Journal of Mines, Metals and Fuels, *73(10): 3067-3072; 2025. DOI: 10.18311/jmmf/2025/49454*

Online ISSN : 0022-2755

Journal of Mines, Metals and Fuels

Contents available at: *www.informaticsjournals.co.in/index.php/jmmf*

AI Driven Discovery and Design of Smart Materials

Mahesh. A. Bote[1], Naeem Shaikh[1], Shruti Pandit[2], A. C. Bhagali[1] and Azhar Mulla[1]

[1]*Sanjay Bhokare Group of Institutes, Miraj - 416410, Maharashtra, India; maheshbote1@gmail.com*
[2]*Pimpri Chinchwad College of Engineering, Pimpri-Chinchwad - 411044, Maharashtra, India*

Abstract

Artificial Intelligence (AI) is revolutionising the discovery, characterisation, and application of smart materials. This review comprehensively explores AI's role in smart materials research, focusing on Machine Learning (ML) for property prediction, generative models for inverse design, and autonomous research systems. AI advancements have accelerated the optimisation of materials like shape memory alloys, piezoelectric materials, and self-healing polymers, enhancing their functionality. However, challenges such as data quality, model interpretability, and scalability persist. This paper addresses these innovations, their limitations, and future directions for AI-driven materials science.

Major Findings: *AI-driven methods, including ML and generative models, significantly enhance smart material discovery by improving prediction accuracy and enabling inverse design. Autonomous systems streamline experimental processes, but data quality and model interpretability remain critical challenges. Emerging trends like foundation models and active learning promise further advancements.*

Keywords: *Artificial Intelligence, Autonomous Research Systems, Generative Models, Smart Materials, Machine Learning, Materials Informatics*

1.0 Introduction

1.1 Definition and Scope of Smart Materials

Smart materials dynamically respond to external stimuli (e.g., temperature, electric fields) by altering properties such as shape, conductivity, or colour[1,2]. Examples include Shape Memory Alloys (SMAs), piezoelectric ceramics, and self-healing polymers. These materials find applications in healthcare (e.g., drug delivery), aerospace (e.g., adaptive structures), and electronics (e.g., wearable sensors)[3,4]. However, their development is hindered by slow experimental processes and data limitations[5,6].

1.2 Traditional Challenges in Smart Materials Discovery

Traditional material discovery relies on trial-and-error, which is time-intensive and limited to known material spaces[7]. Data scarcity and inconsistency further complicate the application of computational methods[8]. Extracting structured data from heterogeneous scientific literature remains challenging, requiring advanced Natural Language Processing (NLP) techniques[9,10].

1.3 Role of AI in Transforming Materials Science

AI, particularly ML and generative models, is transforming materials science by accelerating discovery and optimising material properties. For instance, the Energy-GNoME database identified 33,000 energy materials using AI-driven screening[11]. Autonomous systems, such as AI-enhanced scanning probe

**Author for correspondence*

microscopy, automate characterisation, improving efficiency[12,13]. However, challenges like data quality and model interpretability persist.

1.4 Objectives and Structure of the Review

This review aims to:

- Classify AI techniques used in smart materials research.
- Analyze AI's role in accelerating material discovery and characterization.
- Evaluate the integration of computational and experimental approaches.
- Highlight challenges and propose future directions.

The manuscript is structured as follows: Section 2 discusses AI techniques, Section 3 explores applications, and Section 4 concludes with implications and future directions.

2.0 AI Techniques in Smart Materials Research

2.1 Machine Learning for Property Prediction

ML models, such as Crystal Graph Convolutional Neural Networks (CGCNNs), predict material properties like bandgap and elastic modulus with high accuracy[14]. Unlike housing price prediction, material property prediction requires domain-specific features (e.g., crystal structure). For example, CGCNNs leverage graph-based representations to model atomic interactions, achieving superior performance over traditional regression models[15]. Uncertainty Quantification (UQ) via Bayesian neural networks ensures reliable predictions, critical for practical applications[16]. However, challenges include limited training data and model interpretability.

