Library Progress International
Vol.44 No. 3, July-December 2024: P.23917-23927

Print version ISSN 0970 1052
Online version ISSN 2320 317X

Original Article

Available online at www.bpasjournals.com

The Transformative Role of Artificial Intelligence in Advancing Chemistry: A Comprehensive Review

Divya V[1a*], Aparna V[2b], Ashna Rasheed[3b], Sunitha. V. R[4a], Lakshmy M[5a], Anu K[6a]

*Corresponding author
[a] Assistant Professor, Department of Chemistry, Milad-E-Sherief Memorial College, Kayamkulam, Affiliated to University of Kerala, Kerala, India
[b] Post Graduate student, Department of Chemistry, Milad-E-Sherief Memorial College, Kayamkulam, Affiliated to University of Kerala, Kerala, India

1. divyarajiv001@gmail.com
2. aparnav70@gmail.com
3. ashnarasheed2001@gmail.com
4. sunijith26@gmail.com
5. lakshmym1971@gmail.com
6. anu7anu@gmail.com

How to cite this article: Divya V, Aparna V, Ashna Rasheed, Sunitha. V. R, Lakshmy M, Anu K (2024). The Transformative Role of Artificial Intelligence in Advancing Chemistry: A Comprehensive Review. *Library Progress International,* 44(3), 23917-23927

Abstract
Artificial Intelligence (AI) has had an innovative impact on various industries, and its profoundinfluence on the field of chemistry cannot be overstated. In this comprehensive review, we explore the pivotal role that AI plays in transforming different areas of chemistry, including drug discovery and development, material science, analytical chemistry, and chemical engineering. By harnessing machine learning, deep learning and other advanced AI technologies, scientists have been able to accelerate processes, optimize reactions, and uncover previously unknown compounds with unparalleled efficiency. Additionally, we examine the challenges and ethical considerations associated with integrating AI into chemical research. This review highlights the enormous potential of AI in driving scientific discovery andfostering innovation in the field of chemistry.
Keywords: *Artificial intelligence, Drug Discovery, Material Science, Environmental Chemistry, Electrochemistry, Forensic Chemistry*

Introduction

The integration of AI with chemistry has brought about a significant shift in scientific research methodologies1–3. AI powered algorithms are replacing traditional manual experimentation and data analysis methods, accelerating discovery processes, and optimizing experimental procedures. The review investigates into the historical evolution, recent applications, and prospects of AI in chemistry.

Historically, AI in chemistry originated in the late 20th century with a focus on computational methods for molecular modelling and drug design. Early initiatives concentrated on developing algorithms for molecular dynamic simulations, quantum chemistry calculations, and structure- activity relationship (SAR) analysis4. Noteworthy advancements include the utilization of machine learning algorithms such as artificial neural networks (ANNs) and support vector machines (SVMs) for predicting molecular properties and screening chemical libraries5.

In the contemporary era, AI has permeated every aspect of chemistry, facilitating breakthroughs in drug discovery, material science, catalysis, and chemical synthesis. AI-driven approaches have significantly impacted drug discovery by analysing extensive chemical datasets, predicting biological activities, and identifying potential drug candidates. Virtual screening techniques powered by AI expedite the identification of lead compounds for therapeutic targets4,6,7. Moreover, AI has revolutionized materials science by enabling the design and optimization of novel materials with tailored properties based on their chemical composition and structural characteristics, leading to discoveries in energy storage, catalysis, and electronic devices. In organic

synthesis, AI has played a crucial role in predicting chemical reaction conditions. Machine learning algorithms analyse reaction databases and molecular descriptors to forecast reaction outcomes, propose reaction mechanisms, and suggest optimal conditions. This capability streamlines the synthesis of complex molecules and facilitates the discovery of novel reactions. Figure 1 depicts several crucial domains in which AI is employed within the realm of chemistry. The focus of this discussion is on the most significant applications of AI in the fields of Chemistry, as well as the important tools employed in these applications.

