

# INTERNATIONAL JOURNAL OF MULTIDISCIPLINARY FUTURISTIC DEVELOPMENT

## Deep Learning in Scientific Discovery

Matthew NO Sadiku <sup>1\*</sup>, David Padi <sup>2</sup>, Janet O Sadiku <sup>3</sup>

<sup>1</sup> Roy G. Perry College of Engineering, Prairie View A&M University, Prairie View, Texas, USA

<sup>2</sup> Alumnus, Graduate School of International Business and Leadership, Midwest University, Wentzville, Missouri, USA

<sup>3</sup> Juliana King University, Houston, Texas, USA

\* Corresponding Author: **Matthew NO Sadiku**

---

### Article Info

**P-ISSN:** 3051-3618

**E-ISSN:** 3051-3626

**Volume:** 07

**Issue:** 02

**Received:** 09-07-2026

**Accepted:** 07-08-2026

**Published:** 08-09-2026

**Page No:** 72-80

### Abstract

Traditionally, scientists have relied on mathematical models, laboratory experiments, and computational simulations to investigate complex phenomena. The growing availability of scientific data, advances in computing power, and improvements in neural network architectures have created new opportunities for applying deep learning to scientific discovery. Deep learning involves training artificial neural networks to identify patterns, make predictions, and learn representations from data. It enables researchers to predict molecular structures, identify potential drugs, discover new materials, analyze astronomical phenomena, and develop more accurate models of complex natural systems. This capability makes deep learning particularly valuable in scientific fields where information is high-dimensional, nonlinear, noisy, or too complex for conventional analytical techniques. Deep learning has become an important tool for scientific discovery, enabling researchers to investigate complex phenomena, analyze enormous datasets, and explore scientific possibilities that would be difficult to examine using conventional approaches alone. This paper examines the principles, applications, benefits, challenges, and future prospects of deep learning in scientific discovery.

**DOI:** <https://doi.org/10.54660/IJMFD.2026.7.2.72-80>

**Keywords:** Deep learning, DL, deep machine learning, scientific discovery

---

### 1. Introduction

Scientific discovery is the process of acquiring new knowledge about the natural world through observation, experimentation, analysis, reasoning, and theory development. Throughout history, scientific breakthroughs have been driven by new instruments, mathematical theories, and computational methods. However, the increasing volume and complexity of scientific data have created new challenges that conventional analytical methods cannot address efficiently. Today, deep learning is emerging as a powerful technology to overcome some of these challenges and accelerate scientific discovery. It transforms how scientists investigate complex phenomena, analyze experimental data, and develop new theories. Scientific discovery advances knowledge of the natural world through observation, experimentation, analysis, and developing and testing theories. Advances in scientific instruments, large-scale experiments, sensors, imaging technologies, and computational methods have substantially increased the volume and complexity of scientific data. Artificial intelligence (AI), particularly deep learning, can help researchers analyze these large datasets, identify complex patterns, generate predictions and hypotheses, and guide subsequent scientific investigation <sup>[1]</sup>.

Deep learning is a branch of machine learning that uses artificial neural networks with multiple processing layers to learn data representations at different levels of abstraction <sup>[2]</sup>. Deep-learning techniques are increasingly being applied across scientific disciplines, including biology, chemistry, physics, astronomy, medicine, environmental science, and materials science <sup>[1, 3]</sup>. Examples include predicting three-dimensional protein structures with high accuracy <sup>[4]</sup>, identifying and predicting promising new materials <sup>[5]</sup>, analyzing high-energy particle-collision data to distinguish potential signals from background events <sup>[6]</sup>, and

automatically classifying astronomical objects and galaxy images [7].

These applications demonstrate that deep learning can accelerate important components of the scientific research process. However, AI-generated predictions do not by themselves constitute scientific proof; model outputs must be appropriately evaluated, validated, and, where necessary, confirmed through experiments or other established scientific methods before they are used to support scientific conclusions [1].

## 2. Methodology

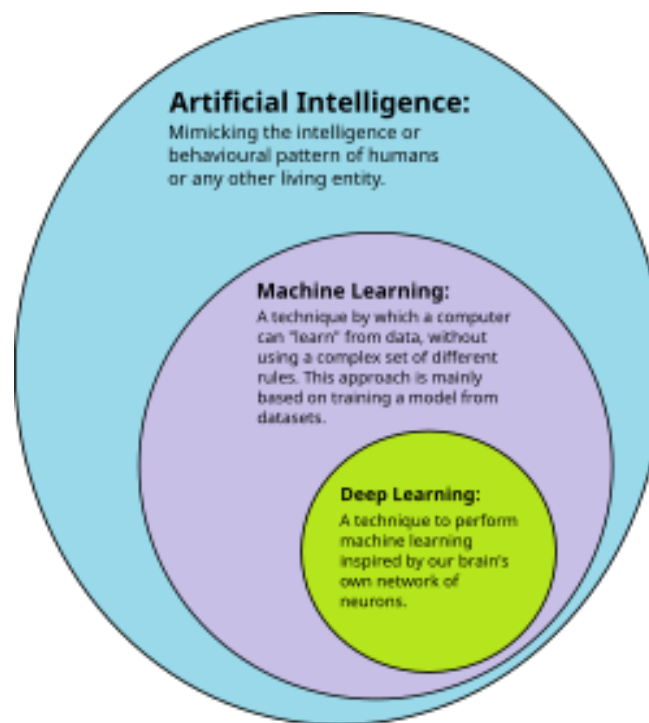
This paper uses a qualitative literature review to research on how deep learning contributes to scientific discovery. A literature review provides a way to bring together findings from existing studies and identify themes and gaps in the evidence [8]. The review draws on scholarly journals, peer-reviewed articles, and selected industry publications concerning applications in medicine, biology, chemistry, physics, astronomy, environmental science, and materials science. These fields provide examples of how artificial

