AI deployment in chemistry: Bibliometric and topic analysis of top-cited papers (2015−2025)

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SUPPORTING INFORMATION

Table S1. Categorization of review papers

Category	# of papers
Narrative, mini-review, recent advances Refs. 6, 8, 9, 14, 15, 19, 20, 21, 22, 23, 24, 32, 33, 35, 36, 39, 41, 43, 44, 47, 53, 58, 60, 61, 63, 66, 68, 70, 75, 76, 79, 80, 82, 86, 87, 88, 89, 92, 97, 98, 100, 101, 110, 111, 112, 114, 117, 118, 119, 120, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 134, 135, 136, 138, 139, 140, 142, 147, 148, 151, 152, 157, 160, 161, 163, 164, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 182, 183, 185, 189, 190, 191, 193, 194, 195, 196, 197, 198, 200, 203, 204, 207, 208, 209, 212, 214, 215, 222, 223, 224	109
Perspective, roadmap, outlook Refs. 37, 38, 40, 67, 83, 108, 121, 157, 184, 206	10
Bibliometic and meta-bibliometric reviews	0
Scoping or mapping reviews Ref. 201	1
Systematic reviews or meta-analysis Refs. 17, 65, 109	3
Source: Authors' work (2025)	

Table S2. Institutions (1 and 2 papers)

Institution(s)	# of papers per institution
Aalto University, Ajou University, Beijing University of Chemical Technology, Canadian Institute for Advanced Research (CIFAR), Centre for Research & Technology Hellas, Chung-Ang University, Fudan University, Guangdong University of Technology, Helmholtz Association, Institute of Coal Chemistry (CAS), Institute of Microelectronics (CAS), Jiangnan University, La Trobe University, Lawrence Berkeley National Laboratory, Leibniz Association, Masaryk University, Minzu University of China, Nanjing Tech University, National Institute of Technology (NIT System), North University of China, NUS Suzhou Research Institute (NUSRI), Pacific Northwest National Laboratory, Polish Academy of Sciences, Polytechnic University of Turin, Royal Melbourne Institute of Technology (RMIT), Semnan University, Shandong University, Shanghai Jiao Tong University, Shenzhen Research Institute (City University of Hong Kong), St Anne's	2

University Hospital Brno (FNUSA), St Anne’s University Hospital Brno (FNUSA-ICRC), State University System of Florida, Sunway University, Technical University of Denmark, Technische Universität Dresden, Tianjin University, University of Birmingham, University of California Berkeley, University of California Davis, University of California Los Angeles, University of California Santa Barbara, University of Münster, University of North Texas Denton, University of North Texas System, University of Nottingham, University of Petroleum & Energy Studies (UPES), University of Shanghai for Science & Technology, University of Warwick, University of Waterloo, Uppsala University, Vector Institute for Artificial Intelligence, Worcester Polytechnic Institute, Wuhan University, Yeungnam University

