

# Applications of Artificial Intelligence and Machine Learning

Chemical Reviews

122, 13006-13042

DOI: 10.1021/acs.chemrev.2c00141

Citation Report

#	ARTICLE	IF	CITATIONS
1	Revealing the role of polymer in the robust preparation of the 2,4-dichlorophenoxyacetic acid metastable crystal form by AI-based image analysis. Powder Technology, 2023, 413, 118077.	4.5	10
2	Iterative model-based optimal experimental design for mixture-process variable models to predict solubility. Chemical Engineering Research and Design, 2023, 189, 768-780.	6.4	3
3	Synthetic Strategies toward Higher Cocrystals of Some Resorcinols. Crystal Growth and Design, 2022, 22, 7578-7589.	3.5	22
4	A synthetic machine learning framework for complex crystallization processes: The case study of the second-order asymmetric transformation of enantiomers. Chemical Engineering Journal, 2023, 465, 142800.	11.9	12
5	Optimized identification of cheese products based on Raman spectroscopy and an extreme learning machine. New Journal of Chemistry, 2023, 47, 6889-6894.	2.5	17
6	Building confidence in deep Learning-based image analytics for characterization of pharmaceutical samples. Chemical Engineering Science, 2023, 278, 118904.	4.0	6
7	Modeling and Predictive Control of Cooling Crystallization of Potassium Sulfate by Dynamic Image Analysis: Exploring Phenomenological and Machine Learning Approaches. Industrial & Engineering Chemistry Research, 2023, 62, 9515-9532.	4.0	15
8	Integrating Machine Learning and Molecular Simulation for Material Design and Discovery. , 2023, 8, 325-340.		6
9	Crystallization: A Tool for Asymmetric Synthesis and Isolation. , 2024, , 81-134.		1
10	Enabling technologies for process intensification in pharmaceutical research and manufacturing. Current Opinion in Chemical Engineering, 2023, 41, 100920.	7.2	13
11	Benefits of Application of Process Optimization in Pharmaceutical Manufacturing: A Panoramic View. , 2023, , 291-304.		1
12	A crystallization case study toward optimization of expensive to evaluate mathematical models using Bayesian approach. Materials and Manufacturing Processes, 2023, 38, 2127-2134.	4.8	42
13	Computer Modeling and Machine Learning in Chemistry and Materials Science: From Properties and Reactions of Small Organic and Inorganic Molecules to the Smart Design of Polymers and Composites. Compounds, 2023, 3, 459-463.	2.6	2
14	Discovery of structureâ€“property relations for molecules via hypothesis-driven active learning over the chemical space. , 2023, 1, .		6
15	Developing diagnostic tools for canine periodontitis: combining molecular techniques and machine learning models. BMC Veterinary Research, 2023, 19, .	2.3	5
16	Opportunities for Machine Learning and Artificial Intelligence to Advance Synthetic Drug Substance Process Development. Organic Process Research and Development, 2023, 27, 1868-1879.	3.9	22
17	MatGPT: A Vane of Materials Informatics from Past, Present, to Future. Advanced Materials, 2024, 36, .	24.4	51
18	Improved modeling of crystallization processes by Universal Differential Equations. Chemical Engineering Research and Design, 2023, 200, 538-549.	6.4	16