intelligence is being used to analyze data, generate predictions, and guide research [1]. The paper organizes the literature around applications in areas such as protein structure prediction, drug discovery, genomics, astronomy, materials discovery, and climate research, then discusses reported benefits, limitations, and challenges.

## 3. Overview of Deep Learning

Deep learning is a branch of machine learning that uses artificial neural networks with multiple processing layers to learn patterns and representations from data. Its value lies in its ability to learn useful features directly from data, reducing the need for researchers to specify every feature in advance. As information passes through a network's layers, the model can learn increasingly abstract representations. This approach has been applied to images, video, speech, text, and biological data [2].

This capacity has made deep learning a central technology in contemporary artificial intelligence [9]. Figure 1 shows that deep learning is a subset of machine learning, and machine learning is a subset of artificial intelligence [10].



**Fig 1:** Deep learning is a subset of machine learning and machine learning is a subset of artificial intelligence [10].

Deep learning can be regarded as a representation or feature-learning approach in which computational models automatically learn useful features from data rather than relying entirely on manually designed features [2]. Different applications may employ different deep learning architectures depending on the nature of the data and the task being performed. Over time, deep learning has developed from a specialized machine-learning approach into a widely used technology within artificial intelligence and data-intensive applications [2, 11]. It has achieved significant results in areas such as automatic speech recognition, image recognition, computer vision, object detection, natural language processing, bioinformatics, drug discovery, and information retrieval [12].

Fundamentally, deep learning refers to machine-learning methods that use multiple layers of processing to transform

input data into progressively more abstract representations [2]. The term “deep” generally refers to the presence of multiple computational layers through which information is transformed. Artificial neural networks consist of interconnected computational units, commonly called neurons, organized into input, hidden, and output layers. In a deep neural network, the input layer receives the original data, while successive hidden layers apply weighted operations and nonlinear activation functions to develop increasingly complex representations. These hierarchical transformations enable the network to learn intricate relationships and patterns that may be difficult to identify using conventional feature-engineering approaches [1, 11].

In a fully connected deep neural network data flows through multiple layers where each neuron performs nonlinear transformations, allowing the model to learn intricate

representations of the data. In a deep neural network, the input layer receives data which passes through hidden layers that transform the data using nonlinear functions. The final output layer generates the model's prediction<sup>[13]</sup>.

Deep learning models are complicated artificial neural networks designed to mimic the human brain. Figure 2 shows a deep learning neural network model<sup>[14]</sup> while Figure 3 shows the key components of deep learning<sup>[15]</sup>. Deep learning powers many technologies we use every day, such

as voice assistants and medical tools. It is especially valuable when working with large quantities of unstructured data. Conventional databases organize information into clearly defined rows and columns, but much of the world's information exists such as photographs, recordings, documents, and videos. Deep neural networks are well suited to extracting patterns from these formats. Its greatest promise, however, emerges when technical capability meets responsible design.

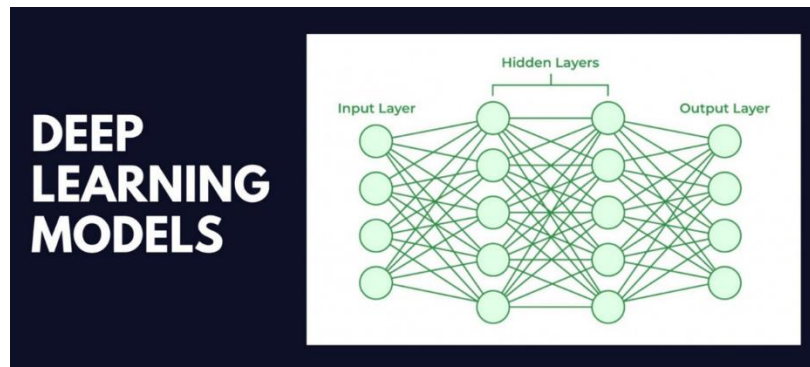


Fig 2: A deep learning neural network<sup>[14]</sup>.

