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AI Deployment in Chemistry: Bibliometric and Topic Analysis of Top-Cited Papers (2015–2025)

Andrea Usenik,[1] Ernest Meštrović,[2] Mirjana Pejić Bach[3,*]

[1] Department of Chemistry, University of Zagreb Faculty of Science, 10000 Zagreb, Croatia
[2] University of Zagreb Faculty of Chemical Engineering and Technology, 10000 Zagreb, Croatia
[3] University of Zagreb, Faculty of Economics & Business, 10000 Zagreb, Croatia
* Corresponding author's e-mail address: mpejic@net.efzg.hr

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Abstract: Over the past decade, artificial intelligence (AI) has moved from a promising novelty to a pervasive discovery engine across the chemical sciences. The goal of this paper is to provide a data-driven overview of how AI is reshaping chemical research and where the next breakthroughs are likely to emerge, using bibliometric and topic analysis. To gain insight into this transformation, the 224 most–cited papers on artificial intelligence (AI) indexed in the Web of Science Core Collection between 2015 and 2024 in the field of chemistry research were analyzed. After extracting complete bibliographic metadata, abstracts, keywords, and references, a two-phase study was conducted: (i) descriptive bibliometrics to profile publication growth, document types, venues, countries, institutions, and funding sources; and (ii) VOSviewer-based text-mining to build co-occurrence networks of keywords and countries, revealing thematic and geographic research fronts. Results show an almost exponential rise in highly cited output, from five papers in 2015 to 184 in 2023, driven primarily by China and the United States. Keyword clustering highlights seven dominant application arenas: (1) electronic-skin sensors and functional nanomaterials, (2) cheminformatics and computer-aided synthesis, (3) sustainable processes and Industry 4.0, (4) deep-learning-enabled drug discovery, (5) neuromorphic devices, (6) energy harvesting and storage, and (7) AI-assisted healthcare and delivery systems. Institutional mapping confirms the Chinese Academy of Sciences as the leading contributor, while collaboration networks illustrate a growing but still uneven global engagement.

Keywords: artificial intelligence, AI, chemistry, chemical sciences, drug discovery, machine learning, materials, pharmaceutical chemistry, sensors.

INTRODUCTION

ARTIFICIAL intelligence has long promised to accelerate the labour-intensive stages of chemical research: hypothesis generation, molecular design, reaction optimisation, and data interpretation. Early prototypes, from expert systems in the 1980s to neural-network property predictors in the 2000s, foreshadowed a more automated future but were limited by data scarcity and computing power. The confluence of three recent developments has changed that landscape dramatically: (*i*) the availability of large, curated chemical and materials datasets; (*ii*) the maturation of deep-learning architectures capable of capturing complex structure–property relationships; and (*iii*) affordable high-performance computing, including GPUs (graphical processing units) and cloud resources. These advances have propelled AI from isolated proofs of concept to mainstream practice in catalysis design,[1,2] polymer discovery,[3] process control,[4,5] analytical spectroscopy,[6–8] and drug development.[9]

Despite notable successes of AI in the last decade, its increasing popularity in all aspects of life, AI in chemistry heavily depends on data quality and solid chemical reasoning. In the case of incomplete datasets, high-yield examples are being highlighted, while those that gave poorer yields or have failed are omitted. To avoid learning from coincidences rather than chemical principles, integrating core principles like stoichiometry and thermodynamics into the algorithm helps omit chemical impossibilities. In order to deploy practical solutions, thorough documentation of each step of the process, starting from data cleaning to managing computational costs, should be provided.

However, chemists are still involved as the “final check” and will surely be until the models and their implementation in chemistry-related fields mature.

Capturing the full scope of the rapidly expanding field of AI in chemistry is challenging. Comprehensive databases such as Chemical Abstracts Services’ (CAS) SciFinder, Scopus, PubMed, and Google Scholar offer wide coverage. However, the Web of Science Core Collection (WoS CC) remains the gold standard for longitudinal bibliometric work in various sciences, therefore also in chemistry.[10,11] Focusing on highly cited papers adds a further lens: citation theory posits that such works delineate “research fronts” that shape subsequent discourse,[12] while empirical studies show that field-normalised top-percentile articles are robust indicators of scientific excellence.[13] Accordingly, this study targets the most-cited WoS (Web of Science) records on AI in chemistry published between 2015 and 2024, a period that encompasses the rise of deep learning and generative models.

The objectives of this study are twofold. First, we quantify growth dynamics, publication venues, and geographic distribution to identify where AI-driven research in chemistry and chemical sciences is gaining the most traction and map collaborative networks of countries and institutions to reveal centres of expertise and partnership patterns. Second, we deploy text-mining techniques to distil the thematic clusters that define current research fronts and future opportunities. By triangulating bibliometric statistics with semantic network analysis, we provide a multidimensional overview that summarizes past progress and pinpoints emerging directions. The remainder of the paper proceeds as follows: The Methodology section details the data collection and analytical workflow; he bibliometric results, keyword and country co-occurrence networks are discussed in the Results section, followed by Conclusions with implications for researchers, funding agencies, and policymakers aiming to harness AI for chemical innovation.

METHODOLOGY

Data and Study Design

The Web of Science Core Collection (WoS CC), comprising the SCI-EXPANDED (Science Citation Index Expanded) and ESCI (Emerging Sources Citation Index) collections, has been utilized as the primary source for recent research on the deployment of artificial intelligence in chemistry.

For bibliometric mapping of AI applications in chemistry, this study relies on the WoS CC because its strict journal-selection criteria and comparatively accurate citation links make it the most dependable dataset for the chemical sciences.[10,12] Analysing the most-cited papers then allows us to isolate the research fronts that drive disciplinary progress, a principle first articulated in the seminal work on citation indexing,[12] and later confirmed by evidence that top-percentile articles offer a field-normalised, robust indicator of scientific excellence.[13]

The following search strategy has been applied (Table 1). Firstly, the primary search was conducted in WoS, using the keywords “artificial intelligence” or “AI” under the topic of Chemistry, defined as a Web of Science Category, which resulted in 17.382 research papers covering the period from 2015 to 2024. Secondly, the search was refined using Highly Cited Papers, resulting in 224 papers (listed in the Supporting Information). The research focuses solely on English-language peer-reviewed literature, and the obtained results have been manually refined to exclude any unrelated papers.

The resultant 224–paper dataset provides a reliable source from which the most trending research fronts can be identified with certainty. The next chapter clarifies the research approach, building on the bibliometric analysis and theme clusters.

Analysis

The analysis is conducted in two phases, using data extracted from WoS CC for each paper, including bibliometric data, abstract, keywords, and references.

Firstly, a bibliometric analysis was conducted, focusing on the research area, document type, type of open access, journal, and conferences for the paper’s publication. Furthermore, the most frequent countries, funding agencies, authors, and institutions are also examined.

Secondly, this data has been used as input for the text mining analysis using the VOSviewer tool.[14] Two advanced functions of VOSviewer are used. First, VOSviewer’s text mining functionality is deployed to construct co-occurrence networks of terms extracted from English-language textual data, such as keywords (both those provided by authors and those assigned). This process utilizes the Apache OpenNLP library, an open-source Java library for processing Natural Language text.[15] Tokenisation, sentence segmentation, part-of-speech tagging, named entity extraction, chunking, parsing, and co-reference resolution are some of the services OpenNLP provides.

VOSviewer envisions bibliometric linkage using a distance-based principle, with the ability to visualize various types of items in a network, such as those based on keywords, authors, or countries. Items are grouped in nodes, and the distance between nodes is normalized.[16] Nodes are located in a two-dimensional space following the principle that strongly related nodes are located close to each other, using the VOS mapping technique. Finally, nodes are allocated to clusters using the smart local moving algorithm.[17,18]

Table 1. Web of Science search strategy

Database	Search term	Years	# of papers
Web of Science Core Collection (SCI-EXPANDED + ESCI)	"artificial intelligence" or AI (Topic) and Chemistry (Web of Science Categories)	1955–2024	17.382
	"artificial intelligence" or AI (Topic) and Chemistry (Web of Science Categories) and Highly Cited Papers	2015–2024	232
	Expert content analysis of papers	2015–2024	224

Source: Authors' work (2025).

This methodology enables co-occurrence analysis to identify the most extensively studied themes and research groups concerning AI deployment in chemistry. To achieve this objective, the analysis focused on the co-occurrence of terms and nations, employing the full-counting extraction approach.

