

Index

a

- absolute rate theory (See also Transition State Theory) 277
- absorption line shape (NMR) 312–315
- activated carbon
 - adsorbents 520–524
 - with hierarchical pore structure 542–543
- activation energy (diffusion) 99, 521, 524, 825, 826
 - variation with carbon number (5A and NaX) 593, 616
 - in DDR-3 569
 - for diffusional motion 131
 - for intracrystalline diffusion 354, 476
 - for linear paraffins 593, 616
 - for long-range self-diffusion 549
 - for low-occupancy diffusion 258
 - for self-diffusion 108
 - van der Waals diameter 585
 - for xenon in NaX 638
- active sites 732, 820
 - for guest molecules 752
- additivity of resistances, principle 146
- adsorption–desorption cycles 408
- adsorption equilibrium 40, 93, 434, 443, 460, 743, 783
- adsorption isotherms 743
 - of CO₂ and CH₄ in ZIF-8 745
- adsorption/desorption kinetics 143–189
 - concentration profiles for 154, 164–167, 174–175, 177–179, 400, 420, 700, 749
 - effective diffusivity ratios 172
 - from liquid phase 686–688
 - numerical simulations 173
- AlPO₄-5 membrane 780
- aluminophosphates 3
- amorphous microporous materials
 - diffusion in microporous carbon 520–524
 - diffusion in microporous glass 518–520
- angular velocity 243, 308
- anisotropic diffusion 10, 601, 703–710, 759
 - in binary adsorbed phase 710
 - diffusion/rearrangement model 451
- anisotropy of real crystals 710–712
- anomalous diffusion 27, 47
 - fractal geometry 49–52
 - probability distribution functions of residence time and jump length 47–49
- aromatic hydrocarbons, diffusion 300, 624–631, 676–686
 - benzene 627–631, 676–681
 - C₈ aromatics 624–627, 681–686
- Arrhenius plots 369, 573, 576, 583, 595, 600, 662, 668–672, 678, 681, 708, 761, 813
- atomistic modeling 202, 203
- axial diffusion 42
- 3A zeolite
 - reduction in window size 593
- 4A zeolite
 - activation energies 585
 - diffusion in 571–573
 - gravimetric uptake curves 591
 - near isothermal behavior 430
 - summary of diffusivity of data for 574, 575
- 5A zeolite
 - comparison of zeolite samples 581, 582
 - for cyclopropane and *cis*-butene in 476
 - diffusion in 573–582, 595–596
 - general patterns for diffusion in 582–586
 - dimensionless HETP (H/d) vs. ($Dm/\epsilon vd$) for sorbates in 479
 - experimental uptake curves 184, 572, 579
 - HETP vs. cyclopropane and *cis*-butene in 476
 - intra-cage jumpss 581

- measurement techniques 581, 582
 - with different crystal sizes 579, 580
 - uptake rate 576, 579
 - PFG NMR signal attenuation curves 580
- b**
- bed of microporous particles, diffusion 545
 - expressions for diffusion in a continuum with 547
 - mathematical modeling, approaches by 546
 - multicomponent systems 550–552
 - temperature dependence 548–550
 - benzene, diffusion of (see also aromatic hydrocarbons) 676–686
 - Arrhenius plot 678, 680
 - benzene microdynamics 680, 681
 - concentration dependence of 679
 - diffusivity data in silicalite/ZSM-5 676, 677
 - frequency response spectra, in silicalite 454
 - self- and transport diffusion 680
 - Berty reactor 441
 - binary Langmuir isotherm (see also Langmuirian system) 14, 15, 46, 65–71, 74, 185, 784, 795
 - biporous adsorbent 143, 144, 156, 158, 429, 445, 461, 463, 465
 - dual diffusion resistance model for 157
 - transient concentration profile, schematic diagram 144
 - uptake curves 156
 - boggsite (BOG) 130
 - Boltzmann distribution
 - initial momenta 287
 - of velocities 271, 282
 - Boltzmann factor 100, 212, 283, 307
 - Boltzmann–Matano method 414
 - Boltzmann transformation 162, 414
 - Born's approximation 328
 - boundary, absorbing 37–39
 - boundary conditions
 - absorbing and reflecting boundaries 35–38
 - diffusion and permeation, combined impact of 40–42
 - matching conditions 39, 40
 - partially reflecting boundary 38, 39
 - boundary surfaces 298, 299
 - branched and cyclic paraffins 666
 - C₆ isomers, comparison of diffusivities for 670–673
 - cyclohexane and alkyl cyclohexanes 669, 670
 - diffusion
 - isobutane at high loadings 674–676
 - linear and branched hydrocarbons, comparison 673, 674
 - 2,2-dimethylbutane 670
 - isobutane at low loadings 667–669
 - summary of diffusivity data 667
 - Brownian migration 7, 8
 - brute force molecular dynamics 275, 277, 287, 291, 294, 297, 299
 - self diffusivity 297
 - time scale limitation of 287
 - iso-butane:
 - diffusion of iso-butane in silicalite 668, 676
 - MOFs 737
 - NaX 610, 613, 615, 622, 623, 642
 - n*-butane
 - *n*-butane–perfluoromethane, selective diffusion measurement 641
 - central torsion angle 209
 - counter-diffusion of isobutane and 720
 - diffusivity data in CuBTC 738
 - diffusion in 5A 578–581
 - diffusion in silicalite 660, 661, 668
 - effective self-diffusion coefficient for 549
 - evolution of distribution 401
 - gravimetric sorption curves, in Linde 5A crystals 579
 - influence of loading on the selectivity 781
 - in NaX crystals 614
 - and *n*-hexane, diffusivities for 673
 - NMR relaxation times 581
 - perm-selectivity 776, 799
 - self-diffusivities of 715, 737
 - variation of diffusivity, with ion exchange 592
- c**
- Ca²⁺ cations 369, 562–564, 591, 619
 - cage-to-cage jumps 104–106
 - cage-type zeolites 64
 - Cahn balance 428
 - canonical partition function 197, 286
 - capillary condensation 97, 98, 216, 217, 518, 534, 544, 552
 - Carberry mixer 614, 615
 - carbonaceous materials, oxidation of 520
 - carbon molecular sieves 18, 521–524
 - size-selective feature of 524
 - carbon nanotubes 64, 118
 - carbon number, variation of diffusivity with 593–595, 616, 661, 662
 - C₈ aromatics (see also aromatic hydrocarbons)
 - diffusion of 624–627, 681, 682
 - equilibrium concentration of isomers 828