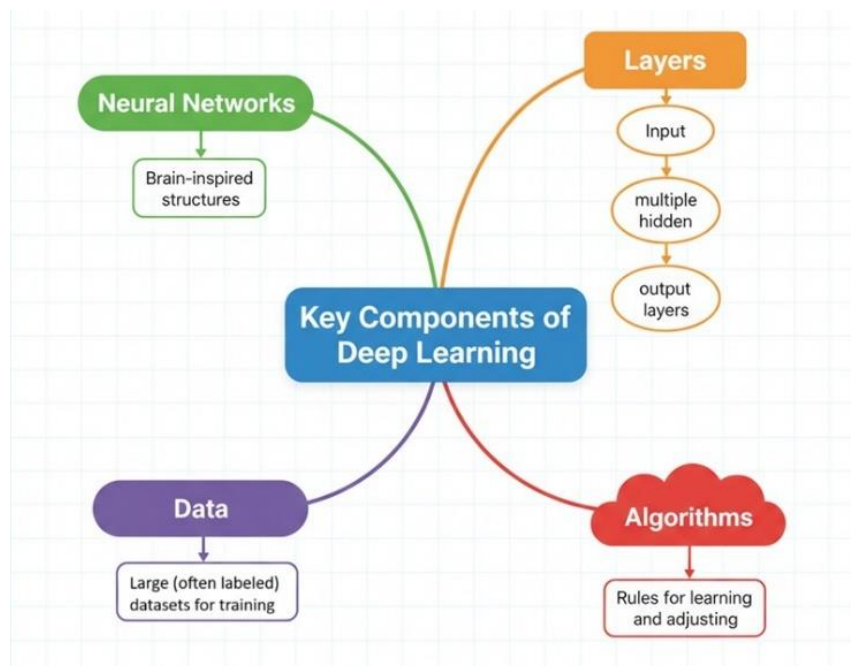


Fig 3: The key components of deep learning<sup>[15]</sup>.

Deep learning is not just a technological advancement. It reflects human intelligence, scaled, accelerated, and embedded in the systems around us. It is most commonly used where there are massive data and a need for intelligent interpretation. As a result, its strongest applications include language processing, image recognition, predictive analytics, and automation<sup>[16]</sup>.

#### 4. Deep Learning in Scientific Discovery

Deep learning is transforming scientific discovery by enabling researchers to analyze large and complex datasets, identify patterns that may be difficult to detect using conventional approaches, generate predictions, and support the investigation of computationally demanding scientific problems. Its integration into scientific research is changing several stages of the discovery process, including data

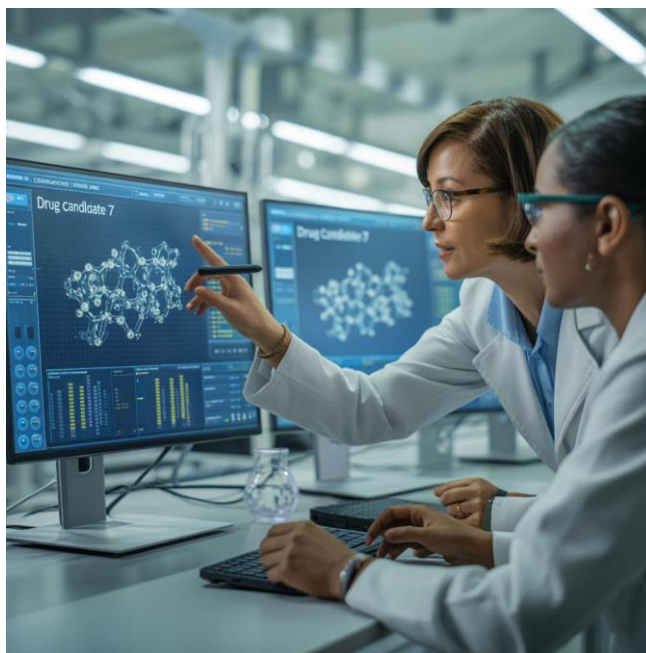
analysis, modeling, hypothesis generation, experimental design, and simulation<sup>[1]</sup>. These capabilities can help researchers investigate complex scientific phenomena and prioritize promising directions for further theoretical or experimental investigation. Despite these capabilities, deep learning does not replace the broader scientific process. Many deep learning models learn statistical relationships from existing observations and make predictions based on patterns represented in their training data. Scientific discovery, however, frequently involves formulating new hypotheses, designing and conducting experiments, challenging existing assumptions, interpreting evidence, and developing explanatory theories<sup>[1]</sup>. Consequently, predictions generated by deep learning models generally require further computational or experimental validation before they can be accepted as scientific findings<sup>[1]</sup>. For example, deep learning

can predict the structures and properties of very large numbers of potential materials, thereby helping researchers identify promising candidates for further investigation the potential by applying deep learning at scale to materials discovery <sup>[5]</sup>. Nevertheless, predicted materials require additional evaluation and, ultimately, experimental synthesis and characterization to establish their physical properties and practical usefulness <sup>[2]</sup>.

Deep learning has therefore created significant opportunities for scientific discovery by enabling researchers to analyze complex datasets, accelerate simulations, identify previously difficult to detect patterns, and support hypothesis generation <sup>[1]</sup>. Applications in medicine, biology, chemistry, physics, astronomy, materials science, and environmental science

demonstrate its potential to expand the methods available for producing scientific knowledge <sup>[1]</sup>. As deep learning systems become more accurate, interpretable, and closely integrated with experimental research, they may increasingly assist scientists in investigating longstanding questions, identifying previously unknown relationships, and developing discoveries that contribute to scientific knowledge and technological progress <sup>[1]</sup>.