A total of 1.900 keywords were extracted from the titles, abstracts, and keywords of publications in WoS, encompassing both Author Keywords and Keywords Plus. The analysis employed a threshold of three keyword occurrences. This approach yielded 110 keywords employed in the text mining analysis.

The analysed publications had authors from 58 nations. The study employed a threshold of three nations, which resulted in the extraction of the 31 nations used in the co-occurrence study.

With this refined dataset in place, the Results chapter presents the results of the bibliometric analysis, along with key themes and patterns emerging from AI-driven chemistry research.

RESULTS

Bibliometric Analysis

From the analysis of papers published over the last decade, as presented in Figure 1, it can be observed that the number of highly cited research papers on the topic of AI in chemistry has shown a steady increase in the past decade. With only five highly cited papers published in 2015 and a relatively low increase in the number of such papers in the two years to follow, a cumulative growth acceleration can be observed from 2018, reaching 26 papers and 42 in 2019. The 2020–2021 period reflects a stronger expansion, with the total number of papers increasing by 37. This increase continued in subsequent years, surpassing 140 and 184 publications in 2022 and 2023, respectively. By 2024, the cumulative number of publications reached 224, demonstrating nearly exponential growth and highlighting the increasing attention directed toward the implementation of AI tools in chemical sciences. This trend is further expected to increase rapidly in the upcoming years due to the rapid development of new AI tools specifically catered to researchers in various fields of chemistry, as well as the increasing involvement of AI-based modules in existing software and platforms. However, a more significant increase in the number of published papers related to AI and chemistry was anticipated, and the trend shown in Figure 1 indicates that AI is still not used as a "magic wand" as one might think.

The distribution of publication types (Table 2), shows that the field is still dominated by review papers (123 out of 224). Among these, narrative, mini-review, and recent-advances articles (109) are by far the most common, while perspectives/roadmaps/outlooks were significantly less

Table 2. Type of document

Type of document	# of papers	%
Reviews	123	54.9
Article	96	42.9
Article; Proceedings Paper	2	0.9
Review; Early Access	2	0.9
Article; Early Access	1	0.4
Total	224	100

Source: Authors' work (2025).

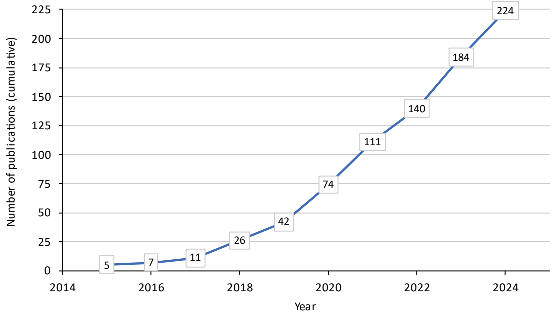

Figure 1. Timeline of publications (cumulative).

Table 3. Journals

Journal(s)	Number of publications	Proportion / %
Advanced Materials	21	9.38
Sensors	15	6.70
ACS Nano, Advanced Science	14	12.50
Advanced Functional Materials, Chemical Reviews	12	10.71
Applied Sciences-Basel	8	3.57
International Journal of Molecular Sciences	7	3.12
Chemical Society Reviews, Nano Energy	6	5.36
Advanced Energy Materials, International Journal of Hydrogen Energy, Journal of Chemical Information and Modeling	5	6.70
Accounts of Chemical Research, Nano Research	4	3.57
ACS Catalysis, Biosensors & Bioelectronics, Chemical Science, Environmental Chemistry Letters, Journal of Chemical Education, Journal of Energy Chemistry, Medicinal Research Reviews, Pharmaceuticals	3	10.71
ACS Sensors, Angewandte Chemie - International Edition, Energy Storage Materials, International Journal of Biological Macromolecules, Journal of Cheminformatics, Journal of The American Chemical Society, Materials Horizons, Molecular Diversity, Molecular Informatics, Nanoscale, Nature Chemistry, Npj Computational Materials, Small, Trac-Trends in Analytical Chemistry, Wiley Interdisciplinary Reviews-Computational Molecular Science	2	13.39
Advances in Colloid and Interface Science, Arabian Journal of Chemistry, Biomacromolecules, Biosensors-Basel, Carbohydrate Polymers, Catalysts, Chemcatchem, Chemistry of Materials, Chemistry-A European Journal, Crystal Growth & Design, Ecomat, Energy & Environmental Science, Food Chemistry, Food Hydrocolloids, Frontiers in Chemistry, Green Energy & Environment, Joule, Journal of Agricultural And Food Chemistry, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Controlled Release, Journal of Materiomics, Journal of Medicinal Chemistry, Journal of Molecular Liquids, Journal of Power Sources, Journal of Separation Science, Micromachines, Molecules, Nanomaterials, Phytochemistry Letters, Plasmonics, Topics in Current Chemistry	1	14.29

Source: Authors' work (2025).

Note: The total number of papers is not displayed in this table, since it depicts the number of papers per journal.

represented (10). Only a very small number of papers were classified as scoping or mapping reviews (1) or as systematic reviews/meta-analyses (3). No bibliometric or meta- bibliometric reviews were identified. Details on the distribution of these types of review papers are presented in Table S1. Overall, this pattern suggests that the field is still in the consolidation and knowledge synthesis phase through broader, narrative reviews, whereas more formal evidence-mapping and quantitatively structured reviews are still quite rare. Additionally, since AI implementation in chemistry-related fields is still in its early stages, it is "easier" to write a (mini-)review article on already published papers than to develop a new way of applying AI tools in research.

Journal distribution of the most cited papers (Table 3) is a clear indicator of the main research fields in which AI is being implemented most thoroughly. Although the papers span peer-reviewed journals covering a broad range of topics, a relatively small set of high-impact journals accounts for the largest share of publications, led by Advanced Materials, Sensors, ACS Nano, and Advanced Science. The presence of multidisciplinary and top-tier journals, such as Nature Chemistry and Angewandte Chemie - International Edition, suggests an increasing interest in and cross-disciplinary relevance of AI-related applications in chemistry among a wider audience. The distribution reflects the current dual nature of the field: while the most visible contributions are clustered in elite, high-impact journals, thereby also increasing their citation counts, the number of papers devoted to AI in the chemical sciences across a wide range of specialized and interdisciplinary journals is also increasing.

While the journals focused on (nano)materials, sensors, and energy dominate the publication landscape, distribution among the publishers is much simpler with clear dominance of journals issued by Wiley and the American Chemical Society (ACS, amounting to 50 % of the 224 papers), whereas MDPI (Multidisciplinary Digital Publishing Institute), Elsevier, Springer / Nature Portfolio, and the Royal Society of Chemistry (RSC) follow.

Countries and Their Co-occurrence

Table 4 reveals a marked geographical imbalance: more than half of the highly cited papers come from China, with 118 papers published, compared to 54 papers from the US.

Table 4. Countries

Countries	# of papers
People's Republic of China	118
United States of America (USA)	54
United Kingdom (UK)	19
Germany	18
South Korea	16
Canada	14
India	13
Australia	12
Singapore	11
Italy, Japan, Sweden	10
Switzerland	9
Spain	6
Iran, Saudi Arabia	5
Czech Republic, Egypt, France, Malaysia	4
Brazil, Denmark, Finland, Greece, Israel, Netherlands, Russia, South Africa, Taiwan, United Arab Emirates	3
Bangladesh, Pakistan, Poland, Turkey, Vietnam	2
Austria, Belgium, Bulgaria, Cyprus, Ecuador, Ghana, Indonesia, Iraq, Ireland, Jordan, Lebanon, Lithuania, Luxembourg, Norway, Portugal, Romania, Slovakia, Thailand, Turkey	1

Source: Authors' work (2025).

Note: The total number of papers is not displayed in this table, since each paper could have more than one author.

Table 5. Cluster countries

Cluster	Countries
1	Australia, Brazil, Denmark, France, Iran, Russia, South Africa, Spain, Sweden
2	England, Finland, Greece, Italy, Netherlands, Singapore, Switzerland
3	Czech Republic, Germany, Israel, People's Republic of China, United States
4	India, Malaysia, Saudi Arabia, South Korea, Taiwan
5	Egypt, Japan, Northern Ireland
6	Canada, United Arab Emirates

Source: Authors' work (2025).