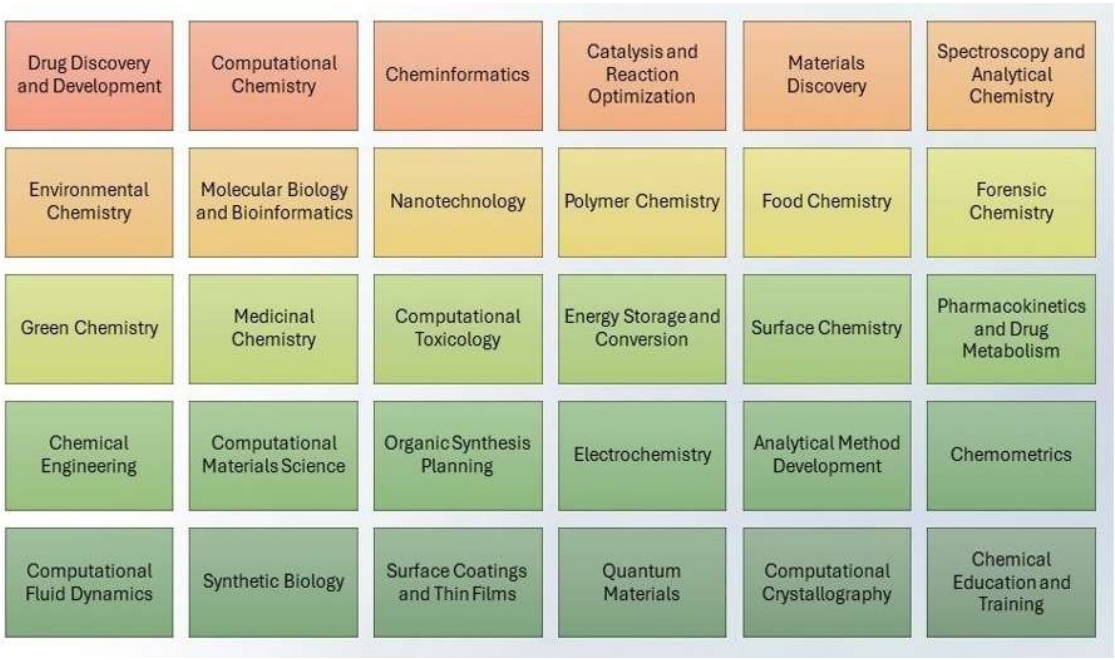

Figure 1: Pivotal domains in which AI is employed within the realm of chemistry.

AI Pharma: Revolutionising Drug Discovery with Artificial Intelligence

The pharmaceutical industry faces challenges with slow, costly, and intricate processes in drug discovery and development. Traditionally, it has relied on trial and error and expert knowledge, which often results in high failure rates. Drug discovery involves identifying therapeutic targets, screening compounds, optimizing leads, and conducting evaluations. Understanding the complexities of biological systems, which consists of networks of genes, proteins, and molecules, is a significant challenge. Overcoming these challenges requires both expertise and advanced computational tools. Figure 2 outlines the principal domains where AI finds application within the realm of drug discovery and development.

AI has become a transformative force in drug discovery. AI provides innovative methods for data analysis, prediction, and hypothesis generation. Machine learning, a subset of AI, has had a significant impact in this field. It enables computers to learn from data and make informed decisions without explicit programming. Through the analysis of vast datasets, AI algorithms can uncover concealed patterns, identify new drug targets, predict the effectiveness and safety of candidate compounds, and even design new molecules8–15.

AI making significant advancements in drug screening and repurposing efforts. The traditional method of high-throughput screening, where large compound libraries are evaluated against specific targets, is time consuming and restricts the number of compounds that can be evaluated. However, AI algorithms improve screening efficiency by predicting the likelihood of activity of a compound based on its chemical attributes and molecular properties. This enables researchers to prioritize compounds with the highest potential, thereby minimizing the need for extensive experimental testing. AI technologies, such as predictive analytics offer solutions to these challenges by analysing clinical trial data to identify appropriate patient groups, refine trial protocols and predict patient's responses to treatment. By utilizing real world evidence from various sources, including electronic health records and wearable devices, AI makes trials more efficient and cost effective, thereby speeding up the availability of new therapies for patients4,8,24–30,16–23,31,32.