Figure 4 scientists working on drug discovery <sup>[17]</sup>. Deep learning can support drug discovery through applications such as molecular-property prediction, protein-structure analysis, candidate identification, and the prioritization of compounds for subsequent experimental investigation <sup>[1]</sup>.



**Fig 4:** Scientists working on drug discovery <sup>[17]</sup>.

## 5. Applications of Deep Learning in Scientific Discovery

Deep learning applications in scientific discovery span molecular biology, drug discovery, genomics, astronomy, materials science, climate research, mathematics, chemistry, and physics <sup>[1]</sup>. AI and deep learning methods increasingly help scientists analyze large datasets, identify complex relationships, generate predictions, and support hypothesis development and experimental design <sup>[1]</sup>.

**Biology and Genomics.** Biology is one of the scientific fields benefiting substantially from deep learning. DNA and RNA sequencing, microscopy, proteomics, and related experimental techniques generate large and complex datasets that can be analyzed computationally to identify biological

patterns and relationships <sup>[1, 18]</sup>. In genomics, deep learning has been applied to tasks such as regulatory genomics, variant calling, predicting mutation effects, and analyzing gene regulation <sup>[18, 19]</sup>.

One important biological application is protein structure prediction. Because the three-dimensional structure of a protein is closely associated with its biological function, accurate structural information can contribute to understanding biological processes and developing therapeutic interventions <sup>[4]</sup>. Experimental determination of protein structures can require substantial time and resources, creating demand for accurate computational approaches <sup>[4]</sup>. Figure 5 shows an example of biological structure <sup>[17]</sup>.

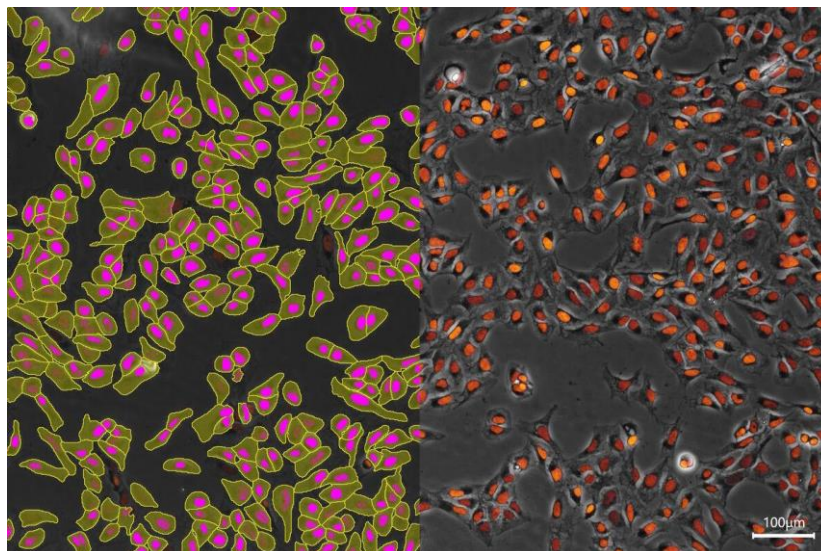


Figure 5 A typical Biological Structure <sup>[17]</sup>.

Drug Discovery and AlphaFold is possible through deep learning also supports drug discovery by helping researchers analyze molecular structures, predict properties, and identify promising candidates for further investigation <sup>[1]</sup>. AlphaFold, developed by DeepMind, is a prominent example of deep learning applied to protein structure prediction. Jumper *et al.* <sup>[4]</sup> demonstrated that AlphaFold could predict three-

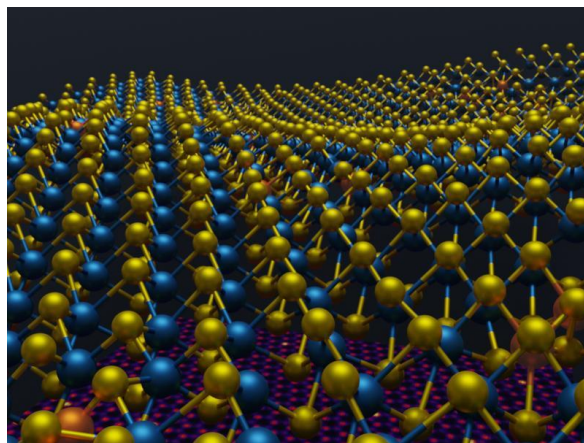
dimensional protein structures from amino acid sequences with accuracy competitive with experimentally determined structures for many proteins evaluated in CASP14. Subsequent research applied AlphaFold across almost the entire human proteome, illustrating the scalability of this approach <sup>[20]</sup>. Figure 6 illustrates AlphaFold protein structure prediction <sup>[21]</sup>.



Fig 6: The Deep Learning System AlphaFold Prediction <sup>[21]</sup>.

