Index

adsorbates 56, 58, 66–7, 69, 86, 91, 185–7, 278, 281, 283, 301–2, 305–6, 310, 312, 429
adsorbents 60–1, 69, 86–7, 89–92, 95–6, 185–6, 307–8, 343, 382, 391, 394, 399, 434, 438–40, 464
adsorption
  absolute 78, 80
  acetylene 135
  excess 78–9
  liquid-phase 423
  nitrogen 63–4
  physical 181
  preferential 118, 120, 122, 129, 144, 155, 283
adsorption applications 390, 409
adsorption-based carbon dioxide separation 348–9, 351, 353, 355, 357, 359
adsorption-based process field 440
adsorption-based selectivity 348–9
adsorption-based separation 302–3, 305, 307, 309–10, 312, 340, 348, 351, 357–9
adsorption behaviors 97, 137, 299, 305, 308, 310, 324, 386, 391
adsorption capacities 54–5, 391, 453, 466–7
adsorption complexes 188, 193, 199
adsorption energies 73, 133, 491, 501, 508
adsorption energy density 301
adsorption enthalpies 14–15, 96–7, 121, 131, 191–2, 195, 197–9, 217
adsorption equilibrium 342, 420, 427
adsorption isotherms 63–5, 69–71, 114, 119, 121, 136–8, 143, 155–7, 159, 195–8, 280–1, 284–5, 343, 346, 426–7
adsorption modeling 86, 393
adsorption selectivity 53, 55, 97, 141, 143, 145–6, 150, 318, 320, 322–3, 349–51, 354, 356, 359, 472–3
adsorption separations 54, 311, 406
adsorption simulations 69, 402
adsorption strengths 80, 98–9
adsorption structures 284, 506
adsorption systems 89, 386
adsorption thermodynamics 254
adsorptive separation 311, 419–20, 425, 464
  cyclic 419
  energy-efficient 308
ammonia, reactive adsorption of 148
aniline 498–9, 533–4

basis set incompleteness (BSI) 180
basis set superposition error (BSSE) 180
benzaldehyde 486, 489, 499, 526, 531–2
benzene 56, 83, 117, 389, 423
BSI, *see* basis set incompleteness
BSSE, *see* basis set superposition error
bulk fluid phase 64, 72, 76, 79, 84
bulk water 471–2

carbon dioxide 120–1, 143–4, 146, 208, 210, 235–6, 300, 340, 342, 346, 348, 350, 352, 354, 364–6
  self-diffusivity of 365, 389
  transport diffusivity of 366
carbon dioxide adsorption 118, 120, 133–4, 143, 145, 151, 193–4, 196, 307–8, 344, 347, 353–4, 356, 393–4, 397, 399, 461–2, 468
  selective 131, 305
carbon dioxide adsorption complexes 194–5
carbon dioxide permeability 317, 362–4
carbon dioxide selectivity 305, 307, 348–60, 362
  adsorption-based 351, 354, 357–8, 360
carbon dioxide separation applications 340, 359, 366
carbon dioxide separations 317, 340–2, 348, 354, 356–9, 361, 363, 381–2, 397, 468
  adsorption-based 348
carbon monoxide adsorption 134, 146–7
carbon nanotubes 96, 257, 276, 282, 284, 341
catalysis 37, 41, 483–4, 486, 488, 490–2, 494–6, 498, 500, 502, 504, 506, 508, 520–2
catalysts 41, 487, 489, 497, 521, 525, 533–9
CBAC, *see* connectivity-based atom contribution
CBS, *see* complete basis set
charge-quadrupole interactions (CQI) 346, 366
chemistry, reticular 366
cluster approach 525–6, 532, 537, 539–40
cluster models 177–8, 180–2, 185, 188, 197, 493, 501, 525–6, 536, 540
COFs, *see* covalent organic frameworks
complete basis set (CBS) 181–3, 190, 256, 258
computational chemists 126, 175
connectivity-based atom contribution (CBAC) 298, 347
coordination chemistry 115, 123
coulombic interactions 307, 342, 344
covalent organic frameworks (COFs) 24, 54, 66, 78, 96, 209, 311, 340, 347
CQI, *see* charge-quadrupole interactions
crystal structure prediction (CSP) 1–3, 5, 7
crystal structures 2, 4–5, 9, 12, 19, 21, 30, 33, 38, 63, 65, 68, 81–2, 119, 453
CSP, *see* crystal structure prediction
Cu atoms 135, 180, 307, 494–5, 530
Cu paddlewheel structure 493–4

DAEs, *see* differential algebraic equations
density functional theory (DFT) 12, 38, 67, 113–14, 119, 122, 128–9, 175–9, 181, 183–4, 186–8, 347, 399–400, 485, 524
deuterium 229, 252–3
DFT, *see* density functional theory
differential algebraic equations (DAEs) 94