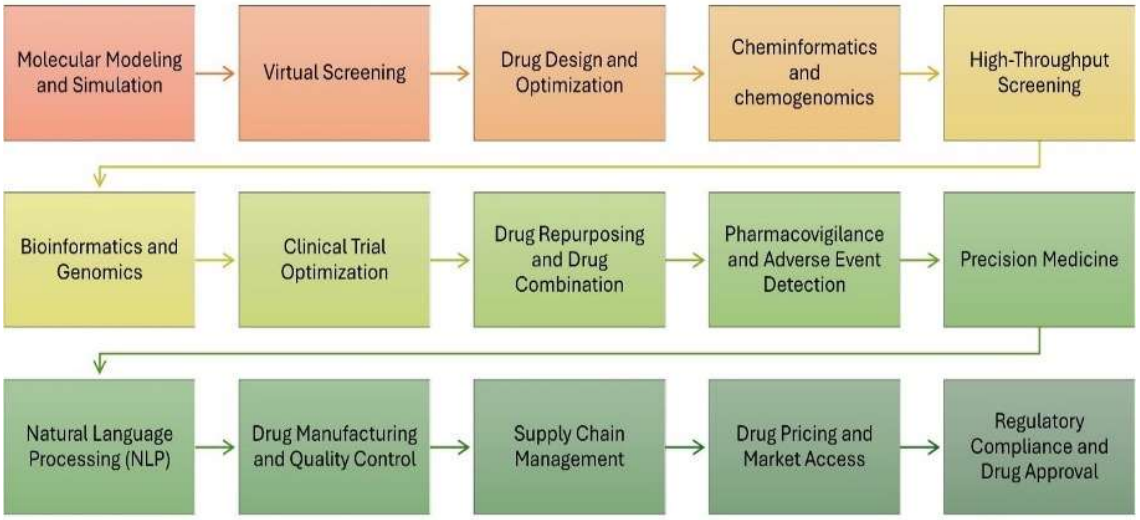

Figure 2: Principal Domains of AI applications in Drug Discovery and Development

However, AI-driven drug discovery does face challenges that need to be addressed. One of the most important challenges is the need for high-quality data to effectively train AI algorithms. Biomedical data, especially clinical and genomic data, often have noise, incompleteness, and bias, which make it difficult for machine learning models. Succeed in AI initiatives in drug discovery, it is crucial to ensure the integrity, quality, and confidentiality of healthcare data. Ethical considerations also play a significant role in integrating AI into healthcare. Careful consideration is required to address issues related to data privacy, consent, bias, and algorithmic fairness, ensuring the responsible and fair use of AI technologies. Furthermore, concerns about potential job loss in the pharmaceutical research sector due to increasing AI automation need attention. However, many experts suggest that AI should augment human expertise rather than replace it. Cross-disciplinary approaches combining biology, chemistry, computer science and data analytics expertise will be essential in realizing the full potential of AI. Additionally, continued investment in infrastructure, talent development and regulatory frameworks will support the widespread adoption of AI technologies in healthcare.

Unveiling the Nano Frontier: The Crucial Role of AI in Material Science and Surface Innovations

The integration of AI technologies in material Science, Nanotechnology, Surface Coatings and Thin films has brought about revolutionary shift in research and development processes. This fusion has lead to significant advancements, presenting unparalleled opportunities for innovation across diverse industries. AI plays a pivotal role in accelerating the discovery of novel materials, enabling precise control over material synthesis. Facilitating multiscale modelling for deeper understanding, and automating experimentation to enhance research productivity and reduce costs33–37.

In material Science, Nanotechnology, Surface Coatings and Thin films, AI- driven predictive modelling, optimization algorithms, pattern recognition, virtual screening, and interdisciplinary collaboration offer numerous opportunities. These technologies empower researchers to forecast material properties with tailored properties and functionalities, streamline synthesis workflows, uncover hidden patterns in complex datasets, evaluate candidate materials in silico, and foster collaboration between experts from various disciplines. However, the integration of AI in these fields also presents several challenges, including issues related to data quality and quantity, interpretability of complex AI models, transferability to new materials, ethical considerations, and technical complexities in integration33–40.

Harmonising Nature: Role of AI in Environmental, Green, and Food Chemistry Advancements

AI technologies offer significant benefits to Environmental Science, Green Chemistry and Food Chemistry by revolutionizing data analysis, process optimization and sustainability efforts. In environmental science, AI facilitates ecosystem monitoring, natural disaster prediction, and climate change assessment by analysing vast datasets including satellite imagery and sensor data, empowering proactive conservation and resource

management strategies. Green chemistry benefits from AI driven models that expediate the discovery of sustainable materials and catalysts, reducing reliance on hazardous materials and promoting safer manufacturing practices. Similarly, AI optimizes agricultural practices in food chemistry by analysing factors such as soil conditions and weather conditions to increase yields sustainably while ensuring food safety through rapid detection of contaminants and spoilage1,41–43. However, addressing ethical, organisational, and educational challenges is crucial to harnessing the full potential of AI in these domains and ensuring responsible deployment for the benefit of society and the environment44.

Powering Progress: The Impact of AI on Electrochemistry and Energy Management

In the realm of electrochemistry and energy storage and conservation, AI technologies have emerged as transformative tools offering substantial benefits alongside notable challenges. Electrochemistry, central to technologies like batteries and fuel cells, stands to benefit from optimization capabilities of AI, driving advancements in energy storage and conservation.

Leveraging AI, researchers can refine processes, predict behaviours, and innovate within these energy domains41,45–50.

Enhanced efficiency is achieved through AI-driven optimization of device design and operation, resulting in improved performance and longevity. Accelerated discovery is facilitated by AI's ability to analyse vast datasets, unveiling patterns and materials that may elude human observation. Real time monitoring and control enabled by AI-powered sensors and systems, ensure proactive maintenance and optimization, enhancing both performance and safety. Furthermore, AI tailors' solutions to specific needs, such as designing optimized battery packs for electric vehicles, promoting resource efficiency and application suitability. Yet, overcoming challenges related to data, interpretability, computational complexity integration and ethics is imperative to fully realize the transformative potential of AI in these critical domains33,40,47,48,50–52.

Unlocking Forensic Mysteries: The Role of AI in Chemical Investigation

Forensic chemistry, the intersection of chemistry and law enforcement, has significantly benefited from the integration of AI technologies, offering enhanced capabilities in evidence analysis, crime scene investigation, and solving complex cases53.

AI algorithms can analyse complex spectral data, such as infrared and mass spectra, to identify substances present in forensic samples. By comparing patterns against vast databases, AI systems can rapidly determine the composition of unknown substances, aiding in the identification of drugs, explosives, and other illicit materials.

AI enables automated recognition of various patterns in forensic evidence, such as fingerprints, shoeprints, and handwriting. Deep learning algorithms excel at identifying subtle patterns and similarities, enhancing the accuracy and speed of evidence analysis.