This is followed by a relatively long "tail" of the distribution – the UK, Germany, and South Korea together account for barely a third of China's output – while most other countries contribute with only a few papers. Alongside strong Asian and North American dominance, European countries show scattered but measurable contributions, suggesting a broad but uneven global engagement in AI-enabled chemistry research across Europe.

The analysis of country-level co-authorship provides insights into which nations exert the strongest influence on highly cited research in the application of artificial intelligence to chemistry, and the extent of international collaboration (Figure 2 and Table 5). The People's Republic of China dominates the landscape with 118 publications, followed by the USA with 54 and England and Germany with 19 and 18 publications, respectively. Other notable contributors include South Korea (16), Canada (14), India (13), and Australia (12).

The VOSviewer network visualization highlights China as the central hub in this field, connected with a wide range of countries across Asia, Europe, and North America. The size of its node reflects both the volume of its contributions and the extent of its collaborative activity. The USA also demonstrates a strong international presence, with significant links to both European and Asian countries, reflecting its global leadership in AI-driven chemical research. England and Germany similarly show strong connections, often acting as bridges between European partners and larger hubs such as China and the USA.

The density and thickness of the connecting lines illustrate frequent collaboration between China and countries such as the USA, Singapore, and Germany, while secondary but notable cooperative links can be seen between the USA and Canada, and between European countries such as England, Switzerland, and Italy. The map further indicates the diversification of research networks, with clusters representing regional strengths — for example, collaborations within Asia (China–Singapore–South Korea), within Europe (England–Germany–Sweden), and transatlantic partnerships (USA–Europe).

This distribution highlights that although China and the USA are the most dominant players in terms of output and centrality, the advancement of AI in chemistry is a truly international effort, where emerging collaborations between Asian and European countries continue to expand the global research front.

Institutions and Their Co–occurrence

When analysing the most frequent institutions, the Chinese Academy of Sciences emerges as the most productive organization, with a total of 29 highly cited publications (Table 6). Not surprisingly, several Chinese universities were among the top 10, positioning China at the forefront of global contributions. A smaller group of institutions follows – Northwestern Polytechnical University, Tsinghua University, Georgia Institute of Technology, and University of Chinese Academy of Sciences – with nine publications each. At the same time, the National University of Singapore stands out with seven. The "middle tier" includes universities with six or five papers each, dominated by Chinese

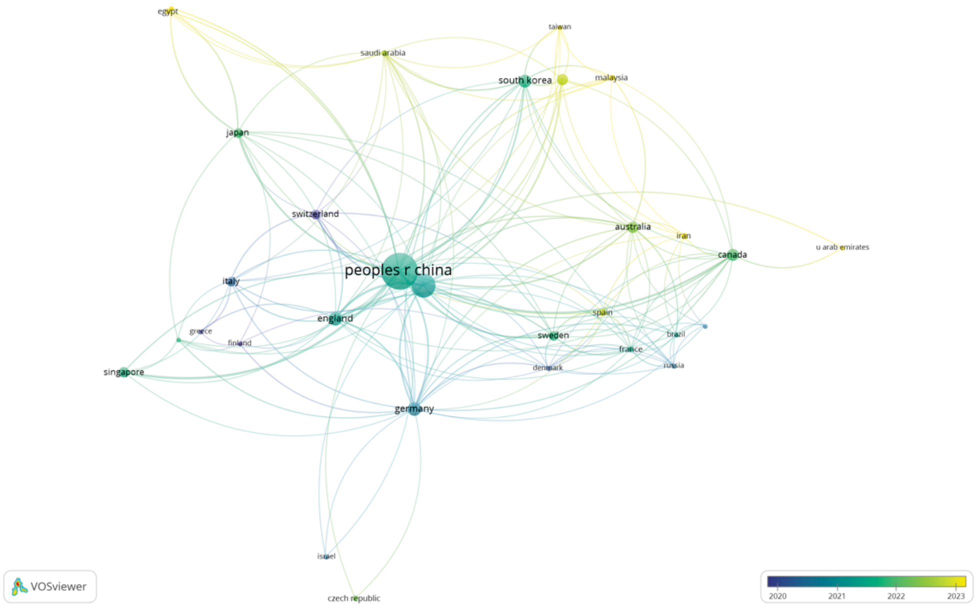

Figure 2. Countries (min. 3 occurrences).

and Asia-Pacific players with some North American presence. The tail of the distribution comprises institutions with three publications, scattered across Europe, the Middle East, and North America, reflecting a broad network of collaboration. In this diverse institutional topography, new research centres are also emerging, which further dynamize the network of cooperation in the field of AI-supported chemistry. From the data presented in Table 6, it is evident that European universities and institutes are underrepresented, with only a few institutions among the top-cited papers in this field.

The institutional network visualized in Figure 3 reveals four clusters of institutional collaboration and co-authorship, each characterized by varying degrees of collaboration intensity and geographic distribution. Due to its largest number of published papers, the largest node in the

Table 6. Institutions

Institution(s)	# of papers per institution
Chinese Academy of Sciences	29
Beijing Institute of Nano-Energy & Nanosystems (CAS)	11
Northwestern Polytechnical University, University of Chinese Academy of Sciences (CAS)	10
Georgia Institute of Technology, Tsinghua University, University System of Georgia	9
National University of Singapore, United States Department of Energy (DOE), University of California System	7
City University of Hong Kong, Guangxi University, Sichuan University	6
Beijing Institute of Technology, Huazhong University of Science & Technology, Shaanxi University of Science & Technology, Southern University of Science & Technology, Stanford University	5
AstraZeneca, Central South University, Donghua University, Egyptian Knowledge Bank (EKB), Hong Kong Polytechnic University, Massachusetts Institute of Technology (MIT), Technical University of Munich, University of Jinan, University of Science & Technology of China (CAS), University of Toronto, Xi'an Jiaotong-Liverpool University, Xi'an Jiaotong University, Zhejiang University	4
A*STAR (Agency for Science Technology & Research), Assiut University, Beihang University, CNRS, Chongqing University, ETH Zurich, Florida Polytechnic University, Islamic Azad University, Kobe University, Max Planck Society, Michigan State University, Monash University, Nanyang Technological University, Ningbo Institute of Materials Technology & Engineering (CAS), Queen's University Belfast, Sejong University, Shanghai University, Shenzhen University, South China University of Technology, Swiss Federal Institutes of Technology (ETH Domain), Technion – Israel Institute of Technology, University of Alberta, University of Bern, University of British Columbia, University of Turin	3

Source: Authors' work (2025).

Note: The total number of papers is not displayed in this table, since it depicts the number of papers per institution. Institutions with 1 or 2 papers published are given in Table S2 in the SI.

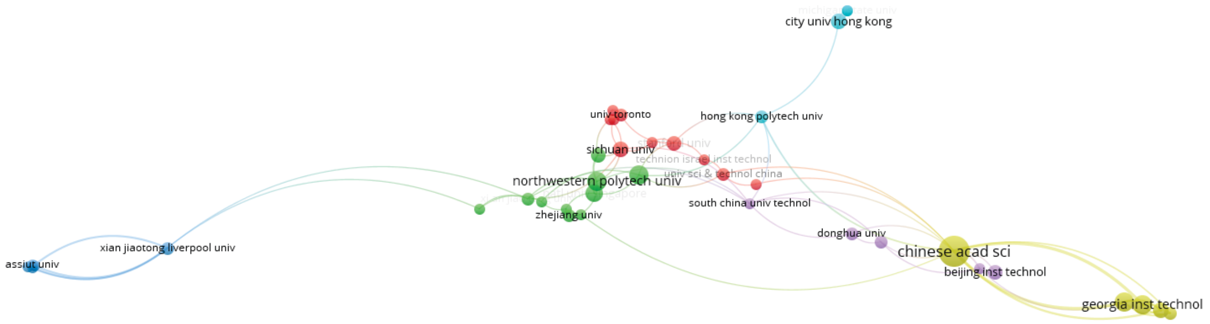

Figure 3. Institutions (min. 3 publications).

network is the Chinese Academy of Sciences (yellow cluster), with strong connections with Beijing Institute of Technology and Georgia Institute of Technology, suggesting a well-established partnership further supported by the thickness of these connection lines, indicating repeated and consistent collaboration. A second cluster (green) centres on Northwestern Polytechnical University, which is tightly connected to other major Chinese universities. This cluster reflects the strong domestic collaborative framework within China, where institutions often pool resources and expertise to advance shared research agendas. Northwestern Polytechnical University further serves as a bridge between multiple sub-networks of universities. Two other clusters (red and blue) point to international collaborations, also mostly populated by Chinese institutions.