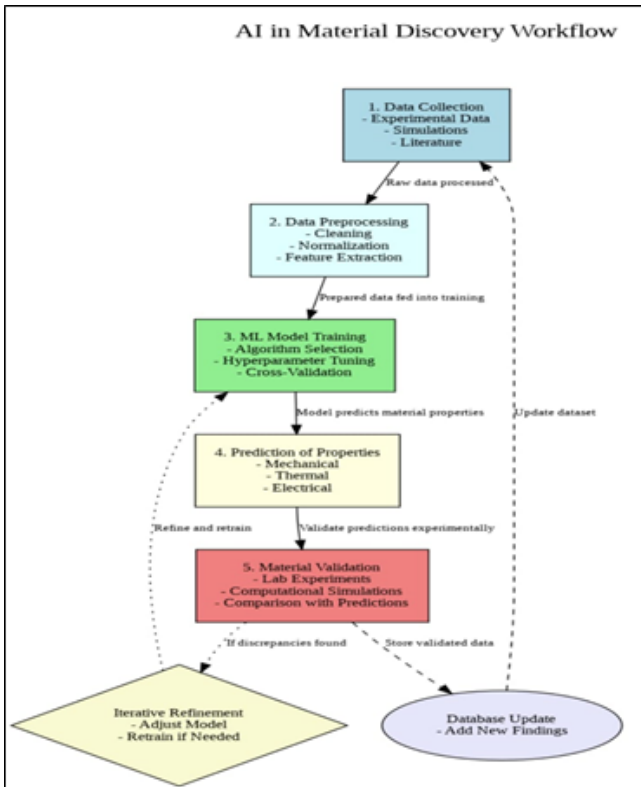


Figure 1. AI in material discovery workflow.

2.2 Data-Driven Approaches and Materials Informatics

Materials informatics integrates ML with experimental databases to predict material properties. Sequential learning frameworks, such as Bayesian Optimisation (BO) and Active Learning (AL), optimise experimental design

Table 1. Comparison of ML models for material property prediction

Model Type	Advantages	Limitations	Example Application
CGCNN	High accuracy, captures atomic structure	Computationally intensive	Bandgap prediction[21]
Random Forest	Interpretable, fast	Limited to tabular data	Elastic modulus[22]
Bayesian Neural Network	Provides UQ	Complex training	Stability prediction[28]

Table 2. Key open-source tools in materials informatics

Tool	Functionality	Example Use Case
Materials Project	Database of computed properties	Bandgap screening[11]
PyMatGen	Structure analysis, ML integration	Crystal structure prediction[21]
DeepChem	Molecular ML models	Drug discovery

by prioritising high-value experiments[17,18]. For example, BO has been used to discover transparent conducting materials[19]. Open-source platforms like Materials Project and PyMatGen facilitate data sharing and model development. Challenges include data heterogeneity and bias, which can skew predictions[20].

2.3 Generative Models and Inverse Design

Generative models, such as Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs), and Diffusion Models, enable inverse design by generating materials with desired properties[21]. The MAGECS framework, combining GANs with bird swarm algorithms, enhances electrocatalyst design for CO_2 reduction, but struggles with mode collapse[22,23]. Diffusion Models outperform GANs in capturing structural diversity, though they require significant computational resources[24]. Challenges include ensuring generative diversity and experimental realizability.

2.4 Simulation and Multiscale Modelling

Multiscale modelling bridges atomic to macroscopic scales using AI-driven surrogate models. Physics-Informed Neural Networks (PINNs) enhance simulation accuracy by embedding physical constraints, reducing reliance on large datasets[25]. For example, PINNs model microstructure evolution in phase field simulations[26]. Bayesian approaches quantify uncertainty, improving prediction reliability[27,28]. Challenges include model interpretability and computational scalability.

2.5 Autonomous Research Systems

Autonomous systems, such as self-driving laboratories, integrate AI with robotics to automate material discovery. Reinforcement Learning (RL) and closed-

Table 3. Generative model frameworks.

