

Index

a

AB inorganic solids, AET stability maps
for 158–159

active learning techniques 244

AFLOW-SYM module 190, 191

aggressive feature selection 237

AiiDA 149–169
workchains 166–168
workflows 166
workfunctions 166

Al–Al interaction potentials 266, 267

anharmonic phonons 198

ASM Phase Diagram Database 90

atomic environment (AE) approach
58, 68, 72, 90, 96, 152, 153, 159,
161, 204, 225–257, 284

Atomic Environment Type (AET)
68–72, 94, 95, 97, 150, 152,
158–159

atomic property parameters, of
chemical elements 157

AtomWork 90

automated computational materials
design frameworks
crystallographic prototypes 183
data generation workflow 183
disordered materials 202–203
material discovery, databases for
182–185
standardized protocols 185–187

autonomous symmetry analysis
189–191

b

back propagation process 229, 234,
235, 246, 265

Bayesian neural networks 245–247

Behler–Parrinello symmetry function
270

binary daltonide inorganic solids 159

2-body correlation function 261, 263,
270, 272, 273

bond-valence imbalance 268

bootstrap aggregation 245

bottom-up approach (BUA) 55

c

chemical element combinations 152,
155, 156

chemical space 177, 223, 248

cod-tools 10, 23–25

compound classes 84

compound formation maps 157–158

computational materials data web
portals 198–199

computational materials science
resources 181

computer-aided materials design 41

configurational entropy 202

convex hull phase diagrams
for multicomponent alloys systems
184

thermodynamically stable
compounds 185

convolutional neural networks 229

- coordination polyhedron 68–70, 150
- cosine distances 256
- Coulomb matrix 177, 226, 228
- crystal classification structures 152
- crystallographic information file (CIF)
 - format 1, 42, 51
- Crystallography Open Database (COD)
 - accessing records 17–18
 - alternative search implementations 20–21
 - CIFs, programmatic use of 24–26
 - data curation policies 12–13
 - data deposition 26
 - data identification 15
 - data maintenance 8–14
 - cod-tools 10
 - error classes 9
 - retraction rate 10
 - version control 11–12
 - data sources 7, 8
 - educational activities 31
 - extracting chemical information 28–30
 - file system based queries 23–24
 - geometry statistics 30–31
 - high-throughput computations 31
 - historic structures 32
 - local copy installations 21–23
 - material identification 27
 - for mining industry 27
 - MySQL 12, 18–20
 - output formats 17
 - principle 7
 - property search 30
 - record number growth 4
 - RESTful interfaces 15–17
 - revisions 13
 - scope and contents 7
 - Web search interface 15
- d**
 - daltonide basic ternary inorganic solids 159
 - deep autoencoders 229, 247
 - deep neural network 235
 - Δ -ML method 242
 - density functional theory (DFT) 7, 50, 107, 149, 164, 174, 186, 242, 253
 - digital ecosystem 103
 - directed acyclic graphs 164, 233, 234
 - dropout technique 236
- e**
 - early-stopping technique 236, 237
 - elastic constants 189, 191–193
 - electronic structure simulations 150
 - embedded atom method (EAM)
 - potentials 276
 - energy vs. structural quasi-entropy
 - correlation 257
 - energy workflow 168, 169
 - European Theoretical Spectroscopy Facility (ETSF) 32
 - evaluation, standardization, derived data (ESDD) software 80, 81
 - Ewald method 258
 - exploratory search 244, 247
 - extended connectivity fingerprinting approach 225
- f**
 - feature bagging process 245
 - feature vectors 261–262
 - fifth paradigm, preconditions for 155
 - fingerprint function property 255, 256
 - first paradigm of science 153
 - fourth paradigm 155–157
 - Friedel oscillations 266, 273
 - frozen phonon method 278
- g**
 - Gaussian approximation potential (GAP) 257, 284
 - Gaussian noise 241
 - Gaussian process (GP) 238, 240–242, 244, 284
 - generalized gradient approximation (GGA) 186
 - Gibbs method 193
 - Gibbs' phase rule 152
 - greedy search 244

h

harmonic phonons 195–197
 Heusler structures 183, 206, 208
 high entropy materials 203
 high thermal conductivity materials 189
 high-throughput computational materials science 182
 high-throughput simulated inorganic solids database 156
 high-throughput virtual screening (HTVS) 235
 Hogwild 237
 Hohenberg–Kohn theorem 185

i

inorganic crystal structure database (ICSD)
 applications of 46–51
 concept of structure types 47–48
 content of 42–46
 decisive factors for 41, 42
 description 41
 Desktop/Web interface 46
 ferroelectricity prediction 47
 high-throughput calculation 50–51
 machine learning algorithm 48–50
 integrated computational materials design frameworks 189
 interatomic force constants (IFC) 192, 196
 International Union of Crystallography (IUCr) 1, 58

k

kernel-based method 238, 240
 Gaussian process 240–242
 support vector machines 238–240
 kernel trick 239
 Kohn–Sham equations 185
 “*k*-points per reciprocal atom” (KPPRA) value 187

l

LAMMPS code 274
 lattice sums method 258–260, 273

lattice thermal conductivity 181, 189, 195, 198, 206, 207
 Lennard-Jones potential 259, 260, 271, 273
 local density approximation (LDA) 186
 local orbital-based packages 187
 logistic function 235
 long short term memory (LSTM) network 232–233
 low thermal conductivity materials 189