Herein described bibliographic data envisages globally connected AI-aided research in chemical sciences, with China and the US leading over half of highly cited papers and dominating collaborations. A complex network spreads over every continent, with regional clusters like those inside Asia and Europe, and trans-Atlantic hubs. Secondary centres such as Singapore, South Korea, England, and Germany link already established countries with the newcomers. Chinese Academy of Sciences and several Chinese universities are far ahead of others in terms of output and collaborations, while North American and European institutions form smaller, strategic clusters. Leadership in AI-driven chemistry is now broader, involving many nations, with key centres driving progress and diverse partners contributing expertise.

Most Cited Papers

An overview of the top 20 most-cited papers is provided in Table 7, which is arranged in order of the number of citations as of May 23, 2025. The variety of subjects demonstrates the significant influence of AI techniques on research in chemistry and materials. Alongside application-focused research that utilizes machine and deep learning for molecular docking, drug development, agriculture, and computational chemistry, there is foundational algorithmic work, such as SchNet's neural network design for atomistic simulations. Smart, energy-conscious materials make up a second distinct subgroup of papers. The list is dominated by textile-integrated sensors, MXene-based composites, triboelectric and piezoelectric nanogenerators, and electronic skin, demonstrating AI's compatibility with wearable and next-generation sensing technologies. Notably, ten of the publications from the past 10 years have already received over 700 citations (eight of which were published less than seven years ago), demonstrating the field's rapid expansion and dissemination of information. Together, these highly cited works show the multifaceted impact that AI now has on the chemical sciences by revealing both methodological advancements (new neural architectures, data-driven modeling frameworks) and revolutionary applications ranging from energy harvesting to flexible electronics to health-focused sensing.

The most cited papers among the 224 included in this study highlight how AI research in chemistry and related sciences has become interdisciplinary, with only a handful of entries (Schütt et al.'s SchNet architecture,[19] Goh et al.'s survey of deep learning in computational chemistry,[20] and Gupta et al.'s review on AI-driven drug discovery[21]) focusing solely on algorithmic development while exceeding 600 citations. This indicates that methodological innovations quickly spread within research areas centred on practical technologies or substances and their advancement. On the other hand, papers dealing with materials innovation and sensor technology clearly dominate the citation count, with two papers (Wu et al.[22] and Dong et al.[23]) exceeding 1000 citations. Although these papers are seemingly unrelated to "core" chemistry, together with the third-most-cited paper (Liakos et al.),[24] which focused on the applications of machine learning in agriculture, these papers outline how the use of AI or machine learning (ML) is often accelerated to a greater extent in chemistry-related sciences due to their direct application in advancing the quality of life. Development of triboelectric nanogenerators depends critically on the physical chemistry of surfaces, polymer-inorganic

Table 7. The most cited papers

Paper	# of citations[a]
C. Wu et al. Triboelectric Nanogenerator: A Foundation of the Energy for the New Era. *Adv. Energy Mater*. **2019**, *9* (1), 1802906. https://doi.org/10.1002/aenm.201802906	1604
K. T. Schütt et al. SchNet – A Deep Learning Architecture for Molecules and Materials. *J. Chem. Phys*. **2018**, *148* (24), 241722. https://doi.org/10.1063/1.5019779	1541
K. Liakos et al. Machine Learning in Agriculture: A Review. *Sensors* **2018**, *18* (8), 2674. https://doi.org/10.3390/s18082674	1448
L. Pinzi et al. Molecular Docking: Shifting Paradigms in Drug Discovery. *Int. J. Mol. Sci*. **2019**, *20* (18), 4331. https://doi.org/10.3390/ijms20184331	1356
D. C. Blakemore et al. Organic Synthesis Provides Opportunities to Transform Drug Discovery. *Nat. Chem.* **2018**, *10* (4), 383–394. https://doi.org/10.1038/s41557-018-0021-z	1118
Y. Zang et al. Advances of Flexible Pressure Sensors toward Artificial Intelligence and Health Care Applications. *Mater. Horiz.* **2015**, *2* (2), 140–156. https://doi.org/10.1039/C4MH00147H	1086
K. Dong et al. Fiber/Fabric-Based Piezoelectric and Triboelectric Nanogenerators for Flexible/Stretchable and Wearable Electronics and Artificial Intelligence. *Adv. Mater*. **2020**, *32* (5), 1902549. https://doi.org/10.1002/adma.201902549	1062
Z. Lei et al. A Bioinspired Mineral Hydrogel as a Self-Healable, Mechanically Adaptable Ionic Skin for Highly Sensitive Pressure Sensing. *Adv. Mater*. **2017**, *29* (22). https://doi.org/10.1002/adma.201700321	972
X. Wang et al. Recent Progress in Electronic Skin. *Adv. Sci*. **2015**, *2* (10), 1500169. https://doi.org/10.1002/advs.201500169	858
N. E. Thomford et al. Natural Products for Drug Discovery in the 21st Century: Innovations for Novel Drug Discovery. *Int. J. Mol. Sci.* **2018**, *19* (6), 1578. https://doi.org/10.3390/ijms19061578	838
Y. Cai et al. Stretchable Ti3C2Tx MXene/Carbon Nanotube Composite Based Strain Sensor with Ultrahigh Sensitivity and Tunable Sensing Range. *ACS Nano* **2018**, *12* (1), 56–62. https://doi.org/10.1021/acsnano.7b06251	785
Y. Zhang et al. Distributed Ti3C2Tx Hollow Microspheres on Thermally Conductive Polyimide Composite Films for Excellent Electromagnetic Interference Shielding. *Adv. Mater*. **2023**, *35* (16), 2211642. https://doi.org/10.1002/adma.202211642	776
H. Chen et al. Exploring Chemical, Mechanical, and Electrical Functionalities of Binders for Advanced Energy-Storage Devices. *Chem. Rev.* **2018**, *118* (18), 8936–8982. https://doi.org/10.1021/acs.chemrev.8b00241	743
Z. Ma et al. Ultraflexible and Mechanically Strong Double-Layered Aramid Nanofiber–Ti3C2Tx MXene/Silver Nanowire Nanocomposite Papers for High-Performance Electromagnetic Interference Shielding. *ACS Nano* **2020**, *14* (7), 8368–8382. https://doi.org/10.1021/acsnano.0c02401	721
Z. L. Wang, Triboelectric Nanogenerator (TENG)—Sparking an Energy and Sensor Revolution. *Adv. Energy Mater*. **2020**, *10* (17), 2000137. https://doi.org/10.1002/aenm.202000137	707
G. Goh et al. Deep Learning for Computational Chemistry. *J. Comput. Chem*. **2017**, *38* (16), 1291–1307. https://doi.org/10.1002/jcc.24764	622
J. Shi et al. Smart Textile-Integrated Microelectronic Systems for Wearable Applications. *Adv. Mater*. **2020**, *32* (5), 1901958. https://doi.org/10.1002/adma.201901958	609
S. A. Grigoriev et al. Current Status, Research Trends, and Challenges in Water Electrolysis Science and Technology. *Int. J. Hydrog. Energy* **2020**, *45* (49), 26036–26058. https://doi.org/10.1016/j.ijhydene.2020.03.109	606
R. Gupta et al. Artificial Intelligence to Deep Learning: Machine Intelligence Approach for Drug Discovery. *Mol. Divers*. **2021**, *25* (3), 1315–1360. https://doi.org/10.1007/s11030-021-10217-3	602
J. Tang et al. Bridging Biological and Artificial Neural Networks with Emerging Neuromorphic Devices: Fundamentals, Progress, and Challenges. *Adv. Mater*. **2019**, *31* (49), 1902761. https://doi.org/10.1002/adma.201902761	602

Source: Authors' work (2025).

[a] Number of citations on 23 May 2025.

interfaces, and charge-transfer phenomena; therefore, recent progress in this area has been driven by data-driven selection of functional groups, time- and cost-efficient virtual screening of dielectric materials, and ML optimisation of surfaces for maximal output. Similarly, the agricultural review outlines some chemometric studies in which ML algorithms help in the spectroscopic or elemental analysis of soil nutrients and plant metabolites, as well as in the authentication of food products – tasks which are in the domain of analytical chemistry. Taking this into account, it is visible that, among the search results, papers related to fields with direct application in everyday life (energy storage and generation, neuromorphic devices and sensors, drug discovery) dominate the citation count, suggesting these fields are profiting and will benefit the most from the implementation of AI / ML models in every aspect of research and development.

