



Index

a

AbsoluteProof software 139
advanced automated synthesis platform 42, 45
AI-assistant chemical and bio-material design 58
AI-driven automated microscopy system 42
AI-powered digital chemical synthesis platform 40, 42
AI prediction 40, 166, 171–172
AI Supervisor and ScholarNet 130–134
AlexNet 73, 85
AlphaFlow 48–52
AlphaFold 165
AnByCz 118
Apple Vision Pro 164
aqueous system research in metaverse 177–181
Arrhenius equation 4
automated chemical reactor system 25
automated chemical synthesis systems 26, 27
automated intelligent machine (AIM) 47
autonomous high throughput experiments 166–172

b

band theory 6
Bayesian neural networks (BNNs) 92
BiaeP 150–155, 157
Big Kahuna System 36, 37, 42
BindingDB 71

Bitcoin 140–142

“black-box” optimization algorithms 79

BlockAudit 144

blockchain in the autonomous laboratory 150–155

blockchain technology 139–145, 150, 157–160, 163

Born–Lande equation 180

Byzantine fault tolerance (BFT) 140, 144

Byzantine Generals Problem 140, 141

c

canonical SMILES 60–63
ChatGPT 19, 114, 131
ChEMBL 70
ChemOS 96
Chempiler program 91
Chemputer system 91, 92
components identification 101–104
computer-aided synthesis planning (CASP) 40, 94, 95
convergence innovation 129
convolutional neural networks (CNNs) 72–74, 89
coolant and moderator materials 10
cooling bath system 23, 24
CrossRef 121
CubeRoot 155–157

d

data balancing 68
dataset preprocessing 68–69
data storage safety 158–159



- decentralized applications (dApps) 142
 decentralized autonomous organizations (DAOs) 142
 decentralized finance (DeFi) 142
 DeepCID 99
 DeepMind 165
 deep neural networks (DNNs) 72, 77, 85, 99
 DeepRIPP workflow 81
 digital chemical synthesis platform 39, 40, 42
 digital currencies 142, 163
 digitalization 29, 165–167
 divergence innovation 129
- e**
 Edisonian design 78
 Emerald Cloud Lab (ECL) 35, 36, 42
 Ethereum 142, 143, 150–154
 Ethereum Blockchain 142, 143, 150, 152, 153
 Ethereum Blockchain & Cloud Storage Platform 150
 Ethereum Virtual Machine (EVM) 142
- f**
 first-principle-based inverse design 78–79
 flow-based automated reaction device 91
 Foldit 165
 Fortnite 164
 fuel cladding materials 10
- g**
 Gaussian approximation potential (GAP) 76, 77
 Gaussian process (GP) 95
 Generalized Gradient Approximation (GGA) 67
 Generative Pre-trained Transformer (GPT) 117
 Gibbs–Duhem integration methods 175
 GlobusLabs 116
- gradient-domain machine learning (GDML) approach 76
 graph attention networks (GATs) 74–75
 graph convolutional neural networks (GCN) 73–75
 graph neural networks (GNNs) 65, 71, 74
 Graph-pKa 66
- h**
 hard drive-based PoW systems 141
 high-performance computing devices 164
 Hohenberg–Kohn theorems 67
 HTC Vive 164
 human-in-loop (HIL) optimization 165–166, 169–171, 173
 human-refined multistep synthesis 94
 hydrolysis 177, 181
 hyper-converged Autonomous Organic Reaction Infrastructure (HAORI) 96, 97
- i**
 IBM RXN for Chemistry (IBM) 39, 92
 ice phase diagram 175
 image captioning (IC) 114
 ImageNet 120, 130
 in-context learning (ICL) 116, 117, 119
 Industry 5.0 163–165
 Inferred Contextual Learning (ICL) 116, 119
 intelligent machines 19
 International Chemical Identifier (InChI) 58, 59, 62–63
 International Chemical Identifier Key (InChIKey) 63
 isomeric SMILES 60
- k**
 Kapok series of advanced automated laboratory equipment 49
 Kohn–Sham equation 66–68, 75–78

l

laboratory information management systems (LIMS) 29
 LangChain's ConversationChain method 121
 Language-Interfaced Fine-Tuning (LIFT) approach 114, 117 framework 117
 large language models (LLMs) 104
 Large Scale Visual Recognition Challenge (LSVRC) 85
 linear notations for molecules 58–63
 Local Density Approximation (LDA) 67

m

machine learning (ML) 21, 29, 36, 58, 68, 69, 71, 72, 75, 76, 78, 80, 81, 89, 94, 95, 99, 108, 114, 182
 MAPI-LLM framework 118
 materials acceleration operation system (MAOS) 166
 message-passing neural networks (MPNN) 75–76
 metal-organic frameworks (MOFs) 34, 35, 146
 Microsoft HoloLens 164
 MIDA boronate-based purification method 91
 molecular graph representation 63
 molecular representation and encoding 58–66
 molecular structure predictor 102, 103

n

Natural Language Processing (NLP) 80, 99, 104, 113, 114, 119
 Neuralink 169
 “no free lunch” theorems 79
 non-fungible tokens (NFTs) 163

o

object-relational mapping (ORM) 144
 Oculus Rift 164
 OpenAlex 121

optimization algorithms 78, 79, 95, 176
 organic semiconductor lasers (OSLs) 95

p

Partial Least Squares (PLS) 98
 Pauling's ionic character theory 181
 physics-endorsed diffusion-like model 171
 physics-inspired neural networks 77
 PlayStation VR 164
 practical Byzantine fault tolerance (pBFT) 140
 principal component analysis (PCA) 98
 process analytical technology (PAT) 94
 Protein Data Bank (PDB) database 70, 71
 PubChem 70, 71
 PubMed 121
 PubPeer 146–148

q

quantum deep field (QDF) 77
r
 reinforcement learning (RL) 48, 51, 89–90
 renewable energy 7–10, 110
 ResNet 73
 Roblox 164
 RoboChem 97
 RoboRXN from IBM 92
 Robot Scientist Adam 31, 42

s

Savitzky–Golay filter 101
 SchNet 75–77
 ScholarBert model 116
 ScholarNet 120, 130–134
 scite 114
 self-referencing embedded strings (SELFIES) 116
 Simplified Molecular Input Line Entry System (SMILES) 58–63, 70, 116



SMILES Arbitrary Target Specification (SMARTS) 59, 62
Soft Independent Modeling of Class Analogy (SIMCA) 98
Spectrum Spiking Neural Network (SpecSNN) architecture 96, 97
Spider Matrix 120, 124–130, 136, 168
Symyx Tools 31, 32, 42

t

tensor networks (TNs) 99–100, 120
TIP4P-Meta 174–176

u

Unchained Labs’ Big Kahuna System 36
U-net architecture 171

Unity 13, 164
Unreal Engine 164

v

variational autoencoder (VAE) 171
Vision and Language BERT (ViLBERT) 114
Vision Transformer (ViT) 114
VisualBERT 114

w

water force field TIP4P-Meta 174
wearable technology 164
Word2Vec 113

z

Ziegler–Natta catalyst 15