A*STAR Institute of High Performance Computing (IHPC), A*STAR Institute of
Materials Research & Engineering (IMRE), A*STAR Singapore Institute of
Manufacturing Technology (SIMTech), Academy of Scientific & Innovative
Research (AcSIR), Adv Technol New Mat Res Inst, Al Maaqal University,
Alexander Fleming Biomedical Sciences Research Center, All India Institute of
Medical Sciences (AIIMS) Rishikesh, Anhui Medical University, Anhui Provincial
Chest Hospital, Aristotle University of Thessaloniki, Arizona State University,
Arizona State University Tempe, Assam University, Astex Pharmaceuticals,
Auburn University, Auburn University System, Australian Nuclear Science &
Technology Organisation (ANSTO), Autonomous University of Barcelona,
Autonomous University of Madrid, Bahçeşehir University, Basque Research &
Technology Alliance (BRTA), Beijing Institute of Fashion Technology, Beijing
Intelligent Pharma Technology Co Ltd, Beijing University of Posts &
Telecommunications, BenevolentAI, BenevolentBio, BigChem GmbH, Bilecik
Şeyh Edebali University, Binzhou Medical University, BioLand Lab, Bridging
Health Foundation, Brigham and Women’s Hospital, Brno University of
Technology, Bulgarian Academy of Sciences, Catholic University of Korea,
CeADAR (Ireland’s Centre for Applied AI), Central Institute of Technology
Kokrajhar, Center for Excellence in Brain Science & Intelligence Technology
(CAS), Center for Excellence in Molecular Cell Science (CAS), Center for Physical 1
Sciences & Technology (Lithuania), Central Queensland University, Central
University Hospital of Asturias, Centre of Polymer-Carbon Materials (Polish
Academy of Sciences), Chaitanya Bharathi Institute of Technology, Chalmers
University of Technology, Chang’an University, Changchun University of Science
& Technology, Changsha University of Science & Technology, Chettinad Academy
of Research & Education, China Academy of Electronics & Information
Technology, China Jiliang University, China Medical University, Chinese
University of Hong Kong, Chitkara University Punjab, Chosun University,
CIDETEC, CIQUS, Clemson University, CNRS Institute of Chemistry (INC),
CNRS Institute of Ecology & Environment (INEE), Collaborative Innovation
Center of Electronics (Beijing), Collège de France, Comenius University Bratislava,
Commonwealth Scientific & Industrial Research Organisation (CSIRO),
Communication University of China, Consiglio Nazionale delle Ricerche (CNR),
Council of Scientific & Industrial Research (CSIR-India), Coventry University,
CSIR-Central Electrochemical Research Institute (CECRI), CTR Materials Science
& Engineering, Czech Academy of Sciences, Czech Technical University in Prague,
Dalian Municipal Central Hospital, Deakin University, Delhi Technological
University, Dept Chem Ångström Laboratory, Dept of Statistics (unspecified),
Dhaka University of Engineering & Technology (DUET), DIT University,

Dongguan University of Technology, Duke University, Duy Tan University, East China University of Science & Technology, École de Technologie Supérieure (Canada), Edith Cowan University, Extreme Light Infrastructure (ERIC), FARMB Digital Agr PC, Federal Center for Technological Education Minas Gerais (CEFET-MG), Fitchburg State College, Florida International University, Fritz Haber Institute of the Max Planck Society, Fukuoka Institute of Technology, Gachon University, Gandhi Institute of Technology & Management (GITAM), Gannon University, German Jordanian University, GlaxoSmithKline, GlaxoSmithKline (UK), Goethe University Frankfurt, Graduate School of Materials Science, Mainz, Griffith University, Griffith University Gold Coast Campus, Guangdong Medical University, Guilin University of Electronic Technology, Guru Jambheshwar University of Science & Technology, Gwangju Institute of Science & Technology (GIST), Hainan University, Harbin Institute of Technology, Harvard Medical School, Harvard University, Harvard University (Medical Affiliates), Hebei University, Heinrich Heine University Düsseldorf, Hellenic Military Academy, Helmholtz Center Munich (German Research Center for Environmental Health), Henan University, High-Tech Org. Fibers Key Lab (Sichuan Prov.), Hokkaido University, Hong Kong Metropolitan University, Hospital Universitario Ramón y Cajal, Hubei University of Automotive Technology, Hubei University of Technology, Hunan Institute of Engineering, Hunan University, Hunan University (Changsha), Hunan University of Science & Technology, Hunan University of Technology, IBM Japan, IBM Research Europe, IBM Research Europe (Zurich), IBM USA, Icahn School of Medicine at Mount Sinai, ICGEB (Cape Town), IBM Research Europe (Daresbury), Indian Institute of Science (IISc) Bangalore, Inha University, Insil Med Hong Kong Ltd, Insil Med Shanghai Ltd, InsiliCom GmbH, Insilico Med AI Ltd, Insilico Med Canada Inc, Inst. of Mechanics (CAS), Institute for Translational Medicine, Institut Universitaire de France, Institute for Basic Science (IBS, Korea), Institute of Biomedical Chemistry, Institute of Chemistry (CAS), Institute of High Pressure Physics (Polish Academy of Sciences), Institute of Organic Chemistry & Biochemistry (Czech Academy of Sciences), Institute of Semiconductors (CAS), Instituto de Investigación Sanitaria del Principado de Asturias (ISPA), International Business Machines (IBM), International Centre for Genetic Engineering & Biotechnology (ICGEB), Iran Polymer & Petrochemical Institute, Iran University of Science & Technology, Islamia College of Science & Commerce, Islamic University of Gaza, Istanbul Technical University, Istituto Nazionale di Ricerca Metrologica (INRiM), Jeonbuk National University, Jilin University, Johan Lundberg AB, Kanazawa University, Karpagam Academy of Higher Education (KAHE), Keimyung University, Khulna University, King Abdullah University of Science & Technology, King Khalid University, King Saud University, Koneru Lakshmaiah Education Foundation (KL University), Korea Advanced Institute of Science & Technology (KAIST), Korea Institute of Industrial Technology (KITECH), Korea University, Korea University of Technology & Education, Kyoto University, Lanzhou University, Lawrence Livermore National Laboratory, Lebanese American University, Leibniz Institute for Catalysis (LIKAT), Leibniz Institute for Solid State & Materials Research Dresden, Liaocheng University, Linköping University, Lomonosov Moscow State University, Maastricht University, Mälardalen University, Malaviya National Institute of Technology Jaipur, Mashhad University of Medical Sciences, Massachusetts System of Public Higher Education, MD Use Innovat S L, Mendel University in Brno, Merck Company, Merck Company (USA), Military Technical College, Minia

