to materials discovery because materials can be represented as graphs.

In a simplified representation:

**Atoms → Nodes**

**Interactions → Edges**

The model can learn structural relationships and predict properties.

Potential applications include predicting:

- Formation energy.
- Band gaps.
- Stability.
- Mechanical properties.

**11. Generative AI for Materials**

Generative AI extends materials discovery beyond prediction.

Instead of asking:

"What properties does this material have?"

researchers can ask:

"What material could potentially provide these desired properties?"

Generative models may propose:

- New compositions.
- New molecular structures.
- New crystal configurations.

These candidates must still undergo physical and experimental validation.

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**12. Inverse Materials Design**

Traditional materials discovery follows:

**Material → Properties**

Inverse design reverses the process:

**Desired Properties → Candidate Material**

For example:

**High Energy Density + Long Cycle Life + Low Cost**

↓

**AI Candidate Generation**

↓

**Material Screening**

This approach can significantly change the materials-development process.

**13. AI and Battery Materials**

Battery technologies are among the most important application areas.

AI can support the development of:

- Cathode materials.
- Anode materials.
- Electrolytes.
- Solid-state electrolytes.
- Electrode additives.
- Battery interfaces.

**14. Lithium-Ion Batteries**

Lithium-ion batteries currently dominate many applications.

AI can optimise:

- Electrode composition.
- Charging strategies.
- Electrolyte formulations.
- Degradation prediction.
- Thermal management.

Materials discovery can also focus on reducing dependence on constrained or environmentally problematic materials.

**15. Sodium-Ion Batteries**

Sodium-ion batteries are receiving increasing attention because sodium is more abundant than lithium.

AI can assist in identifying:

- Cathode materials.
- Anode materials.
- Electrolytes.
- Stable electrode structures.

This illustrates how AI-supported materials discovery can contribute to diversification of energy-storage technologies.

**16. Solid-State Batteries**

Solid-state batteries replace conventional liquid electrolytes with solid materials.

Potential benefits include:

- Improved safety.
- Potentially higher energy density.
- Reduced flammability.

However, challenges include:

- Ionic conductivity.
- Interface stability.
- Manufacturing.
- Mechanical compatibility.

AI can help screen candidate solid electrolytes and interface materials.

**17. Supercapacitor Materials**

Supercapacitors require materials with:

- High surface area.
- High electrical conductivity.
- Fast ion transport.

Potential materials include:

- Carbon-based materials.
- Metal oxides.
- Conducting polymers.

AI can assist in identifying combinations with improved electrochemical performance.

**18. Hydrogen Technologies**

Hydrogen systems require advanced materials for:

- Electrolysers.
- Fuel cells.
- Hydrogen storage.
- Catalysts.

AI can accelerate catalyst discovery by predicting:

- Catalytic activity.
- Stability.

- Adsorption behaviour.

**19. Catalyst Discovery**

Catalysts can improve the efficiency of chemical reactions.

They are important in:

- Hydrogen production.
- Carbon utilisation.
- Fuel cells.
- Chemical manufacturing.
- Environmental remediation.

AI can screen thousands or millions of potential catalyst compositions computationally.

**20. AI for Solar Materials**

AI can support the discovery of materials for:

- Photovoltaics.
- Perovskite solar cells.
- Photocatalysis.
- Solar fuels.

Potential objectives include:

- Improved efficiency.
- Greater stability.
- Lower toxicity.
- Lower production cost.

**21. Resource Efficiency**

Advanced materials can reduce resource consumption by improving:

- Product lifetime.
- Energy efficiency.
- Material strength.
- Corrosion resistance.
- Thermal performance.

AI can accelerate the identification of materials that provide these characteristics.

**22. Lightweight Materials**

Lightweight materials can reduce energy consumption in transportation.

Examples include:

- Advanced aluminium alloys.
- Magnesium alloys.
- Carbon-fibre composites.
- High-strength steels.

AI can optimise material composition and structural performance.

**23. Corrosion-Resistant Materials**

Corrosion creates major economic and environmental costs.

AI can help predict corrosion behaviour based on:

- Material composition.
- Environmental conditions.
- Temperature.
- Humidity.
- Chemical exposure.

This can support longer equipment lifetimes.

**24. Materials for Circular Economy**

AI can support circular materials systems through:

- Recycling optimisation.
- Material identification.
- Waste classification.
- Recovery prediction.
- Secondary-material quality assessment.

Computer vision can identify materials in waste streams.

Machine learning can optimise recycling processes.

**25. Critical Material Substitution**

Modern technologies depend on various critical materials.

Supply risks can arise from:

- Geographic concentration.
- Limited reserves.
- Processing bottlenecks.
- Geopolitical instability.