#	ARTICLE	IF	CITATIONS
19	Optimizing environmental sustainability in pharmaceutical 3D printing through machine learning. International Journal of Pharmaceutics, 2023, 648, 123561.	4.9	17
20	Transforming organic chemistry research paradigms: Moving from manual efforts to the intersection of automation and artificial intelligence. National Science Open, 2023, , 20230037.	3.1	1
21	A step forward in food science, technology and industry using artificial intelligence. Trends in Food Science and Technology, 2024, 143, 104286.	15.7	62
22	Developing a model-driven workflow for the digital design of small-scale batch cooling crystallisation with the antiviral lamivudine. CrystEngComm, 2024, 26, 822-834.	2.5	7
23	A critical review of machine learning algorithms in maritime, offshore, and oil & gas corrosion research: A comprehensive analysis of ANN and RF models. Ocean Engineering, 2024, 295, 116796.	4.9	47
24	Machine Learning-Guided Prediction of Cocrystals Using Point Cloud-Based Molecular Representation. Chemistry of Materials, 2024, 36, 1153-1161.	6.9	16
25	Data-driven identification of crystallization kinetics. AIChE Journal, 2024, 70, .	3.9	12
26	Machine learning for polyphenol-based materials. Smart Materials in Medicine, 2024, 5, 221-239.	9.3	6
27	Inhibition of Crystal Nucleation and Growth: A Review. Crystal Growth and Design, 2024, 24, 2645-2665.	3.5	59
28	Rapid prototyping of a modular optical flow cell for image-based droplet size measurements in emulsification processes. Journal of Flow Chemistry, 2024, 14, 515-528.	1.8	6
29	OpenCrystalData: An open-access particle image database to facilitate learning, experimentation, and development of image analysis models for crystallization processes.. Digital Chemical Engineering, 2024, 11, 100150.	3.5	3
30	A changing paradigm in industrial pharmaceutical crystallization. Nature Chemical Engineering, 2024, 1, 327-329.	0.0	4
31	Artificial Intelligence Assisted Pharmaceutical Crystallization. Crystal Growth and Design, 2024, 24, 4245-4270.	3.5	14
32	Machine Learning Methods to Improve Crystallization through the Prediction of Solute-Solvent Interactions. Crystals, 2024, 14, 501.	2.3	3
33	Enhanced sustainability with crystallization in continuous flow. Current Opinion in Green and Sustainable Chemistry, 2024, 48, 100937.	6.2	2
34	Recent Advances in the Application of Machine Learning to Crystal Behavior and Crystallization Process Control. Crystal Growth and Design, 2024, 24, 5374-5396.	3.5	21
36	Current trends and advancements in crystallization and single-crystal structural analysis of small molecules. Coordination Chemistry Reviews, 2024, 517, 216035.	23.4	26
37	Infrared Microscopy: A Multidisciplinary Review of Techniques, Applications, and Ethical Dimensions. Jordan Journal of Pharmaceutical Sciences, 2024, 17, 267-291.	0.9	3

#	ARTICLE	IF	CITATIONS
38	The Application of Supervised Learning Algorithms in Predicting the Formation Energy of NLO Crystals. Advanced Theory and Simulations, 2024, 7, .	2.9	2
39	Paracetamol polymorphs detection in suspension via a new ex situ Fourier Transform Near Infrared spectroscopy method. Chemical Engineering Research and Design, 2024, 208, 808-819.	6.4	4
40	Nucleation Patterns of Polymer Crystals Analyzed by Machine Learning Models. Macromolecules, 2024, 57, 9711-9724.	5.2	5
41	An Enhanced Deep Learning-Based Pharmaceutical Crystal Detection with Regional Filtering. Crystals, 2024, 14, 709.	2.3	1
42	Deciphering the molecular complexity: Employing density functional theory to probe 2-aminopyridinium 4-methyl benzene sulfonate elucidates synthesis methodologies, spectroscopic trends, reactivity patterns, molecular dynamics, and antibacterial properties. Journal of Molecular Structure, 2025, 1320, 139357.	4.2	2
43	Going beyond the Ordered Bulk: A Perspective on the Use of the Cambridge Structural Database for Predictive Materials Design. Crystal Growth and Design, 2024, 24, 6911-6930.	3.5	3
44	Effect of the Functional Group Position in Coformers on Ternary Cocrystals: A Case of Sulfamoylbenzoic Acids. Crystal Growth and Design, 2024, 24, 7455-7465.	3.5	1
45	Controlling Paracetamol Unseeded Batch Crystallization with NMPC and Inverse Model. IFAC-PapersOnLine, 2024, 58, 31-36.	1.1	1
46	The ARTISTIC Battery Manufacturing Digitalization Initiative: From Fundamental Research to Industrialization. Batteries and Supercaps, 2025, 8, .	4.4	13
47	Artificial Intelligence in X-Ray imaging: advances, challenges, and future directions. , 2024, 2, 0018.		0
48	The synergy of artificial intelligence and nanotechnology towards advancing innovation and sustainability - A mini-review. Nano Trends, 2024, 8, 100052.	7.0	46
49	Teaching cases of eigenvalues and eigenvectors in the context of artificial intelligence. , 2024, , 168-172.		1
50	Advanced drug delivery systems in the management of CNS disorders. , 2025, , 429-449.		0
51	MLAPI: A framework for developing machine learning-guided drug particle syntheses in automated continuous flow platforms. Chemical Engineering Science, 2025, 302, 120780.	4.0	4
52	Predicting Crystalline Material Properties with AI: Bridging Molecular to Particle Scales. Industrial & Engineering Chemistry Research, 2024, 63, 18241-18262.	4.0	4
53	Examining the utilization of web-based discussion tools in teaching and learning organic chemistry in selected Rwandan secondary schools. Heliyon, 2024, 10, e39356.	3.6	6
54	Digital Design of Cooling Crystallization Processes Using a Machine Learning-Based Strategy. Industrial & Engineering Chemistry Research, 2024, 63, 20236-20251.	4.0	7
55	Information Network Security Situation Awareness Based on Artificial Intelligence and Machine Learning Algorithms. , 2024, , 1-6.		0