In order to provide an overview of how exactly (if at all) AI is implemented in the research outlined in the top-cited papers (Table 7), their short summary is given as follows.

In the article of Wu et al.,[22] artificial intelligence is not used as a research tool but more like a background idea: TENGs (triboelectric nanogenerators) are shown as an energy base for sensor networks that give power to AI systems in the time of IoT (Internet of Things). So, AI has an important and practical role in making smart and self-powered devices and systems. In contrast, the contribution of Schütt[19] is predominantly based on artificial intelligence itself, where deep learning is not only used as a supporting tool but becomes the core scientific method for understanding and predicting molecular and material properties through the SchNet architecture. Instead of laboriously designing mechanistic force fields or handcrafted machine learning descriptors, deep learning makes it possible to directly learn system representations from first principles: representations that adapt to the task and level of complexity, whether it involves predicting properties across chemical compound space or modelling force fields within the configurational space of individual molecules.

In the review paper by Liakos et al.,[24] a broad overview and multiple options are presented for applying artificial intelligence in agriculture, primarily through machine learning methods that facilitate the analysis of large datasets collected from various sensor systems. The paper shows how AI can improve crop, livestock, water, and soil management, and how these approaches are gradually evolving into fully intelligent systems that support decision-making and optimize agricultural production. Another review paper by Pinzi and Rastelli[25] illustrates how molecular docking has evolved into a data-driven and AI-assisted discipline, marking a shift in paradigms within drug discovery. The authors highlight that the integration of machine learning, deep learning, and artificial intelligence is transforming traditional docking methods by enhancing scoring functions, pose prediction, and virtual screening accuracy, leading to more efficient and reliable identification of potential drug candidates.

The perspective paper by Blakemore et al.[26] focuses on advancements in synthetic strategies within drug discovery, with machine-assisted and AI-driven synthesis recognized as innovative, forward-looking methods that could greatly speed up and transform chemical innovation. These emerging technologies are seen as a bridge between traditional experimental chemistry and data-driven automation, offering the potential to combine predictive modelling, autonomous experimentation, and continuous synthesis into a unified drug discovery process. Similarly, in the publication by Zang et al.,[27] AI is not the main focus but rather the context in which flexible pressure sensors are developed. The study emphasizes the design and optimization of tactile E-skin systems that can mimic human touch and monitor physiological signals, showing how such sensors can support AI-driven health monitoring and robotic applications.

The review by Dong et al.[23] focuses on the development of fiber- and fabric-based piezoelectric and triboelectric nanogenerators for flexible and wearable electronics. The paper is mainly oriented toward material design and energy-harvesting mechanisms, with artificial intelligence mentioned only as a potential application area. These nanogenerators are presented as self-powered components that could support future AI-integrated wearable systems. In the communication by Lei et al.,[28] the study introduces the development of a bioinspired mineral hydrogel designed as a self-healable, mechanically adaptable ionic skin with high pressure sensitivity. The research primarily concentrates on the material design and functional performance of the hydrogel, which can mimic human skin properties and detect fine mechanical stimuli. Artificial intelligence is referenced mainly as an application field, where such sensors could contribute to AI-driven health monitoring and human–machine interfaces, rather than being the central research focus. In another publication related to electronic skin, Wang et al.[29] provide a comprehensive overview of materials and sensing mechanisms used to achieve flexibility, stretchability, and multifunctionality in e-skin systems. The paper emphasizes advances in self-powered and self-healing designs, focusing on piezoresistive, capacitive, piezoelectric, and triboelectric sensors. Artificial intelligence is discussed as a future integration pathway, where electronic skin could serve as a sensory interface enabling adaptive perception and responsive behaviours in intelligent robotic and biomedical systems. Interest in natural product–based drug discovery is extensively reviewed by Thomford et al.,[30] highlighting the integration of digital and analytical technologies into modern drug development. The paper emphasizes innovative strategies such as omics, automation, and computational modelling, with artificial intelligence and machine learning identified as key tools enabling predictive modelling, virtual screening, and more efficient, data-driven drug discovery.

The study by Cai et al.[31] reports the development of a stretchable $Ti_3C_2T_x$ MXene / carbon nanotube composite strain sensor with exceptional flexibility, conductivity, and sensitivity. The work focuses on material design and performance optimization, with artificial intelligence mainly as an application context where these sensors could play a functional role in adaptive, AI-assisted monitoring and motion-sensing systems. An additional contribution comes from Zhang et al.,[32] who present the fabrication of thermally conductive polyimide composite films containing uniformly distributed $Ti_3C_2T_x$ hollow microspheres. This work emphasizes structural control and optimization to achieve superior thermal management and electromagnetic shielding performance. Artificial intelligence is mentioned only as a potential application area where these materials could support AI-integrated flexible electronics. Overall, the paper is strongly materials-oriented, focusing on microstructural design rather than AI methodology. The review by Chen et al.[33] focuses on design strategies for advanced polymer binders that improve mechanical strength, conductivity, and interfacial stability in energy-storage devices. The paper mainly emphasizes materials design and performance optimization, with artificial intelligence mentioned only as a technological context driving innovation in battery systems for future electronic and AI-based applications.

The article published by Ma et al.[34] reports the development of ultraflexible, double-layered aramid nanofiber–$Ti_3C_2T_x$ MXene / silver nanowire composites with excellent mechanical strength, conductivity, and EMI shielding performance. The work focuses on materials design and structural optimization, while artificial intelligence is only mentioned in connection with potential applications, particularly in smart electronics and wearable systems requiring effective thermal and electromagnetic management. An additional review by Wang et al.[29] summarizes advances in electronic skin materials and sensing mechanisms, including piezoresistive, capacitive, piezoelectric, and triboelectric systems with self-powered and self-healing properties. Artificial intelligence is only noted as a potential application area, where e-skin could facilitate adaptive sensing and feedback in robotics and health monitoring, but the main emphasis remains on materials and device engineering. The review by Goh et al.[20] highlights how deep learning has transformed computational chemistry, enabling more accurate predictions of molecular and material properties. Artificial intelligence is the central theme, with neural networks replacing manual feature engineering through automated representation learning. The paper demonstrates that deep architectures and multitask learning significantly advance QSAR (quantitative structure-activity relationship) modeling, protein prediction, and quantum chemistry simulations. The review by Shi et al.[35] explores smart textile–integrated microelectronic systems for wearable applications, emphasizing material design, fabrication, and device integration. It covers sensors, actuators, antennas, and energy harvesters that support flexibility and multifunctionality in textiles. Artificial intelligence is mainly referenced as a framework for future applications, where such systems could enable AI-assisted health monitoring and human–machine interaction. The main focus remains on materials development and system integration, not on AI methodology. The review by Grigoriev et al.[36] analyses advances and challenges in water electrolysis technologies, concentrating on material design, system efficiency, and large-scale hydrogen production. The work is heavily engineering-oriented, addressing improvements in alkaline, PEM, and solid oxide systems. Artificial intelligence is only marginally mentioned, with a minor role in future process optimization and energy management rather than as a core research element. The review by Gupta et al.[37] offers a detailed overview of how artificial intelligence, machine learning, and deep learning are transforming the entire drug discovery process. The paper is dominated by AI methodology, covering its use in target identification, virtual screening, peptide synthesis, toxicity prediction, and de novo drug design. Deep learning models such as CNNs, RNNs, GANs, and reinforcement learning frameworks are highlighted as essential tools enabling automated molecular prediction and synthesis planning. The authors emphasize that AI dramatically reduces the time, cost, and uncertainty of traditional drug development. Overall, the work presents AI as a key paradigm for next-generation pharmaceutical innovation. The work by Tang et al.[38] reviews progress in connecting biological and artificial neural networks through the development of neuromorphic devices based on materials such as RRAM (resistive random-access memory), PCM (phase-change memory), and CBRAM (conductive-bridge random-access memory). The study focuses on mimicking synaptic behavior and neural plasticity to improve computational efficiency and learning capabilities. Artificial intelligence plays only a minor role, mainly serving as a conceptual framework rather than a research focus. The paper's main contribution lies in advancing the material and hardware foundations for future brain-inspired AI systems.