In physics, deep learning can help researchers analyze experimental measurements, model complex processes, and identify patterns in large datasets <sup>[1, 6]</sup>. Particle physics provides an important example because high-energy particle colliders generate large quantities of collision data in which rare signals must be distinguished from background events. Baldi *et al.* <sup>[6]</sup> demonstrated that deep learning could improve signal-versus-background classification in searches for exotic particles in high-energy physics. In chemistry, deep learning provides computational methods for studying

molecular behavior and predicting chemical reactions. Neural-network models can learn relationships between reactants, reagents, and reaction products, helping chemists predict likely reaction outcomes and plan chemical synthesis <sup>[7]</sup>. For example, researchers has demonstrated a Molecular Transformer approach that predicted reaction products without requiring handcrafted reaction rules <sup>[22]</sup>. Deep learning can also support molecular-property prediction and chemical-space exploration <sup>[1]</sup>. Figure 7 shows an example of a molecular structure <sup>[23]</sup>.



**Fig 7:** A typical molecular structure <sup>[23]</sup>.

Machine learning is increasingly being investigated as a tool for mathematical research and computational problem-solving <sup>[23]</sup>. Models can examine collections of mathematical objects, identify patterns and relationships, and provide information that guides mathematicians in formulating conjectures <sup>[24]</sup>. For example a machine-learning-assisted approach that helped mathematicians identify patterns and formulate conjectures in areas of pure mathematics. However, computationally generated conjectures still require mathematical reasoning and rigorous proof before they can be established as theorems <sup>[24]</sup>.

Deep learning can help researchers discover and design materials with desirable physical and chemical properties by predicting candidate structures and properties before extensive experimental synthesis <sup>[1, 5]</sup>. Researchers demonstrated the large-scale application of deep learning to materials discovery, illustrating how computational predictions can substantially expand the number of candidate stable materials available for further investigation <sup>[5]</sup>. Such approaches may contribute to research on batteries, catalysts, semiconductors, and other technologically important materials.

Astronomy and space science also benefit from deep learning because telescopes, satellites, and observatories generate extensive image and measurement datasets. Deep learning methods can assist with tasks such as astronomical image

analysis, object classification, detection, and extracting patterns from large observational datasets <sup>[1]</sup>. These capabilities allow researchers to process astronomical datasets at scales that would be difficult to analyze manually. In environmental and climate science, deep learning and related AI methods are increasingly used to analyze observations and simulations of the atmosphere, oceans, land, and other components of the Earth system <sup>[1]</sup>. These approaches can support weather and climate modeling and the analysis of satellite and remote-sensing data. Deep learning can also help identify environmental changes in large Earth-observation datasets, although model predictions require appropriate validation and consideration of data quality and uncertainty <sup>[1]</sup>. Autonomous laboratories combine artificial intelligence, machine learning, robotics, automated instrumentation, scientific databases, and experimental feedback to conduct portions of the research process with reduced manual intervention <sup>[1, 25]</sup>. Deep learning and other machine-learning methods can contribute to experiment selection, data interpretation, and iterative optimization. For example, the A-Lab developed by Szymanski *et al.* <sup>[25]</sup> integrates robotics, computational databases, machine-learning-based data interpretation, literature-derived synthesis information, and active learning to accelerate inorganic materials synthesis. Figure 8 shows an example of an autonomous laboratory <sup>[17]</sup>.



**Fig 8:** A typical autonomous laboratory <sup>[17]</sup>.

## 6. Benefits of Deep Learning in Scientific Discovery

Major benefits of deep learning in scientific discovery include faster analysis of large, complex datasets; more efficient experimental design; improved analysis of scientific images; reduced time and costs in selected research activities; and the ability to identify complex patterns that may contribute to the development of new scientific hypotheses. Deep learning can process high-dimensional data generated by modern scientific instruments and experiments, allowing researchers to extract useful information from datasets that may be difficult or time-consuming to analyze using conventional approaches<sup>[1]</sup>.

These benefits extend across numerous scientific disciplines, including biology, medicine, chemistry, physics, astronomy, environmental science, and materials engineering<sup>[1, 5]</sup>. For example, deep learning has advanced protein structure prediction<sup>[4]</sup>, materials discovery<sup>[5]</sup>, high-energy particle analysis<sup>[4]</sup>, and other data-intensive areas of scientific research. However, the benefits depend on factors such as the quality and representativeness of training data, model reliability and interpretability, computational resources, and appropriate experimental validation<sup>[1]</sup>.

One of deep learning's most significant contributions to scientific discovery is its ability to strengthen the relationship between data, prediction, and experimentation. Models can learn patterns from existing scientific data, generate predictions or identify promising candidates, and help researchers prioritize subsequent experiments. Experimental results can then provide additional evidence and data to refine models and guide further investigation, creating an iterative relationship between computational prediction and empirical scientific research<sup>[1, 25]</sup>.

Other benefits of deep learning in scientific discovery include the following:

Deep learning is particularly useful for analyzing the large datasets produced by modern scientific instruments<sup>[1]</sup>. Genome sequencing generates extensive biological data, particle accelerators record vast numbers of collision measurements, and astronomical observatories capture large collections of images and signals. Neural networks can identify complex patterns and relationships within such high-dimensional datasets<sup>[1]</sup>. In genomics, deep learning has been applied to identifying regulatory features in DNA and predicting molecular effects associated with genetic variants<sup>[18, 4]</sup>.