EDD, *see* electron density difference
electron density difference (EDD) 501–2
electronic structure methods 118–19, 121, 123, 125, 127, 129, 131, 133, 135, 157–8
electrostatic charges 390
electrostatic interactions 122–3, 130–1, 138–9, 141, 143–6, 155, 297, 299–300, 304–7, 345–6, 349–51, 392–4, 397, 399, 461–6
electrostatic potential energy surface (EPES) 297, 347
EMD, *see* equilibrium molecular dynamics
enantioselectivity 533–7
EPES, *see* electrostatic potential energy surface
equilibrium molecular dynamics (EMD) 342
ethanol 116, 471–3, 509
ethanol adsorption 472
ethyl cyanoacetate 486, 489, 533

formaldehyde 504, 526, 530
free-energy barriers 239–41, 247

gas adsorption capacities 342
gas mixtures, separation of 296
gas-phase separations 422, 424–5, 440
  adsorptive 420
gas separation 118, 295–6, 298, 300, 302, 304, 306, 308, 310, 312, 314, 320, 322–6, 340, 381–2
  acidic 423
  membrane-based 363
gases, sorptive 69
GCMC, *see* grand canonical Monte Carlo
generalized gradient approximation (GGA) 128, 176, 178, 185, 188, 526
GGA, *see* generalized gradient approximation
grand canonical Monte Carlo (GCMC) 14, 63, 119, 136–7, 142, 145, 176, 215, 280–1, 283, 299, 342, 344, 392, 528

heterogeneous catalysis 497, 524–5, 527, 529, 534
heterogeneous catalysts 488, 520
hexane isomers 87–8, 92–3, 95, 421
highest occupied molecular orbitals (HOMO) 34, 501, 503
HOMO, *see* highest occupied molecular orbitals
hybrid frameworks 5–6, 30, 37
hybrid functionals 34, 185–6, 188
hybrid inorganic-organic framework materials 1
hybrid materials 41, 339, 381, 523
hybrid zeolitic imidazolate framework 488
hybrid zeolitic imidazolate frameworks (HZIFs) 488

hydrogen adsorption 118, 121–3, 126–8, 137–9, 146, 151–2, 154, 257, 280, 386, 427, 527
hydrogen bonds 456, 532–3
hydrogen isotopes 253
hydroperoxide 492–4, 539, 541
hydroperoxide decomposition 485, 492, 494, 540–1
HZIFs, *see* hybrid zeolitic imidazolate frameworks

IAST, *see* ideal adsorption solution theory
ideal adsorption solution theory (IAST) 86–8, 150, 156, 310, 313, 318, 324, 430, 467
imidazole 27, 495–6
interactions
  adsorbate–adsorbent 185, 187, 427
  intermolecular 247
  lateral 133, 193–5, 199, 527
  solid–gas 381, 384, 409
isobutane 72, 81, 432
isoreticular metal–organic frameworks 34, 63, 121, 257, 300, 340, 389, 522
isosteric heats 132–3, 136, 219, 392, 460–3
isosteric heats of adsorption 134, 393, 427–8

Langmuir isotherm 70
Langmuir model 62, 71, 427, 429
  dual 71, 73, 427
lattice energies 13, 19, 23, 25
lattice vibrations 82
LDA, *see* local density approximation
ligand functionalization 14–15, 17, 357
linkers
  2-hydroxypyrimidinolate 493, 540
  imidazolate 353–4, 383, 391
local density approximation (LDA) 129–30, 135, 176, 178, 185, 188
lowest unoccupied molecular orbitals (LUMOs) 34, 501
LUMOs, *see* lowest unoccupied molecular orbitals

metal–adsorbate interactions 149, 152, 159–60
  localized 114, 119, 160
metal–hydrogen interactions 123, 128, 154, 158
metal–organic materials (MOMs) 420, 517–18, 522
methane 58, 72–4, 81–2, 84, 118, 120, 129–30, 145–6, 156–7, 196, 208, 210, 239, 389–90, 396
methane adsorption 6, 17, 120, 130, 140, 142, 156, 196
methane molecules 58, 129, 156, 223, 239
methane storage 141
microporous materials 70, 77, 192, 388, 523, 527
mixed-gas adsorption 362
mixed-matrix membranes (MMMs) 316–19, 361, 363
mixture separations 311, 322
  adsorption-based 302
MMMs, *see* mixed-matrix membranes
mobility, molecular 245, 247
molecular building blocks approach 452
molecular catalysts 486, 521
molecular clustering 77–8
molecular dipoles 459

molecular dynamics 58, 136, 210, 216, 224–5, 227–8, 231, 233, 235, 238–9, 271, 296, 342–3, 388, 456
molecular dynamics simulation 343
molecular mechanics methods 114, 118–19, 136–7, 139, 141, 143, 145, 147, 160
molecular modeling 148, 296–7, 311, 315, 325, 340, 345, 384, 537
molecular sieve membranes 315, 320
molecular sieves 181, 381, 424–5
molecular sieving 294, 421–3
molecule–molecule interactions 71
molecules
  adsorptive 385
  clustering of 77
  dibranched 70–2, 96
  linker 114, 117
  monobranched 96–7
MOMs, *see* metal–organic materials
Monte Carlo simulation 119, 136, 140, 154, 342–3
multicomponent adsorption equilibrium 429–30, 439