- frequency response data for *p*-xylene 684, 685
- gravimetric uptake curves 683
- isomerization of 826
- loop for typical refinery 826
- macroscopic measurements 624, 625
- membrane permeation studies, evidence from 685, 686, 782
- microscopic measurements, comparison with 625, 626
- molecular sieve behavior 659
- *o*-xylene and *m*-xylene, diffusion of 624–626, 686
- in silicalite/ZSM-5 682
- uptake curves 681, 683
- TZLC and TZLC measurements 683, 684
- Car–Parrinello molecular dynamics (CPMD) 257
- carrier gas, effect of 644, 645
- Carr–Purcell–Meiboom–Gill (CPMG) pulse sequences 323–325
- Cartesian coordinates 195, 235, 236, 242, 249, 251, 254
- cascades for separation processes 802
- catalytic cracking 670, 823–825
- cation-free eight-ring structures 567
 - diffusion of CO₂ and CH₄ in DDR 569–571
 - effect of window dimensions 567–569
 - window dimensions, effect of 567–569
- central limit theorem 30, 31, 55, 365, 759
- Cerjan–Miller type algorithms 292
- CHA zeolites
 - diffusion in 568, 601, 791
 - structure 562
- chabazite 562, 564, 565
- Chapman–Enskog kinetic theory 94
- chemical diffusion 8
- chemical potential 12–16, 215, 217
- chemical shielding 318
- chemical shift 318–320, 361, 362, 602, 647
- chromatographic methods 459–482
 - chromatographic column, element of 461
 - chromatographic column, mathematical model for 460
 - form of response curves 463–464
 - time domain solutions 462–463
 - inert carrier 460
 - intraparticle diffusion
 - with adsorbable components 481–483
 - chromatographic column, mathematical model for 460–464
 - concentration profile, direct measurement of 480–481
 - limited penetration regime 480
 - moments analysis 464–468
 - step response 479–480
 - wall-coated column 480
- moments analysis 464–468
- first/second moments 464–466
- HETP/van Deemter equation 466–468
- higher moments, use of 466
- C₆ hydrocarbons 522 (see also benzene, hexane)
- closed-system simulation 222
- clustering effect 32
- CO₂–CH₄/SAPO-34 system 74
- CO₂–CH₄ separation 798
 - membranes performance 798
- coarse-graining 222–224
- coefficients of transport diffusion 8
- coherent scattering function 331, 332
- coke deposition 827, 833, 834
 - on diffusion of methane in H-ZSM-5, effect of 834
- COMPASS force field 198
- compensation effect 40, 311, 315, 383, 416, 549, 550, 802
- competitive adsorption 87
- composite particles 545
 - approaches by mathematical modeling 546
 - MCM-41 556
 - multicomponent systems 550–552
 - temperature dependence 548–550
 - variation of long-range diffusivity, for composite pellet 548
- computer reconstruction 204
- concentration dependent systems, adsorption/desorption curves 172
- concentration profiles, measurement of 480, 481, 819
 - frequency ranges of different techniques 396
 - intracrystalline, of isobutane 700
 - simulated 759
 - through membrane 785
 - transient 152, 695
 - of deuterated propane 748
 - of propane in nanoporous crystal 749
- condensation in capillaries 97, 98, 216, 217, 534, 552
- condensed phase 552, 553
- condition number 238
- configurational integral 197
- configurationally biased insertions 220
- configuration-space probability density 207, 211
- conservation equation 5, 62
- constant-diffusivity system 148, 151, 756