Prediction is central to many areas of scientific research because it enables researchers to formulate and test hypotheses and investigate the behavior of natural systems. Deep learning models can learn relationships from observational and experimental data to support these activities<sup>[1]</sup>. In molecular biology, AlphaFold provides a prominent example: deep learning has enabled highly accurate prediction of three-dimensional protein structures from amino acid sequences<sup>[4]</sup>.

Deep learning may also reduce the time and costs associated with selected stages of scientific research by helping researchers prioritize which experiments to pursue<sup>[1]</sup>. Developing medicines, investigating new materials, and conducting detailed simulations can require substantial financial, computational, and experimental resources. Computational screening can narrow large sets of possibilities before laboratory investigation begins, although model-generated predictions still require appropriate experimental testing and validation<sup>[1, 26]</sup>.

In drug discovery, deep learning can support multiple stages of research, including target-related analysis, molecular-property prediction, virtual screening, and candidate prioritization<sup>[26, 27]</sup>. Neural networks can analyze molecular structures, estimate relevant chemical and biological properties, and help researchers select compounds for further investigation. However, laboratory experiments and appropriately designed clinical trials remain necessary to establish the safety and efficacy of potential medicines<sup>[27]</sup>.

Materials scientists similarly use deep learning to predict properties and identify candidate materials worthy of further investigation<sup>[7]</sup>. Rather than experimentally examining every possible combination of compositions and processing conditions, researchers can use computational predictions to prioritize experiments involving batteries, photovoltaic materials, semiconductors, catalysts, and other technologically important materials. Large-scale deep-learning approaches have demonstrated the potential to substantially expand the number of candidate stable materials available for subsequent experimental investigation<sup>[5]</sup>.

Deep learning also contributes to interpreting scientific images. In microscopy, deep neural networks have been applied to image reconstruction, denoising, segmentation, and identifying and classifying cellular structures<sup>[28]</sup>. In astronomy, machine-learning and deep-learning techniques can assist with tasks such as galaxy classification, object detection, image analysis, and the processing of increasingly large astronomical datasets<sup>[29]</sup>.

Finally, deep learning can support the modeling and simulation of systems that are difficult, costly, or impractical to investigate directly. Models can approximate complex relationships associated with atmospheric processes, molecular interactions, fluid dynamics, and other physical systems<sup>[1, 30]</sup>. Physics-informed neural networks (PINNs) extend this capability by incorporating governing physical principles, such as differential equations, into the learning process. This allows data-driven models to be constrained by established scientific knowledge while solving forward and inverse problems involving complex physical systems<sup>[30, 31]</sup>.

## 7. Challenges of Deep Learning in Scientific Discovery

The use of deep learning in scientific research depends on reliable training data. Scientific datasets may be incomplete, inconsistent, biased, or expensive to obtain, especially when experiments are technically difficult. Models trained in poor-quality data can produce inaccurate predictions and misleading conclusions<sup>[1]</sup>.

Bias presents a related challenge. Training datasets may overrepresent certain populations, regions, or experimental conditions. In one study, chest X-ray classifiers underdiagnosed patients from historically underserved groups, illustrating why researchers should assess performance across relevant populations before applying a model broadly<sup>[32]</sup>.

Interpretability also matters because an accurate prediction does not necessarily explain the process that produced a result. A model might predict a chemical property without revealing its underlying physical mechanism. Researchers should therefore distinguish predictive usefulness from scientific understanding<sup>[1]</sup>.

Models must generalize beyond their training data. A system that performs well under familiar conditions may be unreliable when applied to new molecules or materials. Independent testing under realistic conditions and estimates

of predictive uncertainty are particularly important when a model is used outside its training domain <sup>[33]</sup>.

Computational requirements can limit access to deep learning. Training advanced models can require specialized hardware and substantial electricity, creating challenges for institutions with limited resources. Researchers can address some of these constraints by measuring energy use and considering more efficient approaches <sup>[34]</sup>.

Reproducibility presents another challenge. Other researchers need sufficient information to evaluate methods and verify findings. Documenting datasets, model settings, software, and training procedures is therefore essential to reproducible machine learning research <sup>[35]</sup>.

Ethical concerns require attention throughout the research process. Biomedical datasets may contain sensitive genetic and health information that must be managed securely and used in accordance with participants' consent. Researchers should also acknowledge data sources and disclose relevant limitations and potential conflicts of interest <sup>[1, 36]</sup>.

Finally, deep learning predictions should be interpreted in light of scientific uncertainty. A model can appear confident even when it encounters conditions unlike those represented in its training data. Communicating uncertainty helps researchers decide which predictions warrant further investigation and experimental validation <sup>[33]</sup>.

## 8. Future of Deep Learning in Scientific Discovery

The future of deep learning in scientific discovery is likely to involve the effective integration of deep learning, artificial intelligence, physical models, laboratory automation, human scientific reasoning, domain knowledge, mathematical modeling, and experimental investigation. As these approaches mature, artificial intelligence may help researchers explore previously inaccessible scientific questions and accelerate the development of knowledge that benefits humanity. The future promises even greater possibilities. As computational power increases, scientific datasets expand, and AI models become more sophisticated, deep learning is expected to evolve from a tool primarily used for data analysis into an increasingly active participant in scientific research. It will depend not only on developing more powerful AI models but also on making them more reliable, interpretable, efficient, and scientifically trustworthy.