University, Multimedia University, Nagaoka University of Technology, Nagoya University, Nanjing University, National Centre for Physics (Pakistan), National Cheng Kung University, National Institute for Materials Science, National Institute of Oceanography & Fisheries (NIOF), National Institute of R&D for Cryogenic Isotopic Technologies, National Institute of Technology Agartala, National Pingtung University of Science & Technology, National Research Centre "Kurchatov Institute", National Taipei University of Technology, National Taiwan University of Science & Technology, National University of Defense Technology (China), National Engineering Research Center for Advanced Energy Storage Materials, Netherlands Organisation for Applied Scientific Research (TNO), Newcastle University (UK), NIBR, North Carolina State University, North China University of Technology, North Eastern Indira Gandhi Regional Institute of Health & Medical Sciences, North-West University (South Africa), Northeastern University (China), Northwestern University (USA), Norwegian University of Science & Technology (NTNU), Novamechanics Ltd, NPU Chongqing Technology Innovation Center, Oklahoma State University Stillwater, Oklahoma State University System, Ontario Tech University, Panjab University, Peking University, Pfizer, Pfizer (USA), Pohang University of Science & Technology (POSTECH), Prince of Songkla University, Prince Sattam bin Abdulaziz University, Qingdao University, Qingdao University of Science & Technology, Quinnipiac University, Radi Oncoradi SA, Research Center Jülich, RIKEN, Roche Holding, Royal College of Surgeons in Ireland, Royal Institute of Technology (KTH), Ruprecht Karls University Heidelberg, Russian Academy of Medical Sciences, Rutgers University – New Brunswick, Rutgers University System, RWTH Aachen University, RWTH Aachen University Hospital, Sabancı University, Salesforce, Sandia National Laboratories, Sapienza University of Rome, Saveetha Dental College & Hospital, Saveetha Institute of Medical & Technical Sciences, Seoul National University (SNU), Shaheed Zulfiqar Ali Bhutto Medical University, Shahid Madani University, Shandong Zhongke Naneng Energy Technology Co Ltd, Shanghai COSMAX China Cosmet Co Ltd, Shanghai Engineering Research Center for Intelligent Computing Systems, Shanghai Institute of Technology, Sharif University of Technology, Shenzhen Institute of Advanced Technology (CAS), Shenzhen International Quantum Academy, Shoolini University, Shri Pundlik Maharaj Mahavidyalaya (Nandura), Sinopec, SLAC National Accelerator Laboratory, Soochow University (China), Soongsil University, Sorbonne Université, Southwest University (China), Spartan Innovat, Sri Shakthi Institute of Engineering & Technology, State Key Laboratory of Engines, State University of New York (SUNY) System, Sun Yat-sen University, SUNY Old Westbury, Suzhou Institute of Nano-Tech & Nano-Bionics (CAS), Swansea University, Swinburne University of Technology, Taif University, Tampere University, Tarbiat Modares University, Technical Vocational University, Technical University of Berlin, Technical University of Darmstadt, Technical University of Ostrava, Tel Aviv University, Telkom University, Thanh Hoa University of Culture, Sports & Tourism, The Chinese University of Hong Kong (Shenzhen), Tohoku University, Tongji University, Trinity College Dublin, Triton Systems Inc., Tulane University, Tyréns, UCB Pharma SA, Ulsan National Institute of Science & Technology (UNIST), United Arab Emirates University, Universidad de Burgos, Universidade de Aveiro, Universidade de Santiago de Compostela, Universidade Estadual Paulista, Universidade Federal da Paraíba, Universidade Federal de São João del Rei, Università di Modena e Reggio Emilia, Universität Greifswald, Université de