AI assists forensic chemists in analysing toxicological data by predicting the effects of different substances on the human body and determining the concentration in biological samples. Machine Learning models can correlate toxicological findings with the cause of death, aiding in homicide investigations.

AI techniques are instrumental in processing and analysing vast amounts of digital evidence, including multimedia files, emails, and network logs. Natural language processing (NLP) algorithms extract relevant information from text- based facts, while image recognition algorithms can identify manipulated or forged images, crucial in cybercrime investigations.

AI-powered software systems facilitate case management by organizing and prioritizing evidence, generating investigative leads, and providing decision support to forensic chemists and law enforcement agencies. These systems improve workflow efficiency and assist in resource allocation for complex investigations.

Advancement in Polymer Chemistry harnessing the power of AI Intelligence

AI technology have significantly impacted polymer chemistry offering innovative solutions across various stages of polymer research development and manufacturing processes. One important application lies in the design and optimization of polymer structures for specific properties. Machine learning algorithms can analyse vast databases of polymer structures and properties to identify correlations, facilitating the discovery of novel

materials with tailored characteristics. Deep learning techniques were employed to predict the glass transition temperatures of polymers based on their molecular structures, enabling the rapid screening of potential candidates48,54.

Another crucial aspect is the optimization of polymer synthesis processes. AI driven approaches can optimise reaction conditions, catalyst selection, and polymerization kinetics to enhance efficiency and yield. Researchers at IBM add a MIT has demonstrated the use of AI for automated planning and optimization of chemical syntheses, including polymerization, leading to reduced experimental time and resource consumption.

Moreover, AI contributes to quality control and characterization of polymers. Machine learning algorithms can analyse spectroscopic, chromatographic, and microscopic data to detect defects, impurities, or variations in polymer properties, ensuring product consistency and reliability. A notable example is the application of convolutional neural networks (CNNs) for automated defect detection in polymer films.

Furthermore, AI technologies facilitate the prediction of polymer properties and behaviour under different environmental conditions or processing methods. This aids in the development of predictive models for polymer performance in applications such as drug delivery, packaging, and material for 3D printing.

AI-Driven Advancements in Spectroscopy: Transforming Analysis, Interpretation, and Real-Time Applications

AI technology have significantly impacted spectroscopy, revolutionising various aspects of data analysis and interpretation. One notable application lies in spectral data processing, where

AI algorithms enhance signal-to-noise ratios and improve resolution. For instance, machine learning algorithms can efficiently denoise spectra, allowing for obvious identification of spectral features. Additionally, AI-based method enables automated baseline correction, peak detection, and spectral alignment, streamlining data preprocessing tasks55–57.

Furthermore, AI facilitates spectral interpretation by offering advanced pattern recognition capabilities. Deep learning models such as CNNs and recurrent neural networks (RNNs), excel in recognising complex spectral patterns and identifying subtle spectral signatures associated with specific compound or molecular structures. These models learn from large spectral databases, enabling accurate classification and quantification of analyte in complex mixtures.

Another significant application of AI in spectroscopy is spectrum prediction and modelling. By training on spectral libraries and chemical databases, AI models can predict spectra of unknown compounds or simulate spectra under various experimental conditions. This capability aids in elucidating molecular structures, predicting chemical properties, and optimising experimental parameters.

Moreover, AI-driven spectroscopy enabled real-time analysis and feedback in various fields, including environmental monitoring, pharmaceutical analysis, and material science. Miniaturised spectrometers equipped with AI algorithms offer portable, rapid, and cost- effective solutions for on-site measurement. These devices find application in quality control, process monitoring, and field analysis facilitating decision-making in diverse industries.

Advancement in Analytical Chemistry: Harnessing AI for Precision and Efficiency

Analytical chemistry plays a pivotal role in various industries, ensuring the quality, safety, and efficacy of products through precise measurements and analyses. With the advent of artificial intelligence, the field has witnessed a transformative shift, revolutionised conventional methodologies and enhancing technical capabilities1,3,56,58.

AI technologies such as machine learning and deep learning have found wide-ranging applications in analytical chemistry, facilitating data analysis, pattern recognition and decision- making process. One notable area is spectroscopy, where AI algorithms can interpret complex spectra data with unprecedented accuracy and speed. Additionally, AI-driven chromatographic technique optimises separation processes, improving sensitivity and resolution in compound identification.

Moreover, AI powered chemometrics models enable predictive analytics in chemical sensing, facilitating rapid and reliable detection of contaminants or analytes in diverse matrices. These models not only enhance analytical precision but also streamline workflow efficiencies, reducing time and resource consumption.

Furthermore, AI-driven robotic systems automate sample preparation and handling tasks, minimising human error, and increasing throughput in analytical workflows. Integration of AI with analytical instruments also enabled real-time monitoring and adaptive control, ensuring process stability and product consistency. Thus, from spectroscopy to chromatography and chemical sensing, AI-driven solutions offer unprecedented capabilities, empowering researchers, and industries to tackle complex analytical challenges with and parallel accuracy and speed.