- constant field gradient NMR 359, 377
- constant pressure (infinite volume) systems 175
- constant stress tensor 210
- constraint forces 250, 251
- continuous time random walk (CTRW) 47
- controlled porous glasses (CPG) 339
- corrected diffusivities (D_0) 13, 14, 70, 73, 74, 77–79, 185, 233, 258, 265, 333, 520, 536, 537, 566, 570, 573, 581, 595, 625, 627, 629, 635, 636, 676, 683, 687, 689, 712, 736, 737, 738, 742, 753, 785, 790, 832
- correlation effects 33–35
 - correlated anisotropy 35
 - vacancy correlations 33–35
- correlation factor 34, 35
- correlation function (of electric field vector) 228–230, 338, 340
- correlation time 276, 281, 312, 313, 581
- Coulombic interactions 199, 202, 203
- counter diffusion 68, 91, 101, 119, 130, 135, 186, 187, 400, 439, 498, 718, 720, 742, 814
- covalent organic frameworks (COFs) 264
- crystal framework 747
- crystallite radii 353, 354, 365, 367, 402
- cyclohexane
 - diffusion 519, 520, 672
 - in hierarchical activated carbon 543
 - measurements with 519
 - PFG NMR 541
 - sorption times 694
 - transient uptake curves 554
- d**
- Danckwerts boundary conditions 468
- Darken equation 13, 101, 233
- DDR-3 membrane 790
 - diffusion of CO_2 – CH_4 mixtures in 570
 - SEM photomicrographs 772
 - variation of permeance with kinetic diameter 774
- DDR (ZSM-58),
 - diffusion in 567–571
 - structure of 565
- de Broglie wavelength 326
- density functional theory (DFT) 201, 257
 - approximation 204
- desorption curves
 - theoretical 161, 178, 179
 - experimental 168, 169, 179
- desorption kinetics 160–179
 - effective diffusivity ratios 172
 - experimental concentration profiles 154, 409, 705, 749
 - theoretical profiles 164–167
- detours 760
- deuterated benzene molecules, theoretical ^2H NMR line shapes 322
- deuterated species in PFG NMR 362, 640
- deuterium NMR 322, 323
- diatomic molecule, description of configuration 195
- diffusion
 - activated 87, 99–106, 151
 - face-centered cubic crystal 99
 - anisotropy (*See* diffusion anisotropy)
 - barriers 336
 - bed 158, 159, 160, 179, 180, 431, 432, 444, 591, 624
 - in binary adsorbed phase 64
 - in carbon sieves 522, 524
 - cation in zeolite 402
 - of CO_2 and CH_4 in DDR 569–571
 - co- and counter 395, 400, 438, 718
 - in composite particles 494, 545
 - concentration dependence 5, 14, 74, 101, 114, 172, 508, 535, 536, 609, 621, 629, 634, 643, 734, 737, 749, 790
 - configurational 17, 85
 - corrected 13, 14, 74, 77, 104, 268, 536, 566, 571, 583, 636, 684, 742, 785, 832
 - deviation from ordinary 114
 - driving force 5, 14, 60, 177, 230, 743, 773, 776
 - elementary process 21, 45, 317, 395
 - in fractals 49, 50, 53, 54, 56, 113, 114
 - gas 4, 5, 43, 91, 98, 151, 160, 382
 - inter, two identical species 65
 - intracrystalline 10, 22, 23, 120, 150, 157, 371, 377, 378, 414, 441, 476, 505, 518, 582, 601, 627, 633, 646, 695, 734, 759, 763, 817, 820, 825
 - in ion exchange resins 500
 - Knudsen 96, 370, 503, 518, 533, 792
 - limitation (of reaction) 811
 - in liquid filled pores 80, 538, 687
 - low-temperature 299
 - macroscopic 42
 - measurements (*See* diffusion measurements)
 - model 172, 173, 462
 - molecular dynamics (MD) simulation of 72, 117, 249, 257, 271, 319, 661, 736, 753, 754
 - molecular 92, 96, 532, 548
 - momentum transfer in 5, 94, 271
 - Monte Carlo simulation of 44, 123, 206, 294, 295, 588, 618, 701, 713, 714