By combining these diverse data sources, researchers can gain more comprehensive insights and make predictions that are challenging to achieve with individual data types. Scientific foundation models are another key development. These models, trained on broad datasets, can be adapted for various applications, including molecular analysis, literature review, and materials discovery. Their effectiveness, however, depends on data quality, reliability, interpretability, and thorough validation. Advancements in autonomous laboratories and AI-assisted experimentation enhance the link between computational predictions and physical experiments. These systems can automate experiment selection, analysis, and subsequent steps. For example, they can combine computational insights with robotic experimentation to accelerate new material synthesis. Physics-informed neural networks (PINNs) are also notable, as they blend data-driven learning with established physical principles, allowing for effective modeling of complex systems and solving scientific problems. Overall, the integration of these technologies can accelerate research

across multiple disciplines. However, it is unlikely that AI will completely replace human scientists. Instead, a more likely scenario involves increased collaboration, where AI assists in data analysis and hypothesis generation while researchers provide critical judgment and theoretical understanding. In this partnership, deep learning acts as a powerful tool for scientific discovery rather than a substitute for human intellect and expertise. <sup>[1], 25, 30, 31, 37,39]</sup>

## Conclusion

Deep learning is transforming scientific discovery by providing powerful methods to analyze complex data, predict scientific properties, identify patterns, and generate new research possibilities. It has demonstrated impressive capabilities in prediction, classification, and pattern recognition. Technology offers substantial opportunities to accelerate research, reduce selected experimental costs, and investigate problems that are difficult to address using conventional computational methods. Ultimately, deep learning's greatest contribution to scientific discovery is not merely its ability to process enormous amounts of information, but its potential to help scientists ask new questions, design better experiments, and uncover deeper insights into the natural world. More information about deep learning in scientific discovery can be found in the books in <sup>[39,40]</sup> and in the related journal *Artificial Intelligence Review*.

## References

1. Wang H, *et al.* Scientific discovery in the age of artificial intelligence. *Nature*. 2023 Aug;620:47-60. doi:10.1038/s41586-023-06221-2.
2. LeCun Y, Bengio Y, Hinton G. Deep learning. *Nature*. 2015 May;521:436-444. doi:10.1038/nature14539.
3. Batra R, *et al.* Recent advances and applications of deep learning methods in materials science. *npj Comput Mater*. 2022;8:59. doi:10.1038/s41524-022-00734-6.
4. Jumper J, *et al.* Highly accurate protein structure prediction with AlphaFold. *Nature*. 2021 Aug;596:583-589. doi:10.1038/s41586-021-03819-2.
5. Merchant A, *et al.* Scaling deep learning for materials discovery. *Nature*. 2023 Dec;624:80-85. doi:10.1038/s41586-023-06735-9.
6. Baldi P, Sadowski P, Whiteson D. Searching for exotic particles in high-energy physics with deep learning. *Nat Commun*. 2014 Jul;5:4308. doi:10.1038/ncomms5308.
7. Kim EJ, Brunner RJ. Star-galaxy classification using deep convolutional neural networks. *Mon Not R Astron Soc*. 2017 Feb;464(4):4463-4475. doi:10.1093/mnras/stw2672.
8. Snyder H. Literature review as a research methodology: An overview and guidelines. *J Bus Res*. 2019;104:333-339. doi:10.1016/j.jbusres.2019.07.039.
9. Sadiku MNO, Tembely M, Musa SM. Deep learning. *Int Res J Adv Eng Sci*. 2017;2(1):77-78.
10. Deep learning. Wikipedia [Internet]. Available from: [https://en.wikipedia.org/wiki/Deep\\_learning](https://en.wikipedia.org/wiki/Deep_learning)
11. Goodfellow I, Bengio Y, Courville A. *Deep Learning*. Cambridge, MA: MIT Press; 2016.
12. Schmidhuber J. Deep learning in neural networks: An overview. *Neural Netw*. 2015 Jan;61:85-117. doi:10.1016/j.neunet.2014.09.003.
13. GeeksforGeeks. Introduction to deep learning [Internet]. 2026 May 2. Available from: <https://www.geeksforgeeks.org/deep-learning/introduction-deep-learning/>