AI can search for alternative materials that provide similar functional properties.

This creates an important sustainability objective:

**Performance Preservation + Material Substitution**

**26. AI for Battery Recycling**

Battery recycling is becoming increasingly important as battery deployment expands.

AI can assist with:

- Battery classification.
- State-of-health estimation.
- Sorting.
- Material recovery.

- Process optimisation.

Combining materials discovery with recycling can support a circular battery ecosystem.

**27. Autonomous Materials Laboratories**

One of the most significant emerging developments is the autonomous laboratory.

An autonomous system can integrate:

**AI Model**
↓
**Experiment Selection**
↓
**Robotic Experiment**
↓
**Material Characterisation**
↓
**Data Collection**
↓
**Model Update**

The cycle can repeat automatically.

**28. Closed-Loop Materials Discovery**

Closed-loop discovery creates continuous feedback.

Unlike a traditional linear process:

**Predict → Experiment → Stop**

the system operates as:

**Predict → Experiment → Learn → Predict Again**

This can dramatically increase the efficiency of experimentation.

**29. High-Throughput Experimentation**

Robotic systems can conduct many experiments simultaneously.

AI can determine which experiments provide the most useful information.

This approach is particularly valuable when:

- Experimental space is large.
- Resources are limited.
- Results are uncertain.

**30. Active Learning**

Active learning allows the AI model to choose the next experiment strategically.

Instead of randomly selecting candidates, the model selects experiments that are expected to:

- Improve prediction accuracy.

- Discover high-performing materials.
- Reduce uncertainty.

This can minimise experimental workload.

**31. Bayesian Optimisation**

Bayesian optimisation is useful when experiments are:

- Expensive.
- Time-consuming.
- Limited in number.

The algorithm learns from previous experiments and recommends promising next candidates. This creates an efficient search strategy.

**Table 1. AI Techniques in Materials Discovery**

| AI Technique | Main Function | Materials Application |
|---|---|---|
| Regression | Property prediction | Battery materials |
| Random Forest | Classification/prediction | Material screening |
| Neural Networks | Complex prediction | Material properties |
| Graph Neural Networks | Structure-based prediction | Crystal materials |
| Generative Models | Candidate generation | New materials |
| Active Learning | Experiment selection | Autonomous discovery |
| Bayesian Optimisation | Search optimisation | Battery/catalyst optimisation |
| Computer Vision | Image analysis | Material characterisation |
| Reinforcement Learning | Sequential optimisation | Process optimisation |

**32. AI and Computational Materials Science**

AI does not necessarily replace physics-based simulation.
Instead, AI and simulation can complement each other.
For example:

**DFT Simulation**

↓

Generates high-quality training data

↓

**Machine Learning**

↓

Predicts properties for many additional candidates

This hybrid strategy can reduce computational requirements.

**33. Surrogate Models**

Detailed simulations can be computationally expensive.

Machine-learning surrogate models approximate expensive simulations.

Instead of running a complete simulation every time:

**Input → ML Model → Approximate Property**

This can dramatically accelerate screening.

**34. Digital Materials Twins**

A digital materials twin is a computational representation of a material that integrates:

- Structure.
- Properties.
- Processing information.
- Experimental data.
- Performance history.

Such systems could enable continuous optimisation throughout a material's lifecycle.

**35. Sustainability Metrics**

AI-driven materials discovery should evaluate more than performance.

Potential metrics include:

- Energy density.
- Material abundance.
- Toxicity.
- Carbon footprint.
- Manufacturing energy.
- Recyclability.
- Lifetime.
- Cost.

A material should ideally be evaluated using a multi-objective framework.

**36. Multi-Objective Materials Optimisation**

Materials often involve trade-offs.

For example:

**High Performance**

may conflict with

**Low Cost**

or

**High Energy Density**

may conflict with

Long Cycle Life.

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AI can search for Pareto-optimal solutions rather than optimising a single property.

**Table 2. Sustainability Dimensions for Advanced Materials**

| Dimension | Example Indicator |
|---|---|
| Performance | Energy density |
| Durability | Cycle life |
| Resource Efficiency | Material intensity |
| Environmental Impact | Carbon footprint |
| Safety | Thermal stability |
| Economics | Cost per unit |
| Circularity | Recyclability |
| Supply Security | Material availability |

**37. Data Challenges**

AI requires reliable data.

Materials datasets may contain:

- Missing values.
- Inconsistent measurements.
- Different experimental conditions.
- Duplicated records.
- Small sample sizes.

Poor data can lead to unreliable predictions.

**38. Experimental Data Scarcity**

Compared with other AI fields, materials science often has relatively limited high-quality experimental data.