Framework	Mechanism	Advantages	Challenges
GANs	Adversarial training	High-quality outputs	Mode collapse[24]
VAEs	Latent space encoding	Interpretable latent spaces	Blurry outputs[26]
Diffusion Models	Iterative denoising	Structural diversity	High computational cost[27]

Table 4. Multiscale modelling techniques

Technique	Description	AI Integration	Example Application
Phase Field Method	Simulates microstructure evolution	Neural networks for adaptive meshing[31]	Alloy design
Digital Twins	Real-time process simulation	ML for predictive modeling[30]	Manufacturing optimization
PINNs	Physics-constrained neural networks	Embedded physical laws[29]	Multiscale property prediction

Table 5. Autonomous research systems

System	AI Technique	Functionality	Challenges
NIMS-OS	Bayesian Optimization, RL	Closed-loop experimentation[35]	Scalability
AMASE	Multi-agent systems	Experiment-theory integration[32]	Data bias
AI-SPM	Deep learning	Automated microscopy[34]	Adaptability

loop optimisation, as implemented in NIMS-OS, enable real-time experiment planning[29]. For instance, the AMASE system reduces experimental iterations for phase diagram construction[30]. However, algorithmic biases in training data can lead to systematic errors, necessitating robust validation. Safety and reliability remain critical concerns.

2.6 Emerging Trends

Foundation models, such as GPT variants adapted for materials science, enable generalised property prediction across material classes. Active learning minimises costly experiments by iteratively selecting high-impact data points[31]. Explainable AI (XAI) techniques, like SHAP, enhance model interpretability, fostering scientific trust.

3.0 Applications of AI in Smart Materials Discovery

3.1 Shape Memory Alloys (SMAs)

AI optimises SMA design and characterisation. For example, ML models predict NiTi SMA actuation behaviour with 99% accuracy[32]. Neural networks model nonlinear SMA behaviour, improving computational efficiency[33]. Applications include robotics, biomedical devices, and aerospace actuators[36]. Challenges include understanding complex phase transformations.

3.2 Piezoelectric Materials

AI enhances piezoelectric material performance in wearables and electronics. ML predicts piezoelectric coefficients (e.g., d33) for KNN ceramics, accelerating design[34,35]. AI-driven piezotronics optimise charge transport in III-nitride materials[36]. Scalability and reliability remain challenges.

3.3 Self-Healing Polymers

AI predicts failure points and optimises healing in self-healing polymers, extending the lifespan of flexible electronics[37]. In aerospace, AI designs nanocomposites for structural recovery[38]. Challenges include maintaining performance under extreme conditions.

3.4 Thermochromic and Electrochromic Materials

AI optimises thermochromic materials (e.g., VO2) for smart windows, improving solar modulation[39]. Electrochromic materials like tungsten oxide benefit from AI-driven durability enhancements[40]. Cost and scalability are ongoing hurdles.

3.5 Other Smart Materials

AI enables 4D printing of smart polymers for biomedical applications[41,42]. In manufacturing, AI-IoT systems optimise production[43,44]. Challenges include integrating heterogeneous data for predictive modelling[45,46].

Table 6. Applications of AI in smart materials

Material Type	AI Application	Industry Impact	Reference
SMAs	Actuation prediction	Robotics, aerospace[38]	38
Piezoelectric	Coefficient prediction	Wearables, electronics[41]	41
Self-Healing Polymers	Failure prediction	Electronics, aerospace[43]	43

Table 7. Future challenges and directions

Challenge	Proposed Solution	Expected Impact
Data Quality	Standardized datasets (e.g., Materials Project)	Improved model accuracy
Interpretability	XAI techniques (e.g., SHAP)	Enhanced scientific trust
Scalability	Active learning, cloud computing	Reduced experimental costs

4.0 Conclusion

AI has revolutionised smart materials research by enhancing property prediction, inverse design, and experimental automation[47,48]. ML and generative models enable efficient material discovery, while autonomous systems streamline characterisation[49]. However, challenges like data quality, model interpretability, and scalability persist. Future research should focus on standardised datasets, XAI for transparency, and active learning to reduce experimental costs[50]. Collaborative efforts between material scientists and AI experts will drive the next generation of smart materials.