- phenomena 206, 337
- in porous glass 518, 519, 530, 554
- principles 143
- and reaction 807–809, 816, 832
- regimes, size-selective molecular sieving 85–87
- resistances 94, 156–160, 184
 - macropore and micropore 17
 - in nanoporous media 17, 18
- restricted 75, 125, 276, 381, 382, 530 (*See also* diffusional restrictions, zeolite catalysts)
- self and transport
 - single file 34, 49, 56, 111–121, 123, 135–138, 750
 - in sinusoidal field 107
 - in solids 99
 - Stefan-Maxwell 13, 45, 68, 69 (*see also* Maxwell-Stefan)
 - steric hindrance 75, 498, 539, 566, 623, 688, 779, 825
 - surface 75, 89, 93, 96, 98, 530, 531, 533–536, 539
 - tensor 11, 296, 362, 363, 708
 - thermal 63
 - tracer 21, 32, 741, 743
 - in zeolite A 45, 104, 566–567, 571–600
 - in zeolite X and Y 208, 607–648
 - in ZSM-5 (*See also* silicalite) 653–720
- with simple jump model 44–47
- diffusional restrictions, zeolite catalysts 822
 - activation energies 825, 826
 - catalytic cracking over HZSM-5 824, 825
 - catalytic cracking over zeolite Y 823, 824
 - MTG reaction 830, 831
 - MTO Process 831–833
 - size exclusion 822, 823
 - toluene, selective disproportionation of 828–830
 - xylene isomerization 826–828
- diffusion anisotropy 10, 601, 703–710, 759
 - comparison of measured profiles 704
 - correlation rule for structure-directed diffusion anisotropy 703, 704
 - evidence by PFG NMR measurements 705–707
 - host structure, evidence 364
 - limits of correlation rule 707–710
 - powder measurement 363, 364
 - single-crystal measurements 362, 363
- diffusion coefficients 13
 - anomalous transport diffusion 45
 - liquid phase 67
 - measurement 504
 - thermodynamically corrected 13
- diffusion-controlled system
 - concentration profiles during desorption 496
 - dynamic behavior of 462
 - uptake scales 421
- diffusion measurements
 - alternative approaches 362
 - data analysis 356–358
 - with different nuclei 379, 380
 - different regimes of 364–379
 - intracrystalline 365
 - long-range 368, 369
 - in long-time limit 367, 368
 - in short-time limit 365–367
 - tortuosity factor and mechanism 369, 370
 - experimental conditions, limitations, and options for 355
 - experimental issues for observing light scattering phenomena 339–343
 - extra-large stray-field gradients, benefit of 359
 - filter techniques 341–343
 - Fourier-transform 361, 362
 - gradient pulse mismatch 358
 - impedance by contaminants 360
 - impedance by internal gradients 359, 360
 - index matching 339, 340
 - interference microscopy technique 404
 - by light scattering 337–343
 - mechanical instabilities 358, 359
 - by monitoring molecular displacement 347
 - multicomponent systems, self-diffusion measurement 361
 - optical mixing techniques 340, 341
 - by PFG NMR technique 348
 - pitfalls 358
 - sample preparation 355, 356
 - single-molecule observation 383
 - fluorescence microscopy, basic principles of 384, 385
 - nanoporous materials, correlating structure/mass transfer 388, 389
 - time averaging vs. ensemble averaging 385–388
 - theory 337–339
- diffusion statistical mechanics 227–235
 - mass fluxes in microporous medium 229–232
 - transport in pure and mixed sorbates 232–234
 - self-diffusivity 227–229
- diffusivities 160, 161, 176, 411. *See also* diffusion
 - definition of 4

- long-range 354
 - permeabilities 757
 - diffusivity ratio 170
 - variation 163
 - digital (photo-count) autocorrelation techniques 341
 - 2,2-dimethylbutane (2,2-DMB), permeation fluxes and profiles 788
 - Dirac delta function 280, 460
 - discrepancy between micro and macro diffusivity values 632, 633
 - DDR
 - diffusion of CO₂ and CH₄ in 569–571
 - structure of 565
 - domain decomposition 241
 - Doppler shift 326
 - double refraction method, schematic representation 398
 - drag 45, 60, 98, 742
 - drift velocity 267
 - driving force, for diffusion 5, 12
 - experimental evidence 15, 16
 - gradient of chemical potential 12–15
 - transport and self-diffusivities, relationship between 16, 17
 - dual control volume grand canonical molecular dynamics (DCV-GCMD) 269–272
 - application 269
 - role of control volumes 272
 - dual diffusion resistance model, for biporous particle 157
 - dusty gas model 94
 - dynamical correction factor 281–283, 291
 - dynamically corrected transition state theory 296
- e**
- echo attenuation, for two-region diffusion 376
 - effective diffusivity 151, 170, 171, 524, 525
 - effectiveness factor 808
 - n*-eicosane, atomistic and coarse grained representation 224
 - eight-ring zeolites 561–603
 - anisotropic diffusion in CHA 602, 603
 - 3A zeolites 592
 - carbon number, variation of diffusivity with 593–595
 - cation hydration 563, 564
 - concentration and temperature dependence of diffusivity 566, 567
 - diffusion in NaCaA zeolites 591, 592
 - effective medium approximation 590, 591
 - kinetic behavior of commercial 5A 597–599
 - loading dependence of self-diffusivity 595
 - Monte Carlo simulations 588–590
 - pelletization, effects of 599–602
 - self-diffusivity of water in ZK4 596
 - structure of
 - CHA 564, 565
 - DDR 565
 - LTA 562, 563
 - water vapor, effects of 596, 597
 - window dimensions 565
 - Einstein relation 7, 28, 41, 294, 305, 356, 357, 421
 - for ordinary diffusion 113, 114
 - regime of diffusion 275
 - Einstein–Smoluchowski equation 28
 - electric field (in light scattering) 337, 338, 340
 - electron spin resonance (ESR) 402, 403
 - elementary diffusion processes
 - measurement 305–343
 - by light scattering 337–343
 - by neutron scattering 326–336
 - NMR spectroscopy 306–326
 - empirical tortuosity factors, for diffusion in liquid-filled pores 538
 - energy of activation. *See* activation energy
 - entropy 61, 87, 103, 524
 - production by internal processes 66
 - rate of generation of 61–63
 - entropy of sorption, alkanes in silicalite 221
 - equations of motion 195, 196, 236, 242, 244, 247, 251, 252, 255, 257, 267, 287
 - equilibrium-controlled permeation 779
 - equilibrium isotherm 382, 437, 449, 536, 569, 776, 789
 - equilibrium molecular dynamics (EMD) simulations 227, 235–265, 271
 - constraint dynamics in Cartesian coordinates 249–253
 - domain decomposition 241
 - extended ensemble molecular dynamics 253–257
 - integrating the equations of motion, velocity Verlet algorithm 235–238
 - to mixed sorbates, application 259–265
 - multiple time step algorithms, rRESPA 238–240
 - to pure sorbates, example application 257–259
 - rigid linear molecules, molecular dynamics of 241–244
 - rigid nonlinear molecules 245–249
 - equipartition theorem 255