AI at the Frontier: Revolutionising Space Chemistry for Exploration and Discovery

Space chemistry is an emerging field that seeks to understand the chemical processes occurring beyond earth's atmosphere. With the advent of AI technologies, new avenues have opened for enhancing our understanding of space chemistry59.

AI algorithms aid in the analysis of spectra obtained from celestial bodies, enabling the identification of chemical compounds present in planetary atmospheres and interstellar environments. AI driven simulations facilitate the modelling of complex chemical reactions occurring in space, offering insights into the formation of molecules, such as amino acids and organic compounds, crucial for understanding the origins of life.

AI algorithms sift through vast the datasets collected from space missions, extracting patterns and correlations to unravel the chemical composition of cosmic dust, comets, and asteroid. AI- powered robotic systems autonomously conduct experiments aboard spacecraft, enabling real- time analysis of chemical processes in microgravity environment.

Applications of Artificial Intelligence in Chemistry Education

Chemistry education plays a pivotal role in nurturing the next generation of scientists and professionals. With the rapid advancements in technology, integrating artificial intelligence into chemistry education has emerged as a promising approach to enhance teaching and learning processes. Intelligent Tutoring System (ITS) leverage AI algorithms to provide a personalized and adaptive learning experiences in chemistry education. By analysing learning patterns of students and performance data, ITS can offer tailored instruction, remediation, and feedback catering to individual learning needs. For instance, platforms like Chem101 and ALEKS Chemistry utilise AI-driven algorithms to deliver customized learning pathways and adaptive assessments, thereby optimising learning outcomes4,21,60–6263.

AI powered virtual laboratories simulate real-world chemical experiments, allowing students to explore and manipulate various chemical phenomenon in a safe and controlled environment. These virtual labs offer immersive gaining experiences, enabling students to conduct experiments, analyse results, and gain practical skills without the need for physical equipment. Platforms such as ChemCollective and Virtual ChemLab utilize AI algorithms to simulate chemical reactions, molecular interactions, and spectroscopic analyses, fostering hands-on learning experiences.

AI technique including machine learning and data mining, facilitate the analyses of vast chemical datasets and the prediction of molecular properties and behaviours. By leveraging AI algorithms, researchers can uncover hidden patterns, correlations, and trends in chemical data, aiding in drug discovery, material design, and environmental analysis. Tools such as Cheminformatics and ChemPreditor use machine learning models to predict chemical properties, toxicity, and reactivity empowering educators and researchers with valuable insights. Table 1 represents some of the important and common open access AI Tools for Chemical Education.

Table 1: Open access AI Tools for Chemical Education

Sl. No	Name	Description	Website
1	**ChemCollective**	Provides virtual labs, scenario-based learning activities, tutorials, and concept tests for teaching and learning chemistry	http://chemcollective.org/
2	**Chem101**	Provides personalized learning pathways, adaptive assessments, and interactive content for chemistry education.	https://www.chem101.com/

3	**ALEKS Chemistry**	Utilizes AI algorithms to deliver adaptive and personalized instruction, assessment, and remediation for chemistry students.	https://www.aleks.com/chemistry
4	**Virtual ChemLab**	Offers AI-powered simulations of chemical experiments, allowing students to conduct laboratory activities in a virtual environment.	https://www.chemcollective.org/
5	**Molecular Workbench**	Provides interactive simulations and visualizations of molecular phenomena, facilitating hands-on learning in chemistry education.	https://mw.concord.org/modeler/
6	**ChemReaX**	Offers AI-driven simulations of chemical reactions, equilibrium, and kinetics, enabling students to explore and analyze chemical phenomena.	https://chemapps.stolaf.edu/jmol/jmol.php?model=chemr eaX
7	**Jupyter Notebook**	Used for interactive computing, data visualization, and collaborative work, widely used in chemical education for coding and data analysis tasks	https://jupyter.org/
8	**RDKit**	Used for cheminformatics and molecular modeling, providing algorithms and tools for molecular descriptor calculation, compound screening, and drug discovery.	https://www.rdkit.org/
9	**Cheminformatics Toolkit (ChemTK)**	Offers a collection of open-source tools and libraries for cheminformatics research, including molecule visualization, structure searching, and property prediction.	https://sourceforge.net/projects/chemtk/
10	**Open Babel**	Facilitates molecular structure conversion, format interconversion, and chemical data analysis for educational and research purposes.	http://openbabel.org/
11	**Avogadro**	Used as an open-source molecular editor and visualization software, allowing students and researchers to build and manipulate molecular models for educational and research purposes	https://avogadro.cc/
12	**ChemSpider**	Provides access to millions of chemical structures, properties, and spectra, facilitating chemical research and education.	http://www.chemspider.com/
13	**ChemEdX Data**	Offers open-access datasets for chemistry education research, providing valuable resources for data-driven analysis and experimentation	https://www.chemedx.org/data
14	**PubChem**	Maintained by the National Center for Biotechnology Information (NCBI), offering information on chemical compounds, substances, and bioassays for educational and research purposes.	https://pubchem.ncbi.nlm.nih.gov/

15	**ChemVantage**	Provides interactive tutorials, quizzes, and resources for learning chemistry concepts, offering engaging and accessible educational materials for students and educators.	https://chemvantage.org/

Challenges and Ethical Considerations

Despite its transformative potential, the integration of AI into chemistry processes several challenges and ethical consideration that must be addressed. One concern is the reliance on biased or incomplete datasets, which can lead to erroneous predictions and reinforce existing disparities in scientific research. Moreover, interpretability and the transparency of a model in chemistry raise questions about accountability, reproducibility and the ethical implication of automated decision making64–66.