5.0 References

1. Ramakrishnan T, *et al.* Recent developments in stimuli responsive smart materials and applications: an overview. J Nanomater. 2022; 2022:1–7. https://doi.org/10.1155/2022/4031059
2. Szczypiński FT, *et al.* Can we predict materials that can be synthesized? Chem Sci. 2021; 12(3):830–40. https://doi.org/10.1039/D0SC04321D. PMid:34163850 PMCid:PMC8178993
3. Mroz AM, *et al.* Into the unknown: how computation can help explore uncharted material space. J Am Chem Soc. 2022; 144(41):18730–43. https://doi.org/10.1021/jacs.2c06833. PMid:36206484 PMCid:PMC9585593
4. Hira K, *et al.* Reconstructing materials tetrahedron: challenges in materials information extraction. *arXiv*; 2023.
5. De Angelis P, *et al.* Energy-GNoME: a living database of selected materials for energy applications; 2024.
6. Ottomano F, *et al.* Assessing data-driven predictions of band gap and electrical conductivity for transparent conducting materials. Digital Discovery. 2024. https://doi.org/10.1039/D5DD00010F
7. Hegde V, *et al.* Towards informatics-driven design of nuclear waste forms. Digital Discovery. 2024. https://doi.org/10.1039/D4DD00096J
8. Huang C, *et al.* Material property prediction with element attribute knowledge graphs and multimodal representation learning. 2024
9. Jacobs R, *et al.* Machine learning materials properties with accurate predictions, uncertainty estimates, domain guidance, and persistent online accessibility. Machine Learning: Science and Technology. 2024. https://doi.org/10.1088/2632-2153/ad95db
10. Song Z, *et al.* Inverse design of promising electrocatalysts for CO_2 reduction via generative models and bird swarm algorithm. Nat Commun. 2025; 16(1). https://doi.org/10.1038/s41467-024-55613-z. PMid:39865081 PMCid:PMC11770065
11. Teng L, *et al.* Generative deep learning for the inverse design of materials. Computational Materials. 2024.
12. Habibi M, *et al.* Inverse design with conditional cascaded diffusion models. ASME 2024 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference; 2024. https://doi.org/10.1115/DETC2024-143607
13. Anand G, *et al.* Exploiting machine learning in multiscale modelling of materials. J Inst Eng Ser D. 2022. https://doi.org/10.1007/s40033-022-00424-z
14. Liang H, *et al.* Real-time experiment-theory closed-loop interaction for autonomous materials science. Materials Science. 2024.
15. NIMS-OS: an automation software to implement a closed loop between artificial intelligence and robotic experiments in materials science; 2023.
16. Dutta R, *et al.* Artificial intelligence automates the characterization of reversibly actuating planar-flow-casted NiTi shape memory alloy foil. PLoS ONE. 2022; 17(10):e0275485. https://doi.org/10.1371/journal.pone.0275485. PMid:36260552 PMCid:PMC9581382
17. Nematov S, *et al.* Machine learning-driven materials discovery: Unlocking next-generation functional materials – A minireview. Materials Today Chemistry. 2025. https://doi.org/10.1016/j.mtchem.2025.101684
18. Li Y, *et al.* Materials generation in the era of artificial intelligence: A comprehensive survey. *arXiv preprint*. 2025. https://arxiv.org/abs/2505.16379