14. Somani N. What are deep learning models? IGMGuru [Internet]. 2026 Aug. Available from: <https://www.igmguru.com/blog/what-are-deep-learning-models>
15. Valcheva S. 25 deep learning applications driving AI innovation. Intellspot [Internet]. Available from: <https://www.intellspot.com/deep-learning-applications>
16. Kumar A. Applications of deep learning: Real-world examples and uses. The IoT Academy [Internet]. 2026 Apr 23; updated 2026 May 1. Available from: <https://www.theiotacademy.co/blog/applications-of-deep-learning/>
17. Scientists working on drug discovery: A typical biological structure. AI-generated image [Internet]. Available from: <https://chatgpt.com>
18. Eraslan G, Avsec Ž, Gagneur J, Theis FJ. Deep learning: New computational modelling techniques for genomics. *Nat Rev Genet.* 2019;20:389-403. doi:10.1038/s41576-019-0122-6.
19. Zou J, Huss M, Abid A, Mohammadi P, Torkamani A, Telenti A. A primer on deep learning in genomics. *Nat Genet.* 2019;51:12-18. doi:10.1038/s41588-018-0295-5.
20. Tunyasuvunakool K, *et al.* Highly accurate protein structure prediction for the human proteome. *Nature.* 2021 Aug;596:590-596. doi:10.1038/s41586-021-03828-1.
21. AI AlphaFold protein structure prediction. AI-generated image [Internet]. Available from: <https://chatgpt.com>
22. Schwaller P, *et al.* Molecular Transformer: A model for uncertainty-calibrated chemical reaction prediction. *ACS Cent Sci.* 2019;5(9):1572-1583. doi:10.1021/acscentsci.9b00576.
23. A typical molecular structure. AI-generated image [Internet]. Available from: <https://chatgpt.com>
24. Davies A, *et al.* Advancing mathematics by guiding human intuition with AI. *Nature.* 2021 Dec;600:70-74. doi:10.1038/s41586-021-04086-x.
25. Szymanski NJ, *et al.* An autonomous laboratory for the accelerated synthesis of novel materials. *Nature.* 2023 Dec;624:86-91. doi:10.1038/s41586-023-06734-w.
26. Stokes JM, *et al.* A deep learning approach to antibiotic discovery. *Cell.* 2020;180(4):688-702.e13. doi:10.1016/j.cell.2020.01.021.
27. Paul D, *et al.* Artificial intelligence in drug discovery and development. *Drug Discov Today.* 2021 Jan;26(1):80-93. doi:10.1016/j.drudis.2020.10.010.
28. Moen E, *et al.* Deep learning for cellular image analysis. *Nat Methods.* 2019;16:1233-1246. doi:10.1038/s41592-019-0403-1.
29. Baron D. Machine learning in astronomy: A practical overview. *arXiv [Internet].* 2019. arXiv:1904.07248. doi:10.48550/arXiv.1904.07248.
30. Karniadakis GE, Kevrekidis IG, Lu L, Perdikaris P, Wang S, Yang L. Physics-informed machine learning. *Nat Rev Phys.* 2021;3:422-440. doi:10.1038/s42254-021-00314-5.
31. Raissi M, Perdikaris P, Karniadakis GE. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J Comput Phys.* 2019;378:686-707. doi:10.1016/j.jcp.2018.10.045.
32. Seyyed-Kalantari L, Zhang H, McDermott MBA, Chen IY, Ghassemi M. Underdiagnosis bias of artificial intelligence algorithms applied to chest radiographs in under-served patient populations. *Nat Med.* 2021;27:2176-2182. doi:10.1038/s41591-021-01595-0.
33. Tan AR, Urata S, Goldman S, Dietschreit JCB, Gómez-Bombarelli R. Single-model uncertainty quantification in neural network potentials does not consistently outperform model ensembles. *npj Comput Mater.* 2023;9:225. doi:10.1038/s41524-023-01180-8.
34. Debus C, Piraud M, Streit A, Theis F, Götz M. Reporting electricity consumption is essential for sustainable AI. *Nat Mach Intell.* 2023;5:1176-1178. doi:10.1038/s42256-023-00750-1.
35. Heil BJ, Hoffman MM, Markowitz F, Lee SI, Greene CS, Hicks SC. Reproducibility standards for machine learning in the life sciences. *Nat Methods.* 2021;18:1132-1135. doi:10.1038/s41592-021-01256-7.
36. National Institutes of Health. Using genomic data responsibly under the NIH genomic data sharing policy [Internet]. 2025 Aug 5. Available from: <https://grants.nih.gov/policy-and-compliance/policy-topics/sharing-policies/accessing-data/using-genomic-data>
37. Baltrušaitis T, Ahuja C, Morency LP. Multimodal machine learning: A survey and taxonomy. *IEEE Trans Pattern Anal Mach Intell.* 2019 Feb;41(2):423-443. doi:10.1109/TPAMI.2018.2798607.
38. Bommasani R, *et al.* On the opportunities and risks of foundation models. Stanford, CA: Stanford Center for Research on Foundation Models, Stanford University; 2021. arXiv:2108.07258. doi:10.48550/arXiv.2108.07258.
39. Ramsundar B, Eastman P, Walters P. Deep Learning for the Life Sciences: Applying Deep Learning to Genomics, Microscopy, Drug Discovery, and More. Sebastopol, CA: O'Reilly Media; 2019.
40. Baldi P. Deep Learning in Science. Cambridge: Cambridge University Press; 2021.

### How to Cite This Article

Sadiku MNO, Padi D, Sadiku JO. Deep learning in scientific discovery. *Int J Multidiscip Futur Dev.* 2026;7(2):72-80. doi:10.54660/IJMF.D.2026.7.2.72-80.

### Creative Commons (CC) License

This is an open access journal, and articles are distributed under the terms of the Creative Commons Attribution NonCommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0) License, which allows others to remix, tweak, and build upon the work non-commercially, as long as appropriate credit is given and the new creations are licensed under the identical terms.