Montréal, Université de Picardie Jules Verne (UPJV), Université de Strasbourg, Université Paris-Saclay, Université PSL, Universités de Strasbourg (Etablissements Associés), Universiti Teknologi Malaysia, Universiti Tenaga Nasional, University College Dublin, University College London, University of Adelaide, University of Aizu, University of Allahabad, University of Bonn, University of Calabria, University of California Irvine, University of Cambridge, University of Cape Coast, University of Cape Town, University of Colorado Boulder, University of Colorado System, University of Connecticut, University of Copenhagen, University of Delhi, University of Electronic Science & Technology of China, University of Florida, University of Fort Hare, University of Genoa, University of Glasgow, University of Gothenburg, University of Helsinki, University of Hertfordshire, University of Hong Kong, University of Illinois Chicago, University of Illinois Chicago Hospital, University of Illinois System, University of KwaZulu-Natal, University of Liège, University of Lincoln, University of Liverpool, University of London, University of Luxembourg, University of Massachusetts Amherst, University of Massachusetts System, University of Michigan, University of Michigan System, University of Milano-Bicocca, University of Nebraska Lincoln, University of Nebraska System, University of New Mexico, University of New South Wales Sydney, University of North Carolina, University of North Carolina Chapel Hill, University of Oviedo, University of Oxford, University of Palermo, University of Peshawar, University of Quebec, University of Regina, University of Rostock, University of Sharjah, University of Southern California, University of Sydney, University of Technology Sydney, University of Texas Austin, University of Texas System, University of Tsukuba, University of Vienna, University of Würzburg, UTE University, Uttarakhand Technical University, Vallurupalli Nageswara Rao Vignana Jyothi Institute of Engineering & Technology (VNR VJIET), Vellore Institute of Technology (VIT), Vietnam National University Ho Chi Minh City (VNU-HCM System), Vignan's Foundation for Science & Technology Research (VFSTR), Vilnius University, VIT Vellore, VNU-HCM An Giang University (AGU), Wuhan Textile University, Xi'an Technological University, Xiamen University, Xiamen University Malaysia Campus, Xidian University, Xinjiang Technical Institute of Physics & Chemistry (CAS), Yanshan University (Qinhuangdao), Yanshan University (main), Yantai Institute of Coastal Zone Research (CAS), Yıldız Technical University, Yonsei University, Yuri Gagarin State Technical University of Saratov, Zhengzhou University

Source: Authors' work (2025)

List of publications (alphabetically by title)

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