19. Cheng Z, *et al.* AI-driven materials design: A mini-review. *arXiv preprint*. 2025. https://arxiv.org/abs/2502.02905
20. Xie Y, *et al.* Generative AI for design of nanoporous materials: Review and future prospects. Digital Discovery (RSC). 2025. https://doi.org/10.1039/D5DD00221D
21. Wang A, *et al.* Crystalline material discovery in the era of artificial intelligence. arXiv preprint. 2025. https://arxiv.org/abs/2408.08044
22. Liu S, *et al.* Materials Expert–Artificial Intelligence (ME-AI) for materials discovery. arXiv preprint. 2023. https://arxiv.org/abs/2312.02796
23. Cao L, *et al.* AI methods in materials design, discovery and manufacturing: A review. Advanced Engineering Informatics. 2024. https://doi.org/10.1016/j.aei.2024.101005
24. Gubernatis JE, Lookman T. Machine learning in materials design and discovery: Examples from the present and suggestions for the future. Phys Rev Materials. 2018. https://doi.org/10.1103/PhysRevMaterials.2.120301
25. Lee EH, Jiang W, Alsalman H, Low T, Cherkassky V. Methodological framework for materials discovery using machine learning. Phys Rev Materials. 2022. https://doi.org/10.1103/PhysRevMaterials.6.043802 Physical Review Journals+1arXiv+1
26. Baird SG, *et al.* Data-driven materials discovery and synthesis using machine learning methods. arXiv preprint. 2022. https://doi.org/10.48550/arXiv.2202.02380 arXiv
27. Li W, Chen P, Xiong B, *et al.* Deep learning modeling strategy for material science: from natural materials to metamaterials. J Phys Mater. 2022. https://doi.org/10.1088/2515-7639/ac5914 Physical Review Journals+4IOPscience+4Physical Review Journals+4
28. OllmannKocer E, Ko TW, Behler J. Neural network potentials: A concise overview of methods. Annu Rev Phys Chem. 2022.
29. Chen C, Ong SP. A universal graph deep learning interatomic potential for the periodic table. Nature Comput Sci. 2022.
30. Deng B, Zhong P, Jun K, *et al.* CHGNet: a pretrained universal neural network potential for charge-informed atomistic modelling. Nature Machine Intelligence. 2023.
31. Moi J, Spallarossa D, Bonetti S, *et al.* The quest for new materials: the network theory and machine learning perspectives. arXiv. 2025.
32. Liu Y, Jovanovic M, Mallayya K, *et al.* Materials expertartificial intelligence for materials discovery. arXiv preprint. 2023.
33. Vergara D, Lampropoulos G, FernándezArias P, AntónSancho Á. Artificial intelligence reinventing materials engineering: A bibliometric review. Appl Sci. 2024. https://doi.org/10.3390/app14188143
34. Tabor DP, *et al.* Accelerating the discovery of materials for clean energy in the era of smart automation. Nat Rev Mater. 2018.
35. Butler KT, Davies DW, Cartwright H, Isayev O, Walsh A. Machine learning for molecular and materials science. Nature. 2018.
36. SanchezLengeling B, AspuruGuzik A. Inverse molecular design using machine learning: generative models. Science. 2018.
37. Pilania G. Machine learning in materials science: from explainable predictions to autonomous design. Comput Mater Sci. 2021.
38. Morgan D, Jacobs R. Opportunities and challenges for machine learning in materials science. Annu Rev Mater Res. 2020.
39. MannodiKanakkithodi A, Chan MK. Computational datadriven materials discovery. Trends Chem. 2021.
40. Friederich P, Häse F, Proppe J, AspuruGuzik A. Machinelearned potentials for nextgeneration matter simulations. Nat Mater. 2021.
41. Pollice R, *et al.* Datadriven strategies for accelerated materials design. Acc Chem Res. 2021.
42. Westermayr J, Gastegger M, Schütt KT, *et al.* Perspective on integrating machine learning into computational chemistry and materials science. J Chem Phys. 2021.
43. Jha D, *et al.* Enabling deeper learning on big data for materials informatics applications. Sci Rep. 2021.
44. Jha D, Gupta V, Liao W-K, Choudhary A, Agrawal A. Moving closer to experimental level materials property prediction using AI. Sci Rep. 2022.
45. Gupta V, *et al.* MPPredictor: an AIdriven web tool for compositionbased material property prediction. J Chem Inf Model. 2023.
46. Wahl CB, *et al.* Machine learning enabled image classification for automated data acquisition in the electron microscope. MRS Commun. 2023.
47. Pereira T, Abbasi M, Ribeiro B, Arrais JP. Diversity oriented deep reinforcement learning for targeted molecule generation. J Cheminform. 2021.
48. Mercado R, *et al.* Graph networks for molecular design. Machine Learn.: Sci Technol. 2021. SpringerLink
49. Lookman T, Balachandran PV, Xue D, Yuan R. Active learning in materials science with emphasis on adaptive sampling. NPJ Comput Mater. 2019.
50. Kim C, Chandrasekaran A, Jha A, Ramprasad R. Activelearning and materials design: high Tg polymers example. MRS Commun. 2019.