Additionally, there are concerns about data privacy, intellectual property rights, and the potential misuse of AI driven technologies for wicked purposes such as chemical warfare or bioterrorism. As AI continues to permeate every aspect of chemical research, it is imperative to establish robust regulatory frameworks, ethical guidelines, and standard for data sharing, algorithm validation, and responsible conduct of research.

Future directions

Anticipating, the integration of AI chemistry envisioning to reshape the research landscape and catalyze scientific advancement across various disciplines. One promising avenue is the development of autonomous laboratories equipped with robotic systems and AI-driven platforms for high throughput experimentation and data analysis. The automated workflows can accelerate the pace of discovery while conducting iterative experiments, analysing result in real-time, and iteratively optimising reaction conditions.

The synergy between AI and quantum chemistry holds immense potential for modelling complex molecular system and predicting their behaviour with unprecedented accuracy. Quantum machine learning algorithms can leverage quantum computing capabilities to solve computationally intractable problems in chemical simulation, molecular dynamics, and materials design. This convergence of AI and quantum chemistry could revolutionize our understanding of molecular interaction and pave the way for the discovery of novel materials and therapeutics.

AI powered platform for collaborative research and knowledge sharing are poised to enhance interdisciplinary collaboration and accelerate scientific innovation. By leveraging cloud-based infrastructure and data sharing protocols, researchers can collaborate on large-scale projects, access shared resources, and integrate diverse datasets to address complex scientific challenges. This collaborative approach to research can foster creativity, accelerate discovery, and catalyst breakthroughs in chemistry and beyond.

Conclusion

In conclusion the integration of artificial intelligence into chemistry has revolutionized research methodologies, accelerated scientific discovery, and transformed the various subfields such as drug discovery, materials science and chemical synthesis. From predicting molecular properties to optimising reaction conditions, AI-driven approaches have demonstrated immense potential to reshape the future of chemistry. However, realising the full benefits of AI in chemistry requires addressing challenges related to data quality, algorithm transparency and ethical considerations. Buy fostering interdisciplinary collaboration and embracing responsible innovation, we can harness the power of AI to address pressing challengers in chemistry and unlock new opportunities for scientific exploration and technological advancement.

References

1. Baum, Z. J. et al. Artificial Intelligence in Chemistry: Current Trends and Future Directions. J. Chem. Inf. Model. 61, 3197–3212 (2021).
2. Gray, N. A. B. Artificial intelligence in chemistry. Anal. Chim. Acta 210, 9–32 (1988).