- ergodic hypothesis 338
- ethane selectivity, for permeation 789
- ethyl benzene, piezometric uptake curve 435
- Eulerian angles 245–247
- Ewald summation technique 203
- excess chemical potential 218
- relation to fugacity 218
 - calculation by Widom insertion 219
 - calculation by configurationally biased insertion 222
- experimental evidence
- findings referred to single-file diffusion 132, 135
 - catalysis 138, 139
 - pulsed field gradient NMR 135, 136
 - quasi-elastic neutron scattering 136, 137
 - tracer exchange and transient sorption experiments 137, 138
 - ideal vs. real structure of single-file host systems 132–135
- experimental methods
- classification 19–24
- external field non-equilibrium molecular dynamics (EFNEMD) 266–269, 271
- f**
- Fabry–Perot interferometers 342
- fast tracer desorption 376, 601
- Feynman–Hibbs correction 636
- Fickian diffusivity 14, 16, 46, 90, 103
- dependencies 334
 - equation 6, 416, 485
 - model 792
- Fick's first law 4, 12, 61, 356, 378, 406
- Fick's second law 5, 265, 414
- film resistance 20, 144, 179, 441, 489, 809, 812, 817
- filter techniques (light scattering) 341, 342
- Fincham's LEN algorithm 257
- finite single-file systems 119
- catalytic reactions 123
 - adapting analysis for normal diffusion 123–125
 - dynamic Monte Carlo simulations 123
 - molecular traffic control 130–132
 - rigorous treatment 125–129
 - mean square displacement 119, 120
 - tracer exchange 120–122
- flame ionization detector (FID) 470, 484
- flexible zeolite model 201
- fluctuation in number of sorbed molecules 213, 214
- fluctuations in composition 229, 481
- fluid–solid contactors 143
- fluorescence microscopy 819
- fluorine compounds (diffusion of) 637, 638
- focal plane array (FPA) detector 405
- force fields 197–203
- Fourier transform 314, 318, 330, 334, 342, 453
- of PFG NMR spin echo attenuation 339, 352, 359, 361, 371, 374, 528, 734
 - of stationary NMR spectrum 313
- Fourier transform IR spectroscopy (FTIR) 399, 400, 405, 437
- fractal geometry 49–52
- fractal model, for system of parallel cylindrical pores 52
- frames of reference 9, 10
- for binary system 10
 - diffusivity for adsorbed phase 10
 - interdiffusion process 9
 - total volumetric flux 9
- framework type code (FTC) 202
- free energy methods 217–222
- free induction decay 313, 314
- free volume theory 108, 612
- frequency response 22, 23, 436, 451, 455, 627, 681, 684, 686
- experimental systems 452–454
 - in flow system 455, 456
 - measurements 519
 - limits 451–452
 - temperature frequency response 451
 - theoretical model 448–451
 - tracer exchange rates 447
- g**
- gas diffusion 382
- gaseous adsorption systems 473
- gasoline range (C₅–C₁₀)
- hydrocarbons 830
- gasoline yield 831
- gas–solid adsorption systems 43
- gauche*–*trans* conformational isomerizations 238
- Gaussian approximation 330
- Gaussian curve 329
- Gaussian distributions 42, 203
- probability 305, 421
- Gaussian response 463
- Gear predictor-corrector algorithm 253
- Geiger–Müller counter 446
- generalized Maxwell–Stefan equations (see also Maxwell–Stefan model) 67
- application of 72
 - diffusion in adsorbed phase 68–70
 - general formulation 67, 68