nitrogen adsorption simulations 64
NMR, *see* nuclear magnetic resonance
nuclear magnetic resonance (NMR) 83, 121, 232

organic ligands 13, 209, 234, 237, 246, 311, 322–3, 339, 403, 517, 521
organic linkers 9, 16–17, 19–20, 34–5, 39, 176, 184, 349–50, 406, 408, 485–6, 494, 519, 522–3, 530
organic molecules 5, 421
organometallic compounds 522

path-integral expressions 267
path-integral Monte Carlo (PIMC) 271, 285
PCPs, *see* porous coordination polymers
permeation 317, 360, 401, 403
permeation selectivities 312–13, 316–19, 321, 363
PES, *see* potential energy surface
PIMC, *see* path-integral Monte Carlo
pore size distributions (PSDs) 66–7, 99–100
porous coordination polymers (PCPs) 207–8, 210, 212, 214, 216, 218, 220, 222, 224, 226, 228, 230–2, 234, 246, 339
porous materials 30, 60–2, 94, 118, 176, 302, 342, 452, 483–4, 523
potential energy surface (PES) 84, 150, 196, 297, 347, 537
pressure swing adsorption (PSA) 55, 93, 312, 348, 351, 382, 419, 424–5, 434
propane 135, 198–9, 309, 389, 395–6, 405, 422, 425–9, 432, 434, 439
propane adsorption 150, 199, 309, 427, 429
propylene 135, 150, 155, 198–9, 309, 422, 425–9, 432, 434, 439, 485, 490, 526, 530
propylene adsorption 150–1, 155
PSA, *see* pressure swing adsorption
PSDs, *see* pore size distributions

QENS, *see* quasi-elastic neutron scattering
QM, *see* quantum mechanics
QSDFT, *see* quenched solid density functional theory
quantized molecules 285, 287
quantum dynamics 286–8
quantum mechanics (QM) 70, 251, 278, 287, 296, 345, 485, 491, 523, 526, 535
quantum particles 257, 259, 275, 285
quantum sieving 282, 284
quasi-elastic neutron scattering (QENS) 233, 244, 365
quenched solid density functional theory (QSDFT) 67

Rietveld refinement 9, 12–13
ring-polymer configurations 260
ring polymers 259–62, 265, 268, 270–1, 274, 279

selective adsorption 53, 310, 321, 348
self-diffusivity 77–8, 82, 210, 231–3, 235, 239, 247, 343, 365, 389–90
separation
  chemical 308, 521
  liquid-phase 421
separation devices 54–5, 99
simulated annealing 4–5
simulated moving bed (SMB) 419, 423–4, 439
simulations, rigid-framework 82
single-component adsorption 69, 71, 73, 75, 77, 79, 81, 83, 135, 142, 304
single-component isotherms 87–8
small molecule adsorption 113–14, 116, 118, 120, 122, 124, 126, 128, 130, 132, 134, 136, 138, 140, 148–50
SMB, *see* simulated moving bed
sorbates 209–10, 215, 222, 235–6, 239, 247
sorption thermodynamics 207, 209, 217–18, 246

temperature swing adsorption (TSA) 424–5
transition metal cations 176
transition metal ions 175
transition metals 19, 34, 200, 208, 383
TSA, *see* temperature swing adsorption

UFF, *see* universal force field
universal force field (UFF) 137–9, 142, 153, 198, 209, 219, 254, 324, 345, 386–7, 396, 398, 400, 526, 530

vacuum swing adsorption (VSA) 353, 434, 438
vapor permeation 472–4
VSA, *see* vacuum swing adsorption

water adsorption 75, 148, 471–2
water adsorption isotherms 191
water/ethanol mixtures 473–4
water molecules, coordinated 307, 486

xylene isomers 420–3, 529

zeolite framework 9, 222, 523

zeolite imidazolate frameworks 340
zeolites 4, 19–21, 30, 53, 65–6, 81–3, 341–2, 360, 363, 390, 434, 483–4, 488, 523, 526
  traditional 348–9, 359, 363
zeolitic imidazolate frameworks (ZIFs) 15–17, 26–7, 29–30, 37–8, 207–8, 210–11, 308, 350, 353–4, 381, 383–5, 388–95, 399, 401–3, 405–9
zeolitic-like hybrid materials 381–2, 384, 386, 388, 390, 392, 394, 396, 398, 400, 402, 404, 406, 408
zeolitic topologies 392
zeotypes 20, 24
zero-point vibrational energy (ZPVE) 32, 128, 131, 192
ZIF materials 30, 392, 401, 403, 405–9
ZIF structures 208–9, 225, 386, 390, 403
ZIFs
  see zeolitic imidazolate frameworks
  adsorption behavior of 391
zinc 26–7, 34–5, 38, 127, 129, 132, 264, 317, 319, 321, 354, 356, 362, 364, 506
zinc atoms 457, 506–7, 533
ZPVE, *see* zero-point vibrational energy