3. Gasteiger, J. Chemistry in Times of Artificial Intelligence. ChemPhysChem 21, 2233– 2242 (2020).
4. Ma, J., Sheridan, R. P., Liaw, A., Dahl, G. E. & Svetnik, V. Deep neural nets as a method for quantitative structure-activity relationships. J. Chem. Inf. Model. 55, 263– 274 (2015).
5. Wei, J. N., Duvenaud, D. & Aspuru-Guzik, A. Neural networks for the prediction of organic chemistry reactions. ACS Cent. Sci. 2, 725–732 (2016).
6. Nielsen, A. A. K. & Voigt, C. A. Deep learning to predict the lab-of-origin of engineered DNA. Nat. Commun. 9, (2018).
7. Jumper, J. et al. Highly accurate protein structure prediction with AlphaFold. Nature 596, 583–589 (2021).
8. Ramsundar, B. et al. Massively Multitask Networks for Drug Discovery. (2015).
9. Kourou, K., Exarchos, T. P., Exarchos, K. P., Karamouzis, M. V. & Fotiadis, D. I. Machine learning applications in cancer prognosis and prediction. Comput. Struct. Biotechnol. J. 13, 8–17 (2015).
10. Yann Lecun, Yoshua Bengio, G. H. Deep learning. Nature 521, 436–444 (2015).
11. Brown, N. et al. Artificial intelligence in chemistry and drug design. J. Comput. Aided. Mol. Des. 34, 709–715 (2020).
12. Sabe, V. T. et al. Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. Eur. J. Med. Chem. 224, 113705 (2021).
13. Graham L.Patrick. An introduction to medicinal chemistry. (2009).
14. Neves, B. J. et al. QSAR-Based Virtual Screening : Advances and Applications in Drug Discovery. 9, 1–7 (2018).
15. Li, H., Zheng, M., Luo, X. & Zhu, W. in Drug Discovery and Development. 1–9 (2008) doi:10.1002/9780470048672.wecb098.
16. Verma, J., Khedkar, V. M. & Coutinho, E. C. 3D-QSAR in Drug Design - A Review. Curr. Top. Med. Chem. 10, 95–115 (2010).
17. Zhang, S., Golbraikh, A., Oloff, S., Kohn, H. & Tropsha, A. Development , Applications , and Virtual Screening of Chemical Databases Using. J.Chem.Inf.Model 46, 1984–1995 (2006).
18. Divya, V., Pushpa, V. L., Sarithamol, S. & Manoj, K. B. Computational approach for generating robust models for discovering novel molecules as Cyclin Dependent Kinase 4 inhibitors. J. Mol. Graph. Model. 82, 48–58 (2018).
19. Pulla, V. K., Sriram, D. S., Viswanadha, S., Sriram, D. & Yogeeswari, P. Energy- Based Pharmacophore and Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) Modeling Combined with Virtual Screening to Identify Novel Small-Molecule Inhibitors of Silent Mating-Type Information Regulation 2 Homologue 1 (SIRT1). Journal of Chemical Information and Modeling vol. 56 (2016).
20. Palacios, J. Computer Aided Design of Drug Delivery Systems.
21. Alexander, I., Tetko, I. V & David, T. of Overfitting. 826–833 (1995).
22. An, Y., Sherman, W. & Dixon, S. L. Kernel-based partial least squares: Application to fingerprint-based QSAR with model visualization. J. Chem. Inf. Model. 53, 2312–2321 (2013).
23. Henrich, S. et al. Computational approaches to identifying and characterizing protein binding sites for ligand design. J. Mol. Recognit. n/a-n/a (2009) doi:10.1002/jmr.984.
24. Walter, R. et al. Shortcomings in the clinical evaluation of new drugs: acute myeloid leukemia as paradigm. Blood 116, 2420–2428 (2010).
25. Tindle, J., Gray, M., Warrender, R. L., Ginty, K. & Dawson, P. Application Framework for Computational Chemistry (AFCC) Applied to New Drug Discovery. Int. J. Grid High Perform. Comput. 4, 46–62 (2012).
26. Trotter, M. Support Vector Machines for QSAR Analysis. Computer (Long. Beach. Calif).
27. Grinter, S. Z. & Zou, X. Challenges, applications, and recent advances of protein- ligand docking in structure-based drug design. Molecules 19, 10150–10176 (2014).
28. Wu, J. & Jiang, R. Prediction of deleterious nonsynonymous single-nucleotide polymorphism for human diseases. Sci. World J. 2013, (2013).
29. Yue, P. & Moult, J. Identification and analysis of deleterious human SNPs. J. Mol. Biol. 356, 1263–1274 (2006).