- Gibbs–Duhem equation 229, 231
 Gibbs energy 98, 210, 218, 286
 Gibbs ensemble Monte Carlo (GEMC) 215
 Glueckauf approximation 465
 Goring's diffusion measurements 825
 gradient relaxation molecular dynamics (GRMD) 265, 266, 268
 Graham's law 4
 grand canonical Monte Carlo (GCMC) simulations 212, 257, 264, 265, 269, 332, 745
 – selection criteria 269
 grand partition function 211
 gravimetric methods
 – gravimetric uptake (GU) measurements 427–432, 520
 – tracer exchange rates 427
 – bed diffusional resistance, intrusion of 431–432
 – experimental system 428–429, 432
 – heat effects, intrusion of 429–430
 – negligible thermal effects, criterion for 430–431
 – response curves analysis 429
 Green–Kubo equation 229, 233
 guest diffusion
 – in ferrierite 722, 723
 – in nanoporous materials 35
 guest uptake, nanoporous host 413
 gyromagnetic ratio 308, 330, 352, 357, 369, 637, 639
- h**
- Habgood model 785, 789
 Hahn echo (HE) pulse sequences 323
 Hahn's spin echo (runners' model) 323, 324
 Hamilton's equations of motion 196
 Hartree–Fock theory 201
 H₂/CH₄ perm-selectivity 800
 heat fluxes 62, 63, 816
 heat transfer
 – limitations 455
 – resistance 182, 184, 429, 470, 815–817
 Heaviside step function 279, 280, 290
 He–CH₄ carriers 483
 height equivalent to theoretical plate (HETP) 467, 476
 Heisenberg's uncertainty principle 197
 Helmholtz energy 197, 211, 218, 286
 Henry constants 491, 633, 775
 – of alkanes in silicalite 221
 Henry's law 14, 201, 218, 233, 460, 510
 – region 482, 503, 506, 774, 813
 heptane–benzene mixture, experimental uptake curves 188
 Hermite interpolation scheme 202
 Hessian matrix 284, 288
 hexamethyldisilazane 533
n-hexane 519
 – activation energies for long-range self-diffusion 549
 – adsorption branch perm-porosimetry curves for 795
 – Arrhenius plot 672
 – blocking effect 835
 – cracking 823, 825, 830
 – diffusivities
 – derived from high temperature 673
 – measurements 519
 – in Na75CaX 619
 – in porous silicon 537
 – in silicalite 208, 687, 795, 796
 – effective self-diffusion coefficient 549
 – hydroisomerization of 139
 – and 3-methylpentane, over NaA 822
 – relative effective diffusivities for 366
 – saturation capacities for H-ZSM-5 and silicalite. 657
 – self-diffusivities of 536
n-hexane–silicalite
 – experimental perm-porosimetry curves, comparison of 796
 hierarchical pore systems 539
 – activated carbon with interpenetrating micro- and mesopores 541–544
 – in mesoporous zeolites 544, 545
 – ordered mesoporous material SBA-15 539–541
 HKUST-1 structure 732, 733
 homodyne measurement 340
 van Hove correlation function 329
 hydrogen bonding 521
 hydrothermal treatment (of zeolite A) 597, 598
 hyperpolarization 308
 hysteresis effects 215, 541, 553–555, 554, 631
 HZSM-5 based catalysts 824, 831
- i**
- ideal adsorbed solution theory (IAST) 789
 ideal gas 12, 209, 210, 215, 219, 220
 imidazolate (IM) 739
 inert carrier 460, 644, 645
 inertia tensor 245
 infrared microscopy measurements (IRM) 397, 519
 infrequent event techniques 105, 275–301

- dynamical correction factor 281–283
- example applications 296–300
- kinetic Monte Carlo simulation 293–295
- diffusivities in zeolites 296–300
- master equation 292, 293
- analytical solution 295, 296
- multidimensional transition state theory 283–289
- of multistate multidimensional systems 290, 291
- numerical methods for 291, 292
- rate constant expression 276–281
- self-diffusivity
 - at high occupancy 300
 - at low occupancies 296–300
- for simulating diffusion in microporous solids 275–300
- statistical mechanics 276–292
- time scale separation 276–281
- tracking temporal evolution in network of states 292–296
- transition state theory (TST) approximation 281–283
- inhomogeneous field effect 316
- integral measurements 169, 443
- integral sorption curves
 - analysis 170
 - for butylene and propylene 169
- interaction energy 102, 103, 307, 317, 320, 325, 380, 567, 743
- interference microscopy (IFM) 154, 379, 395, 397, 399, 400, 819, 821
 - diffusion measurements 750
 - monitoring intracrystalline concentration profiles 403–408, 408–415
 - Boltzmann's integration method 414–415
 - data analysis 406–408
 - principles of measurement 403–406
 - self-diffusivities and transport diffusivities 412
 - surface resistances, relevance of 413
 - transient sorption experiments, visualizing guest profiles 412–413
- interferometer, Fabry-Perot 342
- intermolecular interactions 219
- interstitial diffusion 283
- intracrystalline barriers 696, 697
 - evidence from PFG NMR diffusion studies 701, 702
- intracrystalline diffusion 10, 17, 85, 124, 354, 366, 367, 377, 379, 417, 482, 518, 561, 599, 602, 693, 758, 811, 817, 820, 835
 - for hydrocarbons in H-ZSM-5 819
 - measurements 486
 - PFG NMR measurements of 358, 377
 - intracrystalline mean life time 124, 137–139, 375
 - intraparticle diffusion 459
 - chromatographic measurements 470
 - dead volume 471
 - experimental conditions 470–472
 - chromatographic method
 - with adsorbable components 481–483
 - chromatographic column, mathematical model for 460–464
 - concentration profile, direct measurement of 480–481
 - limited penetration regime 480
 - moments analysis 464–468
 - step response 479–480
 - wall-coated column 480
 - experimental data, analysis of 472–473
 - axial dispersion, intrusion of 477–479
 - liquid systems 473
 - vapor phase systems 473–477
 - long-column approximation 468
 - heat transfer resistance 470
 - nonlinear equilibrium 469–470
 - pressure drop 468–469
 - membrane permeation measurements 501–510
 - temporal analysis of products (TAP) system 500–501
 - zero-length column (ZLC) method 483
 - counter-current ZLC (CCZLC) 498
 - deviations 489
 - extensions of 497–500
 - fluid film resistance 489
 - fluid phase hold-up 490–491
 - heat effects 492–493
 - intraparticle diffusion control, theory 485–486
 - isotherm nonlinearity, effect of 491–492
 - liquid phase measurements 498–500
 - macroporous particles, diffusion 488–489
 - practical considerations 493–497
 - principle of 483–485
 - short-time behavior 486–488
 - surface resistance, measurement 489–490
 - tracer ZLC 497–498
- intrinsic diffusivity 776
- intrinsic selectivity 774
- IR micro-imaging/microscopy (IRM) 379, 395, 400, 403, 740
 - intracrystalline concentration profiles, monitoring 403–408, 408–415
 - Boltzmann's integration method 414–415