A model trained mainly on computational data may not accurately reflect:

- Manufacturing constraints.
- Defects.
- Impurities.
- Real operating conditions.

Therefore, experimental validation remains essential.

**39. Model Interpretability**

Materials scientists may need to understand why an AI model predicts that a material will perform well.

Interpretability can help researchers identify:

- Important chemical features.
- Structural characteristics.
- Relevant physical mechanisms.

Explainable AI can therefore improve trust in AI-supported materials discovery.

**40. Generalisation**

A model may perform well on known materials but poorly on entirely new compositions.
This is particularly important for discovery because the objective is often to identify materials outside the training dataset.
Improving out-of-distribution generalisation remains an important research challenge.

**41. Reproducibility**

Materials research should ensure that AI predictions can be reproduced.
Important requirements include:

- Transparent datasets.
- Clear model descriptions.
- Standardised evaluation.
- Experimental validation.

Open and interoperable materials databases can help address these challenges.

**42. Computational Sustainability**

AI itself requires computational resources.
Large models may consume:

- Electricity.
- Hardware.
- Cooling resources.

Therefore, sustainable materials discovery should evaluate the environmental cost of the AI system itself.
The relevant metric is not simply:

**Discovery Speed**

but:

**Discovery Benefit / Computational + Experimental Resource Cost**

**43. Proposed AI-Driven Materials Discovery Framework**

The proposed framework contains nine stages.

**Stage 1 — Data Collection**

Gather experimental, computational, and literature data.

↓

**Stage 2 — Data Integration**
Standardise and clean materials information.
↓
**Stage 3 — Feature Representation**
Represent composition, structure, and processing.
↓
**Stage 4 — AI Modelling**
Train predictive or generative models.
↓
**Stage 5 — Candidate Generation**
Identify promising materials.
↓
**Stage 6 — Computational Screening**
Use simulations to eliminate unsuitable candidates.
↓
**Stage 7 — Experimental Validation**
Synthesize and test selected materials.
↓
**Stage 8 — Feedback**
Return experimental results to the AI model.
↓
**Stage 9 — Optimisation**
Iteratively improve material candidates.

**44. Sustainable Energy Storage Framework**

For energy storage, the framework can be extended:

**Energy Requirement**
↓
**Target Properties**
↓
**AI Candidate Generation**
↓
**Material Screening**
↓
**Electrochemical Simulation**
↓
**Prototype Cell**
↓
**Performance Testing**
↓

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**Lifecycle Assessment**

↓

**Scale-Up**

**45. Resource-Efficient Materials Manufacturing**

AI can optimise manufacturing parameters such as:

- Temperature.
- Pressure.
- Processing time.
- Raw-material quantities.

This can reduce:

- Energy use.
- Material waste.
- Production time.

**46. Additive Manufacturing**

AI can optimise additive manufacturing processes.

Potential applications include:

- Lightweight structures.
- Complex geometries.
- Reduced material waste.
- Process optimisation.

AI can predict relationships between:

**Process Parameters → Material Structure → Performance**

**47. AI and Materials for Water Efficiency**

Advanced materials are important for:

- Desalination membranes.
- Water filtration.
- Pollutant removal.
- Water purification.

AI can accelerate the identification of membrane materials with desirable:

- Selectivity.
- Permeability.
- Durability.

**48. AI and Carbon Capture Materials**

Carbon-capture technologies require materials capable of selectively capturing $CO_2$.

AI can help screen:

- Porous materials.

- Metal-organic frameworks.
- Adsorbents.
- Membranes.

Potential objectives include:

- High selectivity.
- Low regeneration energy.
- Long-term stability.

**49. AI and Metal-Organic Frameworks**

Metal-organic frameworks possess highly tunable structures.

The number of possible combinations is enormous.

AI can help predict:

- Gas adsorption.
- Structural stability.
- Selectivity.

This makes them an important field for AI-assisted materials discovery.

**50. Barriers to Commercialisation**

A promising material is not automatically commercially viable.

Commercialisation requires consideration of:

- Raw-material availability.
- Manufacturing scalability.
- Equipment requirements.
- Safety.
- Cost.
- Regulation.
- Recycling.

The transition from:

**AI Prediction → Laboratory Material → Industrial Product**

remains a major challenge.

**51. Technology Readiness**

Materials discovery should therefore consider technology-readiness levels.

**Early Stage**

Computational prediction.

**Intermediate Stage**

Laboratory validation.

**Advanced Stage**
Prototype testing.

**Commercial Stage**
Industrial manufacturing.
AI can accelerate early stages, but scale-up remains dependent on engineering and economics.

**52. Intellectual Property**
AI-generated material candidates create new questions concerning:
- Ownership.
- Patents.
- Data rights.
- Inventorship.
- Proprietary datasets.