30. Sahigara, F. Defining the Applicability Domain of QSAR models : An overview. Mol. Descriptors - Free online Resour. Tutorial 7, 1–6 (2007).
31. Achutha AS, Pushpa VL, S. S. Theoretical insights into the anti-SARS-CoV-2 activity of chloroquine and its analogs and in silico screening of main protease inhibitors. J.
Proteome Res. 19, 4706–17 (2020).
32. Stetson, L. C., Pearl, T., Chen, Y. & Barnholtz-Sloan, J. S. Computational identification of multi-omic correlates of anticancer therapeutic response. BMC Genomics 15, S2 (2014).
33. Zhao, X. G. et al. JAMIP: an artificial-intelligence aided data-driven infrastructure for
computational materials informatics. Sci. Bull. 66, 1973–1985 (2021).
34. Xie, T. & Grossman, J. C. Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties. Phys. Rev. Lett. 120, (2018).
35. Ulissi, Z. W., Singh, A. R., Tsai, C. & Nørskov, J. K. Automated Discovery and Construction of Surface Phase Diagrams Using Machine Learning. J. Phys. Chem. Lett. 7, 3931–3935 (2016).
36. Raccuglia, P. et al. Machine-learning-assisted materials discovery using failed experiments. Nature 533, 73–76 (2016).
37. Han, C., Ma, T., Huyan, J., Huang, X. & Zhang, Y. CrackW-Net: A Novel Pavement Crack Image Segmentation Convolutional Neural Network. IEEE Trans. Intell. Transp. Syst. 23, 22135–22144 (2022).
38. Yamada Y, Gohda S, Abe K, Togo T, Shimano N, Sasaki T, Tanaka H, Ono H, Ohba T, Kubo S, O. T. Carbon materials with controlled edge structures. Carbon N. Y. 122, 694–701 (2017).
39. Sanchez-Lengeling, B. & Aspuru-Guzik, A. Inverse molecular design using machine learning:Generative models for matter engineering. Science (80-.). 361, 360–365 (2018).
40. Shen, L., Zhou, J., Yang, T., Yang, M. & Feng, Y. P. High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications. Accounts Mater. Res. (2021) doi:10.1021/accountsmr.1c00246.
41. Kamkar, M. et al. Artificial Intelligence (AI) for Sustainable Resource Management and Chemical Processes. ACS Sustain. Chem. Eng. 12, 2924–2926 (2024).
42. Green, C. P., Engkvist, O. & Pairaudeau, G. The convergence of artificial intelligence and chemistry for improved drug discovery. Future Med. Chem. 10, 2573–2576 (2018).
43. Bystrzanowska, M. & Tobiszewski, M. Chemometrics for selection, prediction, and classification of sustainable solutions for green chemistry—a review. Symmetry (Basel). 12, 1–21 (2020).
44. Danezis, G. P., Tsagkaris, A. S., Camin, F., Brusic, V. & Georgiou, C. A. Food authentication: Techniques, trends & emerging approaches. TrAC - Trends Anal. Chem. 85, 123–132 (2016).
45. Stanev, V., Choudhary, K., Kusne, A. G., Paglione, J. & Takeuchi, I. Artificial intelligence for search and discovery of quantum materials. Commun. Mater. 2, 1–11 (2021).
46. Serhan, M. et al. Total iron measurement in human serum with a smartphone. AIChE Annu. Meet. Conf. Proc. 2019-Novem, (2019).
47. Mosavi, A. & Bahmani, A. Energy consumption prediction using m[1] A. Mosavi and
A. Bahmani, "Energy consumption prediction using machine learning; a review," Energies, no. March, pp. 1–63, 2019. Energies 1–63 (2019) doi:10.20944/preprints201903.0131.v1.
48. Goodenough, J. B. & Park, K. S. The Li-ion rechargeable battery: A perspective. J. Am. Chem. Soc. 135, 1167–1176 (2013).
49. Hautier, G., Fischer, C., Ehrlacher, V., Jain, A. & Ceder, G. Data mined ionic substitutions for the discovery of new compounds. Inorg. Chem. 50, 656–663 (2011).
50. Zhang, L. & Zhao, X. S. Carbon-based materials as supercapacitor electrodes. Chem. Soc. Rev. 38, 2520–2531 (2009).
51. Chmiola, J. et al. Anomalous increase in carbon capacitance at pore sizes less than 1 nanometer RID B-2167-2008. Science (80-.). 313, 1760–1763 (2006).
52. Rossener Regonia, P. & Pelicano, C. M. Understanding the Performance of (Ni−Fe−Co−Ce)Ox-based Water Oxidation Catalysts via Explainable Artificial Intelligence Framework. ChemElectroChem 202300647, 1–12 (2024).
53. Mohsin, K. Artificial Intelligence in Forensic Science. Int. J. Forensic Res. 4, 172–173 (2023).
54. Mannodi-Kanakkithodi, A., Pilania, G., Huan, T. D., Lookman, T. & Ramprasad, R. Machine Learning

Strategy for Accelerated Design of Polymer Dielectrics. Sci. Rep. 6, 1–10 (2016).
55. Galán-Freyle, N. J. et al. Artificial intelligence assisted mid-infrared laser spectroscopy in situ detection of petroleum in soils. Appl. Sci. 10, (2020).
56. Pan, L., Zhang, P., Daengngam, C., Peng, S. & Chongcheawchamnan, M. A review of artificial intelligence methods combined with Raman spectroscopy to identify the composition of substances. J. Raman Spectrosc. 53, 6–19 (2022).
57. Kothari, R. et al. Raman spectroscopy and artificial intelligence to predict the Bayesian probability of breast cancer. Sci. Rep. 11, 1–17 (2021).
58. Dar, Ayaz Mahmood, S. M. Analytical & Bioanalytical Techniques Molecular Docking : Approaches , Types , Applications and Basic Challenges. J. Anal. Bioanal. Tech. 8, 8–10 (2017).
59. Coley, C. W. et al. A robotic platform for flow synthesis of organic compounds informed by AI planning. Science (80-.). 365, (2019).
60. Vladimir Jakus. ARTIFICIAL INTELLIGENCE IN CHEMISTRY. Chem. Commun. 57, 2413–2451 (1992).
61. Schwaller, P., Gaudin, T., Lányi, D., Bekas, C. & Laino, T. 'Found in Translation': predicting outcomes of complex organic chemistry reactions using neural sequence-to- sequence models. Chem. Sci. 9, 6091–6098 (2018).
62. de Almeida, A. F., Moreira, R. & Rodrigues, T. Synthetic organic chemistry driven by artificial intelligence. Nat. Rev. Chem. 3, 589–604 (2019).
63. Baker, R. S., D'Mello, S. K., Rodrigo, M. T. & Graesser, A. C. Better to be frustrated than bored: The incidence and persistence of affect during interactions with three different computer-based learning environments. Int. J. Hum. Comput. Stud. 68 (4), 223–241 (2010).
64. Amodei, D. et al. Concrete Problems in AI Safety. 1–29 (2016).
65. O'Hagan, A. et al. Uncertain judgements: Eliciting experts' probabilities. Uncertain Judgements Eliciting Expert. Probab. 1–321 (2006) doi:10.1002/0470033312.
66. Jin, W., Barzilay, R. & Jaakkola, T. Chapter 11: Junction Tree Variational Autoencoder for Molecular Graph Generation. RSC Drug Discov. Ser. 2021-Janua, 228–249 (2021).