- data analysis 406–408
- principles of measurement 403–406
- self-diffusivities and transport diffusivities 412
- surface resistances, relevance of 413
- transient sorption experiments, visualizing guest profiles 412–413
- irreversible adsorption model 176
- irreversible process 351
- isosteric heat of sorption 214, 218
 - of alkanes in silicalite 221
- isomerization of xylenes 659, 826, 827
- isothermal approximation 63, 64, 182–185, 492
- isothermal binary system 5
- isothermal diffusion model 167
- isothermal–isostress simulations 210
- isothermal linear dual-resistance systems 151–160
 - surface resistance plus internal diffusion 151, 152
 - transient concentration profiles 152–156
 - two diffusional resistances (biporous solid) 156–160
- isothermal linear single-resistance systems 145–151
 - external fluid film/surface resistance control 145, 146
 - macropore diffusion control 149–151
 - micropore diffusion control 146–149
 - particle shape effect 149
- isothermal MD simulation 132
- isothermal nonlinear systems 160–179
 - adsorption/desorption rates and effective diffusivities 170–172
 - adsorption profiles 162–165
 - approximate analytic representations 172
 - desorption profiles 165–167
 - experimental uptake rate data 167–170
 - linear driving force approximation 172, 173
 - macropore diffusion control 160, 161
 - micropore diffusion control 160
 - semi-infinite medium 161, 162
 - shrinking core model 173–176
 - surface resistance control–nonlinear systems 176–179
- isotherm nonlinearity effect 491
- isotropic diffusion 7, 363
- isotropic medium 10

j

- jump models 331
- Juttner modulus 808

k

- Kelvin equation 793
- kinetic energy function 196
- kinetic equation 278
- kinetic Monte Carlo simulation (KMC) 276, 293–295
 - for prediction of diffusivities in zeolites 296–300
- kinetic theory of gases 88, 421
- Kirchhoff's law 293
- Knudsen diffusion 17, 49, 88, 89, 92, 150, 382, 501, 503, 504, 518, 525, 800
- Knudsen flux 96, 98, 792
- Koch curve 50, 51

l

- Lagrange multipliers 251, 252
- Lambert–Beer law 406
- laminar fluid film 145
- Langmuirian systems 162, 167, 176, 431, 491, 503, 776, 787, 789
 - effective integral diffusivity with diffusivity ratio, variation 171
 - flow through membrane and time delay 507
 - theoretical adsorption and desorption curves for 178
 - transient behavior of 506
- Langmuir isotherm 46, 74, 101, 173, 736, 784, 795
- Laplace transform 444, 467
- large-scale atomic molecular massively parallel simulator (LAMMPS) 241
- Larmor condition 308, 311
- Larmor frequencies 314, 315
 - of nuclear spins 361
- lattice coordination number 34
- Legendre transformation 196, 210, 211
- LEN algorithm 243, 244
- Lennard-Jones interactions 254
- Lennard-Jones (LJ) potential 199, 202, 238
- Lennard-Jones simulations 271
- levitation effect 131, 132, 617
- light scattering 305, 326, 337, 339, 340
- linear alkanes
 - Arrhenius plots 662
 - comparison of self-diffusivities of *n*-alkanes at low loadings 661
 - diffusivity data for *n*-alkanes 660
 - loading dependence of diffusivity 665
 - macroscale measurements 663, 664
 - microdynamic behavior 665
 - microscale measurements 661
 - molecular simulations 665, 666