Across all the analyzed publications, artificial intelligence (AI) played notably different roles depending on the research field and focus. It was central and transformative in studies such as those by Schütt et al.,[19] Goh et al.,[20] and Gupta et al.,[21] where deep learning and machine learning architectures directly shaped methodologies for predicting molecular properties, understanding quantum systems, and accelerating drug discovery. A strong applied AI component was also evident in Liakos et al.[24] and Pinzi and Rastelli,[25] where AI enhanced agricultural optimization and data-driven molecular docking, respectively. In contrast, works like Blakemore et al.,[26] Thomford et al.,[30] and Tang et al.[38] position AI as a complementary or emerging framework, supporting automation, synthesis planning, or neuromorphic modeling without being the central method. Most material-oriented studies, such as those by Zang et al.,[27] Dong et al.,[23] Lei et al.,[28] Ma et al.,[34] and Zhang et al.,[32] mention AI only as a potential application field, especially in wearable, robotic, or health-monitoring systems.

Overall, AI's dominant scientific impact appears in computational chemistry, molecular modelling, and drug discovery, while in materials science and energy research, it serves mainly as an enabling or contextual technology. This highlights its interdisciplinary integration but uneven methodological penetration across research domains.

Keywords Co–ocurrence

By implementing VOSviewer, the study analysed all 224 articles (listed in the Supporting Information) and extracted the keywords with at least 3 occurrences, categorized into seven clusters (Figure 4). The size of the node reflects the frequency of the keywords, with larger nodes indicating more common keywords, and the closeness of the connections between two specific keywords influences the thickness of the line between them.

Keyword-related data extracted from the selected papers are listed in Table 8, with the cluster keywords presented in the second column, and the cluster topics in the third column, and were assigned based on the keywords and the papers representative of each cluster. The exception is Cluster 6, for which no representative papers could be found in which AI is directly implemented or used in chemical research, and are therefore omitted.

CLUSTER 1: ELECTRONICS, (NANO)MATERIALS, SENSORS

The first cluster resembles studies on the integration of chemically engineered nanomaterials into advanced electronic and sensing systems, wherein artificial intelligence enables rapid progress in materials development and signal processing. Graphene-enhanced electronic skins achieve sub-kilopascal pressure sensitivity by optimizing junctions and polymer interlayers.[29] Meanwhile, carbon-based frameworks are common at the device level: IoT-compatible carbon nanotube structures offer high charge mobility and durable surface chemistry for multiplexed sensing and actuation.[39] Expanding into textiles, microelectronic silver-nanowire or conductive-polymer components fabricated via weaving or printing can create durable and breathable functional fabrics equipped with power supply, heating, and haptic feedback functionalities.[35] Recent progress in 2D transition-metal carbides (MXenes) shows that manipulating surface terminations and interlayer chemistry, both experimentally and via data-driven models, yields membranes for pollutant capture.[40] Generative AI is now fully incorporated in the exploration of this Mo-based MXenes with specific redox activity, proposing termination sets of atomic thickness.[41] Chemical selectivity is equally critical, especially in the detection of volatile organic compounds. Hierarchical carbon foams doped with heteroatoms detect VOCs (volatile organic compounds) at ppb levels, with neural nets analysing cross-sensitivity.[42] Machine learning also improves biosensor accuracy, translating spectra into analyte fingerprints in seconds.[43] Papers representative of this cluster demonstrate how AI and machine learning aid chemists in bridging synthesis, structure, and function from surfaces to devices, transforming nanomaterials for advanced electronics and sensors.

CLUSTER 2: CHEMISTRY, CHEMINFORMATICS, MACHINE LEARNING, (RETRO)SYNTHESIS

This cluster outlines the importance of AI and, even more specifically, machine learning, for enhancing the development of wider chemical sciences by directing processes from catalyst design to synthesis planning. This can be seen on a material level, where supervised and generative models accelerate catalyst screening[1] and analyze ab initio data to identify structure-activity patterns in

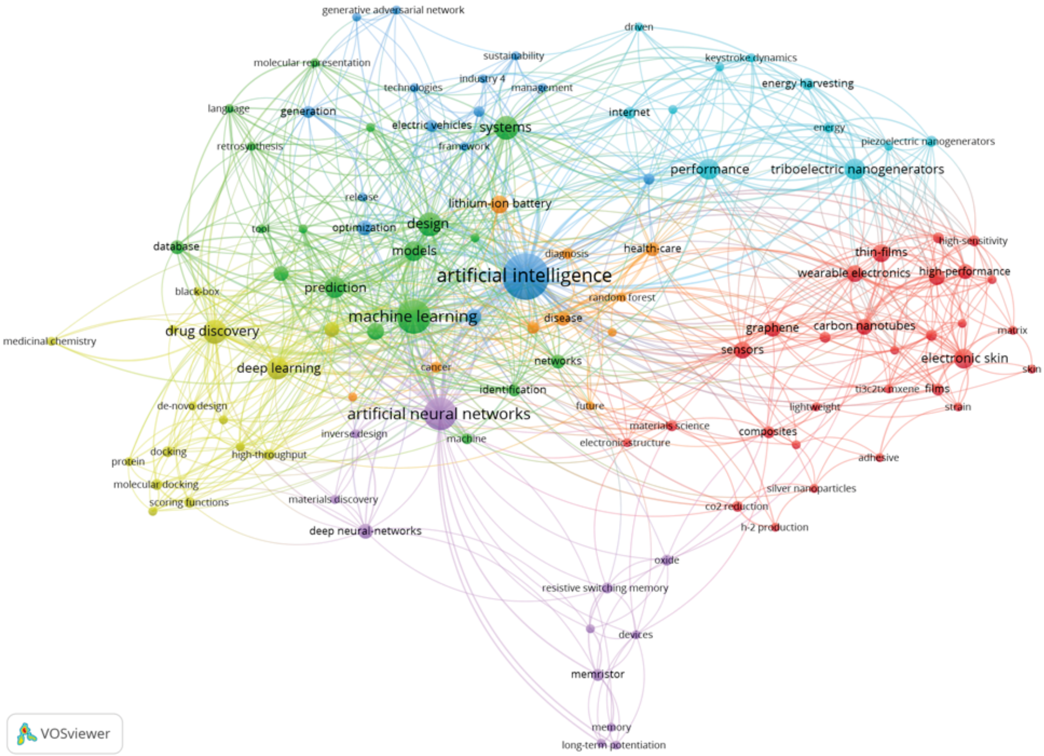

Figure 4. Keywords (min. three occurrences).

Table 8. Cluster keywords and cluster topics.

Cluster	Cluster keywords (alphabetically)	Cluster topic / Example papers
1	adhesive, carbon nanotubes, CO_2 reduction, composites, electromagnetic interference shielding, electronic skin, electronic-structure, electronics, field-effect transistors, films, flexible pressure sensors, graphene, H_2 production, high-performance, high-sensitivity, lightweight, materials science, matrix, MXene, pressure sensors, sensors, silver nanoparticles, skin, strain, strain sensors, thin-films, $Ti_3C_2T_x$ MXene, transition-metal carbides, wearable electronics	Electronics, (Nano)materials, Sensors[29,35,39–43]
2	cheminformatics, chemistry, classification, database, design, discovery, identification, language, machine, machine learning, models, molecular representation, networks, precision agriculture, prediction, retrosynthesis, systems, tool	Chemistry, Cheminformatics, Machine Learning, (Retro)synthesis[1,2,6,19,44–52]
3	artificial intelligence, challenges, density-functional theory, electric vehicles, framework, generation, generative adversarial networks, industry 4, internet of things, management, multiobjective optimization, optimization, release, sustainability, technologies	AI, Sustainability, Computational Chemistry, Industry 4.0, IoT[53–60]
4	big data, black-box, de-novo design, deep learning, docking, drug discovery, high-throughput, medicinal chemistry, medicine, molecular docking, protein, scoring functions, target identification, virtual screening, visualization	Drug discovery, Deep Learning, Docking, Medicinal Chemistry[20,25,61–68]
5	artificial neural networks, deep neural networks, devices, inverse design, long-term potentiation, materials discovery, memory, memristor, oxide, phase-change materials, resistive switching memory, synaptic plasticity	Neural networks, Memory Devices, Neuromorphism[38,69–77]
6	driven, electrode, energy, energy harvesting, internet, keystroke dynamics, performance, piezoelectric nanogenerators, transparent, triboelectric nanogenerators, vibration	Energy(a)
7	cancer, diagnosis, disease, drug-delivery, future, healthcare, lithium-ion battery, lung-cancer, random forest, support vector machine	Healthcare and Drug Delivery[27,78–84]

Source: Authors' work.