Organizations developing AI-driven materials platforms will need clear intellectual-property frameworks.

**53. Skills and Interdisciplinary Research**
The field requires collaboration among:
- Materials scientists.
- Chemists.
- Physicists.
- Data scientists.
- AI researchers.
- Chemical engineers.
- Manufacturing engineers.
- Sustainability specialists.

Interdisciplinary teams are therefore essential.

**54. Future Directions**
**54.1 Foundation Models for Materials**
Large models trained on diverse materials datasets could support multiple discovery tasks.

**54.2 Autonomous Laboratories**
Robotics and AI may increasingly operate closed-loop experimental systems.

**54.3 Quantum-AI Materials Discovery**
Quantum computing may eventually complement AI for molecular and materials simulation.

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### 54.4 Sustainable-by-Design Materials

Future AI systems could optimise performance and sustainability simultaneously.

### 54.5 Circular Materials Intelligence

AI could track materials from extraction through manufacturing, use, recycling, and reuse.

## 55. Future Research Agenda

Future research should focus on:

1. Standardised materials datasets.
2. Explainable materials AI.
3. Experimental-data integration.
4. Autonomous experimentation.
5. Multi-objective optimisation.
6. Lifecycle-aware materials discovery.
7. AI-assisted recycling.
8. Critical-material substitution.
9. Sustainable AI infrastructure.
10. AI–quantum hybrid materials modelling.

## 56. Questionnaire

**Scale: 1 = Strongly Disagree, 5 = Strongly Agree**

| No. | Statement |
|---|---|
| 1 | AI can significantly accelerate advanced materials discovery. |
| 2 | Machine learning can reduce the number of materials experiments required. |
| 3 | AI can improve the development of advanced battery materials. |
| 4 | AI-assisted materials discovery can support resource efficiency. |
| 5 | Autonomous laboratories can improve experimental productivity. |
| 6 | Sustainable criteria should be incorporated into materials discovery. |
| 7 | AI models require greater access to high-quality experimental materials data. |
| 8 | Explainability is important when using AI for scientific materials discovery. |
| 9 | AI can contribute to reducing dependence on critical materials. |
| 10 | AI-driven materials science will become increasingly important for sustainable technology development. |

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**57. Discussion**

The convergence of AI and advanced materials science represents a major shift in the way new materials can be discovered.

Traditional materials development is often characterised by sequential experimentation.

AI enables researchers to explore much larger design spaces computationally before entering the laboratory.

The greatest potential arises when AI is combined with:

- Physics-based modelling.
- High-throughput computation.
- Automated experimentation.
- Advanced characterisation.
- Lifecycle assessment.

This creates a closed-loop materials innovation ecosystem.

However, AI predictions should not be interpreted as proof of material performance.

A computationally predicted material may fail because of:

- Difficult synthesis.
- Structural instability.
- Impurities.
- Manufacturing constraints.
- Unexpected degradation.
- Cost limitations.

Consequently, the future of AI-enabled materials discovery is likely to be human–AI collaboration, rather than complete automation.

Materials scientists provide:

- Physical knowledge.
- Experimental judgement.
- Domain expertise.

AI provides:

- Large-scale search.
- Pattern recognition.
- Prediction.
- Optimisation.

Together, these capabilities can accelerate scientific discovery.

**58. Conclusion**

AI-enabled materials discovery has the potential to accelerate the development of technologies required for sustainable energy and resource efficiency.

Its applications extend across:

- Lithium-ion batteries.
- Sodium-ion batteries.

- Solid-state batteries.
- Supercapacitors.
- Hydrogen systems.
- Catalysts.
- Solar materials.
- Carbon capture.
- Water purification.
- Lightweight materials.
- Recycling technologies.

The most promising approach is not simply to use AI to predict material properties but to integrate AI into a complete discovery ecosystem involving data, simulation, experimentation, automation, and lifecycle assessment.

The proposed framework can be summarised as:

Materials Data → AI Prediction → Computational Screening → Automated Experimentation → Validation → Feedback → Sustainable Optimisation

The sustainability dimension is particularly important. Future materials should not be evaluated solely according to performance. Their:

- Resource requirements.
- Environmental impact.
- Safety.
- Cost.
- Durability.
- Recyclability.
- Supply-chain resilience.

must also be considered.

Ultimately, AI can transform materials discovery from a predominantly trial-and-error process into a more data-driven, predictive, iterative, and sustainability-oriented scientific process. When combined with advanced simulation, autonomous laboratories and responsible materials engineering, AI has the potential to shorten discovery cycles while helping develop the next generation of energy-storage and resource-efficient technologies.

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