m

Molecular ACCess System (MACCS) keys 225
 machine learning interatomic potentials 256
 aluminum 265–267
 carbon 267–271
 for global relaxation 258
 feature vectors 261–262
 lattice sums method 258–260
 helium and xenon 271–272
 statistical approach
 three-body potential 286
 two-body potential 284–285
 Ti₄H₇ system 281
 magnetic materials 50, 208
 material property and structure databases 2
 maximum-convex-volume rule 69
 maximum gap rule 69
 mean shift technique 49
 metallic glasses 202–205
 mineral names 43, 60, 83, 84
 MNIST handwritten digit problem 228
 modified Z method 280
 molecular dynamics (MD) technique 56, 107, 108, 253–286
 molecular fingerprints 223
 moment tensor potentials 284
 Monkhorst–Pack scheme 187
 Morgan circular fingerprint 226, 237
 Morton curve 228
 Morton index 228
 multiphase inorganic solids 151

n

neural fingerprints 231
 neural memory 232
 nickel-based superalloys 205
 noise kernels 244
 Novel Materials Discovery (NoMaD)
 32, 181, 200

o

Open Quantum Materials Database 50
 optimal brain damage (OBD) algorithm
 263, 264
 overfitting 51, 172, 174, 230, 231,
 235–237, 245, 282

p

PAULING FILE project 56, 57, 80,
 89–91, 103, 154, 156, 161, 163
 ASM Phase Diagram Database 90
 AtomWork 90
 Binaries Edition 90, 92, 93
 bottom-up approach 55
 chemical formulas and phase names
 83
 computer-aided checking 80–81
 creation and development 57
 crystal structure database entry
 assigned atom coordinates 67–68
 atomic environment types 68–72
 categories 58–59
 cell parameters from plots 72
 data selection 58
 database fields 59–62
 distribution 85, 86
 requirement for 57
 standardized crystallographic data
 63–67
 structure prototypes 62–63
 data quality 80–84
 digital ecosystem 103
 distinct phases 81–84
 holistic overviews 91–92
 megadatabase 84–89
 ordering of chemical elements
 atomic environment principle
 96–97

ordering tendency principle
 97–98
 simplicity principle 94–95
 symmetry principle 95–96
 Pearson's Crystal Data 90–91
 phase classifications 84
 phase diagram section 72, 74
 physical properties section
 data selection 75–76
 database fields 76
 Powder Diffraction File PDF4+ 91
 SpringerMaterials 91
 unlimited retrieval possibilities 89
 Pearson's Crystal Data 90–91
 phase-oriented inorganic solids
 database 154
 phonon density of states (PDOS) 194,
 196, 197, 277, 278
 plane wave based packages 186
 plane-wave DFT 166
 potential energy surface (PES) 177,
 253
 Powder Diffraction File PDF4+ 91
 Predicted Crystallography Open
 Database (PCOD) 14
 probabilistic back propagation (PBP)
 paradigm 245–246
 programmatically accessible online
 repositories 200–202
 property classes 75, 76, 84
 prototype classification 91, 149,
 153–155, 157, 159, 161, 163
 prototypes of crystalline inorganic solids
 152, 155
 pseudo-code implementation, of
 dropout 236

q

quantum molecular dynamics (QMD)
 273
 quantum simulation strategy 151–153,
 161–163
 quasientropy 256
 quasi-harmonic Debye–Grüneisen
 193–195

- quasi-harmonic Debye model 198
 quasi-harmonic phonons 197–198,
 207
- r**
- radial distribution function (RDF) 177,
 279, 280
 random forest method 244, 245
 rational quadratic kernel 240–244
 ReaxFF method 269, 270
 recursive neural networks (RNNs)
 232, 234
 REpresentational State Transfer (REST)
 15
 restricted Boltzmann machines (RBM)
 228, 229
 Reuss approximation 191, 193
 rsync method 22
- s**
- second paradigm of science 153
 single-phase inorganic solids 151, 152,
 154, 155, 169
 SMILES format 28–30
 space filling curve 228
 SpringerMaterials 91
 squared exponential kernel 239–240,
 242
 Standard Solid State Pseudopotentials
 (SSSP) library 165–166
 standardized crystallographic data 59,
 63, 65–67, 90
 stochastic gradient descent with
 mini-batching 237
- stoichiometric ratio condition principle
 159, 161
 structural quasi-entropy 256, 257
 structure classes 24, 84
 structure type pool (STP) 63
 superalloys 100, 202, 205, 209
 support vector machines (SVMs)
 238–240
- t**
- tanh function 235
 Theoretical Crystallography Open
 Database (TCOD) 4, 11, 14, 32,
 181
 thermoelectric materials 181, 189,
 205–207
 third paradigm of science 153
 Thompson sampling 246, 247
 top-down approach (TDA) 55
- u**
- uncoordinated database producers,
 types of 155, 156
 USPEX code 253, 256, 258–260
- v**
- vibrational entropy 197, 202
 virtual experiment for materials design
 (VEMD) project 56, 100, 101
 Voigt approximation 191
- z**
- zeolite-structure-predictor (ZSP)
 48