(a) Example papers omitted due to insufficient correlation between AI and the chemical research (see elaboration below under *Cluster 6: Energy*).

heterogeneous catalysis.[2] Inverse design of thermal metamaterials similarly uses discriminative networks and optimizers to control heat flow.[44] Membrane researchers apply ensemble learners to complex descriptors such as polymer composition, pore structure, and pH–expediting pathways from formulation to performance,[45] whereas those dealing with batteries and newer energy sources integrate predictive models, high-throughput DFT (density–functional theory), and public databases to rank materials and monitor health in real time, thereby reducing experimental costs.[46] On the molecular scale, models like SchNet offer quantum-level interatomic potentials, enabling fast and accurate reactive dynamics.[19] Active learning approaches wave-function data fitting to produce nanosecond photodynamics and spectra predictions at lower cost,[47] while full excitation spectra can be derived from coordinates almost instantly using AI-derived models.[6] In synthesis, neural-symbolic and sequence-to-sequence planners now match retrosynthetic experts by trimming impractical routes.[48,49] These systems are enhanced by techniques like transfer learning and Bayesian optimization, which extract value from limited experimental data, an ongoing need in chemical research.[50] Protein and enzyme engineers additionally use representation learning to map structure (sequence)-function relationships, suggesting beneficial mutations or new (bio)catalysts with high accuracy.[51,52] Papers representative of this cluster demonstrate a mutual relation between chemists and AI-based systems where the former co-develop experiments and algorithms, perform catalytic, materials, and biosynthetic challenges, generating rich data streams. Domain-aware neural networks interpret that data into practical design rules, and synthesis-planning AI completes the process by mapping out feasible synthetic routes.

CLUSTER 3: ARTIFICIAL INTELLIGENCE, COMPUTATIONAL CHEMISTRY, SUSTAINABILITY, INDUSTRY 4.0, IOT

Studies in this cluster illustrate how AI–enabled chemical sciences, with a specific focus on computational chemistry, are advancing sustainable technologies and data-centric manufacturing processes. The implementation of FAIR–compliant (Findable, Accessible, Interoperable, and Reusable) databases and automated DFT pipelines now supports active-learning frameworks that select subsequent calculations or experiments, thereby constructing chemistry-specific "digital backbones" for the discovery of greener materials.[53] When integrated with high-throughput robotic systems and Bayesian optimization, these infrastructures facilitate autonomous design cycles whereby formulations and processing conditions are iteratively refined with minimal human intervention, thus reducing the time-to-market for catalysts, polymers, and energy materials.[54] Energy-related sciences predominate the sustainability agenda, and AI applications in chemistry, especially batteries and new energy materials, are increasingly growing. Surrogate models trained on extensive datasets predict key properties such as voltage, phase stability, and degradation pathways in lithium-ion batteries, guiding synthesis efforts toward more durable and safer energy storage solutions.[55] AI techniques support material conservation and waste valorisation. Machine learning pipelines classify municipal polymers and metals, predict biogas yields, and optimize catalytic pyrolysis, integrating circular economy metrics into chemical process control.[56] Inverse design methodologies supported by graph neural networks and generative models enable the creation of recyclable, mechanically functional metamaterials with customized stiffness/density profiles, which are then evaluated for synthetic accessibility.[57] Similarly, evolutionary algorithms explore the composition–structure spaces of meta-atoms, enabling the design of ultrathin optical components with bespoke spectral responses while minimizing critical element consumption.[58] At the intersection of the Internet of Things (IoT), chemists are engineering battery-free triboelectric soft robots, whose polymeric and ionic-gel surfaces convert mechanical stimuli into charge signals decoded by cloud-hosted neural networks to enable applications such as virtual shopping interfaces and leak detection.[59] For in situ analytical applications, convolutional and recurrent neural networks are utilized to denoise and interpret Raman and surface-enhanced Raman spectroscopy (SERS) spectra, allowing researchers to monitor catalytic intermediates and trace pollutants with sub-second latency.[60] These studies show how chemists can incorporate AI at every level of chemical research, from predicting electronic structures to optimizing processes across entire plants, all while emphasizing sustainability, circularity, and industrial practicality in their decisions.

CLUSTER 4: DRUG DISCOVERY, DEEP LEARNING, DOCKING, MEDICINAL CHEMISTRY

Artificial intelligence methods now influence all stages of modern medicinal chemistry endeavours. When datasets containing compound information are limited or exhibit significant bias, transfer-learning frameworks facilitate the adaptation of large, pre-trained models to specific therapeutic targets, thereby maintaining predictive accuracy while substantially decreasing the number of new structure-activity relationship (SAR) experiments required.[61] Concurrently, ligand-based modelling has advanced through the QSAR without borders paradigm, which integrates deep neural descriptors with rigorous uncertainty quantification and cross-domain validation, enabling chemists to rely on in silico prioritization even during late-stage lead optimization.[62] Structure-based approaches have experienced a comparable evolution. Contemporary docking strategies focus on flexible receptor ensembles, ligand-efficient scoring functions, and machine learning re-scorers, together enhancing early enrichment during virtual screening processes.[25] Nevertheless, critical assessments such as PoseBusters highlight ongoing deficiencies: many neural docking engines continue to produce sterically implausible poses and struggle to generalize to novel chemotypes, underscoring the necessity for chemically informed validation protocols prior to synthesis.[63] Deep generative models now rapidly produce hit-and-lead ideas, surpassing manual idea generation. Comprehensive evaluations of de novo design methodologies track the development from rule-based fragment growth to reinforcement learning agents that optimize multiple medicinal chemistry objectives simultaneously.[64] For instance, REINVENT 4 exemplifies this transition; its open-source platform allows project teams to incorporate synthetic accessibility filters, substructure alerts, and potency predictors directly into the reward function, resulting in compound libraries that are both novel and synthetically feasible.[65] Community benchmarks like GuacaMol offer standardized metrics and datasets, allowing ongoing proof that successive generative algorithms progress beyond structural novelty to encompass synthesizability and property control.[66] Broader prospective analyses have confirmed that AI-driven computer-aided drug design is transforming routine medicinal practices, spanning target identification, hit expansion, and toxicity assessment.[67,68] Supporting these technological advancements are foundational educational resources that assist bench chemists in interpreting latent molecular representations, diagnosing overfitting, and understanding the limitations of deep learning within chemical space.[20] Collectively, papers representative of this cluster illustrate a shift in the field from the era of "AI-assisted discovery" toward a thorough implementation of AI, where experimental data, algorithmic insights, and chemical intuition progress from a concept to experimentally validated lead compounds.

CLUSTER 5: NEURAL NETWORKS, MEMORY DEVICES, NEUROMORPHISM

Research on neuromorphic materials is increasingly centred on a chemistry-focused toolkit that connects atomistic design to synaptic functionality. Explainable learning pipelines now inform composition and processing choices, enabling chemists to trace how dopants, defects, or phase boundaries influence device behaviour.[69] At the device level, MXene / ZnO heterojunction-based two-terminal memories demonstrate how surface terminations and oxide chemistry can be co-engineered to integrate sensing, memory, and low-level logic into a single "in-sensor" computing element.[70] Similarly, principles of these materials underpin artificial sensory neurons that convert mechanical stimuli into long-term potentiation via ion migration in elastomeric oxide films,[71] and full-skin electronic platforms that use carbon electrodes, proton-conductive gels, and resistive-switching nanofilms to facilitate perception-to-cognition signal flow.[72] Comprehensive reviews contextualize these advances within a broader roadmap. One survey analyses oxide, chalcogenide, ferroelectric, and organic chemistries in terms of defect energetics, switching kinetics, and compatibility with neural-network training, guiding the design from memristor stacks to inference hardware.[73] Another links phase-change and resistive-switching phenomena to biological plasticity, highlighting how valence changes and filament dynamics at the atomic scale emulate Hebbian learning.[38] Inverse–design approaches employ gradient-based and generative methods to discover photonic and plasmonic architectures that compute with photons, enabling ultralow-heat neural accelerators.[74] Additionally, all-optically gated IGZO (indium gallium zinc oxide) memristors utilize wavelength-dependent oxygen vacancy (de)trapping to realize spike–timing–dependent plasticity without electrical write pulses, combining semiconductor processing with photonic bandwidth.[75] At the system level, one review assesses various materials, from 2D carbides to ferroelectric perovskites, evaluating their endurance, linearity, and stochasticity against network training needs, identifying areas for improved electrolyte control and defect passivation.[76] Finally, views on deep-learning hardware scaling highlight that materials discovery must align with algorithmic sparsity and model compression to ensure neuromorphic platforms outperform traditional CMOS (complementary metal-oxide-semiconductor) in energy efficiency.[77] Together, these studies demonstrate that chemical intuition, guided by interpretable machine learning, is crucial to neuromorphic hardware, starting from, e.g., materials enabling photonic synapses capable of computing at the speed of light, thereby laying the foundation for next-generation artificial neural networks.