#	ARTICLE	IF	CITATIONS
56	Crystal Structure Prediction Using Generative Adversarial Network with Data-Driven Latent Space Fusion Strategy. Journal of Chemical Theory and Computation, 2024, 20, 9627-9641.	5.5	9
57	Neural Network Inverse Model Controllers for Paracetamol Unseeded Batch Cooling Crystallization. Industrial & Engineering Chemistry Research, 2024, 63, 19613-19627.	4.0	8
59	Machine Learning Algorithm to Predict Methane Adsorption Capacity of Coal. Energy & Fuels, 2024, 38, 23422-23432.	5.3	5
60	Unveiling novel grub-style pentacene crystals driven by hierarchical self-assembled crystallization. Macromolecular Research, 2025, 33, 625-631.	2.8	0
62	Applications of machine learning for modeling and advanced control of crystallization processes: Developments and perspectives. Digital Chemical Engineering, 2025, 14, 100208.	3.5	7
63	Lactate-related gene signatures as prognostic predictors and comprehensive analysis of immune profiles in nasopharyngeal carcinoma. Journal of Translational Medicine, 2024, 22, .	6.5	14
65	Unveiling the potential of metal-organic framework-based membranes: Transforming material science for a sustainable future. Separation and Purification Technology, 2025, 361, 131332.	8.8	2
67	Unveiling diabetes onset: Optimized XGBoost with Bayesian optimization for enhanced prediction. PLoS ONE, 2025, 20, e0310218.	2.5	13
68	The role of 5G network in revolutionizing agriculture for sustainable development: A comprehensive review. Energy Nexus, 2025, 17, 100368.	10.9	13
69	Hybrid Semi-mechanistic and Machine Learning Solubility Regression Modeling for Crystallization Process Development. Crystal Growth and Design, 2025, 25, 1111-1127.	3.5	0
70	Modern, Efficient, and Differentiable Transport Equation Models Using JAX: Applications to Population Balance Equations. Industrial & Engineering Chemistry Research, 2025, 64, 4541-4553.	4.0	3
75	Advances in Pharmaceutical Oral Solid Dosage Forms. , 2025, , 111-142.		1
87	Data-driven Digital Design of Pharmaceutical Crystallization Processes. , 0, 4, 2604-2609.		0
88	Development of a Hybrid Model for the Paracetamol Batch Dissolution in Ethanol Using Universal Differential Equations. , 0, 4, 2592-2597.		0
89	Imaging Based Fault Detection and Diagnosis of Potassium Dihydrogen Phosphate Batch Crystallization Process. , 2025, , 1-6.		0
103	Artificial intelligence in chemical engineering process monitoring and predictive maintenance. , 0, , 287-311.		0
114	Neutron macromolecular crystallography. , 0, , .		0