CLUSTER 6: ENERGY

Among all clusters, this one sits at the hardware end of the spectrum and is the least centred on chemistry: its main advancements are electromechanical devices such as piezoelectric and triboelectric nanogenerators (PENGs and TENGs), textiles, and interfaces that turn motion into electrical energy. The research in these papers intersects with chemistry mainly through materials selection, surface chemistry, analytical and processing tools like microfluidics, mass spectrometry, air filtration, and battery-free power systems used for chemical sensing networks. Therefore, AI threads through these research fields almost solely through processing of the data obtained from such generators or sensors, and since this is of marginal interest for chemists and scientists working in chemistry-related fields, detailed elaboration of papers representative of this cluster has been omitted.

CLUSTER 7: HEALTHCARE AND DRUG DELIVERY

Although Core AI methodologies in healthcare are explained in the review by Chaddad et al.,[78] who review the fast-growing field of explainable AI (XAI) for medical imaging, discussing several diagnostic pipelines to make malignancy predictions transparent to clinicians. An et al.[79] give a sector-wide inventory of supervised, unsupervised, and deep-learning models now used for electronic health-record mining and vital-sign forecasting; their own illustrative case study shows how hybrid ML improves early-warning scoring in hospitals. Governance, privacy, and oversight of using AI in medicine are important topics related to implementing such models in people-related sciences.[80] The authors explain how federated learning, encryption, and privacy layers work in AI medical analytics. They review projects that follow HIPAA (Health Insurance Portability and Accountability Act) rules and use deep learning. The use of AI in (nano)medicine and its linkage with data science demonstrates how AI models assist in designing nanoparticle-drug carriers by predicting attributes like size, zeta-potential, and drug-loading based on synthesis parameters, and how variational auto-encoders speed up virtual screening of nano-antivirals.[81] Adir et al.[82] illustrate “precision nano-oncology” by integrating high-throughput nanoparticle libraries with machine learning meta-models, such as gradient boosting and graph neural networks, which learn tumor-specific biodistribution patterns. They also showcase reinforcement learning loops that iteratively generate new nano-formulations for in vivo testing. Another subclass of papers in this cluster corresponds to Internet of Medical Things (IoMT) enabled biosensing and smart wearables, outlining an AI–enabled IoMT architecture where edge devices stream multi-modal biosignals, such as a skin-adhesive ECG patch,[83] IoMT-integrated electrochemical biosensors for point-of-care infection testing.[84] Flexible pressure-sensor skins are also one of the most-covered topics in this cluster;[27] however, similar to Cluster 6 and unlike those dealing with drug delivery, papers related to healthcare have less correlation between AI and the chemical part of the research, and more so between the processing of the signals and acquired data.

To summarize, the seven clusters can be understood as sitting on a practical ladder of AI adoption, with three main tiers across the chemical sciences. At the top of the ladder, AI is already part of everyday lab life in areas such as cheminformatics and retrosynthetic planning (Cluster 2) and computer-aided drug discovery and docking (Cluster 4). Here, machine-learning workflows are now considered standard practice. The middle tier includes advanced materials design and Industry 4.0 process optimisation (clusters 1, 3, and 5). In these fields, AI is used regularly but not universally: the experiments can proceed without it, but it significantly accelerates discovery and development. At the bottom tier, AI is still mostly exploratory in triboelectric and other energy-harvesting research (Cluster 6) and in AI-assisted healthcare sensors (Clusters 7). Investigations done here are dominated by proof-of-concept studies, and long-term, routine use in the lab is only starting to appear. Seen this way, the three tiers help show where AI is already essential, where it is steadily gaining ground, and where there is still plenty of room for future growth and implementation.

CONCLUSION

AI has transformed over the last ten years from a specialized curiosity to a potent force behind advancement and discovery in the chemical sciences. Four key findings that characterize this change and are essential to its future development are found in the herein presented bibliometric analysis of the 224 most-cited WoS papers (2015–2024) are as follows:

1. Output has been increasing steadily. From 2015 to 2024, there were 224 highly cited papers, indicating rapid adoption of AI tools into laboratory workflows and significant progress. The papers' broad distribution across review and research papers, prestigious high-impact journals, and more specialized ones indicates that there is still a need to organize the body of knowledge on these subjects.
2. The nations that dominate these fields are both centralized and interconnected, with China and the USA together accounting for slightly more than half of the influential literature, as might be expected. These nations do, in fact, make up the core of the densest networks of collaboration, but they are also a part of a truly global network that spans 58 nations, with new hubs in Singapore, South Korea, the UK, and Germany serving as links between established leaders and upstarts. Third, although they have different themes, AI applications in chemistry and related fields come together to form logical clusters.
3. Citations are dominated by seven main research areas: 1) materials and electronics, 2) cheminformatics and (retro)synthesis, 3) computational chemistry and IoT, 4) drug discovery and medicinal chemistry, 5) neuromorphic devices and neural networks, 6) energy, and 7) healthcare and drug delivery. This demonstrates how the technology is changing the field's foundational elements (data representation, reaction planning, property prediction) as well as its frontiers (wearable electronics, precision medicine). Finally, it is important to note that the majority of highly cited papers do not directly apply AI tools to the chemical portion of the study, as demonstrated in the detailed survey of the 20 most cited papers, even though these tools typically aid in selecting the best materials and optimizing their characteristics.
4. It remains difficult to manage data and ensure chemical validity. Datasets that are incomplete or biased, evaluation methods that aren't consistent, and models that are kept secret can all make trust and reproducibility less reliable. To keep progress going, it's important for communities to work together to share data, improve benchmarking, and create models that work in the real world.

These results have many effects and implications, as they stress how important it is for researchers to have skills spanning across fields by pointing out that the most important work is happening at the crossroads of automated experimentation, chemical intuition, and algorithm development. Funding organizations and policymakers could increase participation beyond the current concentration of Asian and American researchers and speed up the sharing of knowledge with regions that are not well represented by making planned investments in shared data infrastructure, international exchange programs, and computer resources. To raise scientific standards and cut down on hype, journal editors and reviewers should make it harder to share datasets, make code available, and judge uncertainty. At the same time, chemists should adopt AI and automation skills alongside chemical intuition, generate and share FAIR, domain-rich datasets, and use autonomous labs with active-learning loops under human oversight. Industry and the wider community should also embed AI-driven discovery in R&D pipelines and strengthen partnerships with academia to support open innovation and shared datasets.

Last but not least, this study has some practical limitations as it only includes highly cited WoS records in English, underrepresenting recent preprints, non-English publications, and low-profile innovations that might advance in the years to come. To obtain a more comprehensive, up-to-date picture of the research landscape, future studies should incorporate additional databases, conduct normalized citation analyses, and track preprint-to-publication progress. Despite this, the evidence is unmistakable: AI has emerged as a crucial collaborator in chemical discovery, and its influence is only expected to increase as autonomous labs, computational power, and data quality all come together. Even though artificial intelligence was first introduced in the chemical sciences a few decades ago, we are currently witnessing its pinnacle of development, and it is evident that the future of chemistry will be significantly altered. Adopting these key principles, namely trustworthy data, intelligible algorithms, and iterative experimentation, will put chemists in the best position for the next wave of innovations in materials, energy, healthcare, and other fields.

Supplementary Information. Supporting information to the paper is attached to the electronic version of the article at: https://doi.org/10.5562/cca4229.

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