- variation of PFG NMR self-diffusivity 666
- linear and branched hydrocarbons, differences in diffusional behavior 702, 703
- linear driving force (LDF) model 462, 465
 - approximation 173
- linear response theory 230
- linear system 165, 171
- line width 312–314, 317, 320, 361, 647
- liquid-filled pores
 - diffusion 538, 539
 - at high loadings 80, 81
 - flux expressions reduce to 81
 - Habgood model 81
 - mutual diffusion effects 81
- liquid phase diffusion 538
- liquid scintillation counting (LSC) 446, 447
- liquid ZLC measurements 500
- loading dependence 75
 - molecular simulation 78
 - self-diffusivities 75–77
 - structural defects, effect of 78, 80
 - transport diffusivities 77, 78
- long tail behavior 470
- Löwenstein's rule 201
- LTA zeolites (see also Zeolite A)
 - cation sites 562, 563
 - diffusion in 565–567, 571–601
 - structure 562–564
 - diffusion of water vapor 595, 596
 - membrane 797
- m**
- macrodiffusivity 43
- macro FTIR technique 437
- macro IR sorption rate measurements, experimental system 438
- macro/meso-pore sizes 518
- macropore control 150, 169, 493
- macropore diffusion 42–44, 151, 176, 179, 463
 - analysis 185
 - controlled system 160, 164
 - determination, in catalyst particle under reaction conditions 526, 527
 - diffusional resistance 476
- macropores 17, 18, 143, 463, 510, 546, 550, 556
- macroporous catalysts 807
- macroscopic experiments 761
- macroscopic flux 267
- macroscopic TZLC technique 541
- magic angle spinning (MAS) 323, 324
 - PFG NMR 358
 - self-diffusion studies 745
- magnetic dipole moment 308
- magnetic field, spin orientations in 309
- magnetic interaction energy 307
- magnetic moments, superposition 310
- magnetic resonance tomography (MRT) 348
- magnetization, specific (nuclear)
 - longitudinal 315
 - transverse 308
- Markov chain 206, 207
- mass fluxes 229
- mass transfer processes 9, 47, 173, 449, 456
 - coefficient 41, 145, 483
 - resistance at interface 40
- mass transfer rates 145
- mass transfer resistance 455, 460, 469, 477
- master equation 292, 293, 295, 296
 - analytical solution 295, 296
- matching condition 39, 40, 113
- mathematical modeling of sorption kinetics 145–185
- matter wave 326
- Maxwell–Boltzmann distribution 235
- Maxwell–Stefan diffusivities 227, 234, 262, 263, 737, 741, 742, 744, 748
- Maxwell–Stefan model 68–72, 784–791
 - diffusion in macro- and mesopores 74, 75
 - membrane permeation 73, 74, 784–791
 - parameter estimation 72, 73
- McBain balance 428
- MCM-41 crystal
 - anisotropic self-diffusion of water in 530
 - high-accuracy localized reaction 822
 - source and characterization 528, 529
- mean free path 88, 91, 368, 369, 551
- mean jump lengths 48
- mean square displacement 7, 8, 27, 28, 33, 48, 56, 117, 119, 275, 349, 363, 381, 525, 701, 710, 711
- membrane permeation measurements 501–510, 673, 684
 - steady-state permeability measurements 501–502
 - time lag measurements
 - linear systems 504–505
 - nonlinear systems 506–507
 - single-crystal membrane technique, evaluation of 507–508
 - single-crystal zeolite membrane 505–506
 - transient and steady-state measurements, comparison 510
 - transient Wicke–Kallenbach experiment 508–510
 - Wicke–Kallenbach steady-state method 503

- intracrystalline diffusion 503–504
- macro/mesopore diffusion measurements 503
- memory 9, 31, 47, 113, 114, 235, 276, 708, 710
- Menger sponge 50, 51
- mesopores 17, 75, 87, 96, 528, 544, 608, 619
- mesoporous membranes, diffusion through 530
 - measurement 400
- mesoporous silica 531, 532
 - modified mesoporous membranes 533
 - permeance measurements 532, 533
- mesoporous Vycor glass 530, 531
- metal organic frameworks (MOFs) 4, 113, 264, 416, 729, 730
 - breathing effects 751–754
 - CuBTC, guest diffusion 736–738
 - diffusion in MIL-53 751–754
 - HKUST-1 732
 - for H₂ separation 799–800
 - membranes 771
 - MOF-5, guest diffusion 733–736
 - pore segments in single-file arrangement 747–751
 - porous solids, class of 730–732
 - potential use of 732
 - surface resistance 754
 - activation energies 761–762
 - experimental observations 754–757
 - generalization of model 761
 - intracrystalline barriers 761
 - simulation results 758–759
 - surface barrier, conceptual model 757
 - surface permeability and intracrystalline diffusivity 759–760
 - with three-dimensional pore networks 760
 - unblocked entrance windows, fraction of 760–761
 - zeolitic imidazolate framework 8 (ZIF-8) 739
 - experimental self- and transport diffusivities 740–744
 - membrane-based gas separation 744–746
- Zn(tbip) 747–751
- methane
 - capillary condensation, binodal curves for 217
 - NMR diffusivity of 835
 - self-diffusivity 261
- methanol
 - adsorption 155
 - concentration, transient profiles 409
 - deuterated 387
 - diffusion and reaction 832
 - to gasoline (MTG) reaction 830–831
 - in NaX crystals 77
 - to olefins (MTO) reaction 831–833
 - over HZSM-5 831
 - uptake 417
 - to yield dimethyl ether (DME) 831
- methanol–ferrierite, theoretical transient adsorption and desorption curves 178, 179
- 3-methylpentane, cracking 823
 - in silicalite 208
- 2-methylpentane (2-MP), permeation fluxes 788
- Metropolis Monte Carlo 206
- MFI crystal structure 654, 655, 697–699
 - molecular sieve behavior 659
 - saturation capacity 655–659
 - for H-ZSM-5 and silicalite 657
 - zeolite crystals, self-diffusivity of water 381
- MFI-type zeolites 653
- micropore-controlled systems 151
- micropore diffusion 149
 - diffusional resistances 465, 807
- micropore/macropore diffusivities 445
 - chromatographic method, application of 464
- microporous carbon 398. *See also* carbon molecular sieves
 - diffusion in 520, 521, 524
 - PFG NMR 521
 - properties 52
- microscale studies 688
 - ammonia 689–691
 - hydrogen 691 692
 - tetrafluoromethane 688–689
 - water and methanol 689
- microscopic diffusivities 42–44
- microscopic techniques 412
- MIL-88A–D 752
- MIL-53 (Al, Cr), breathing behavior 751
- MIL-88 solids 731
- MIL-47 yield self-diffusivities 753
- mixed adsorbed phase, diffusion in 712
 - blocking effects by co-adsorbed second guest species 712
 - methane in presence of benzene 712, 713
 - methane in presence of pyridine and ammonia 713, 714
 - *n*-butane in presence of isobutane 714–716
- mobile phase model 106
 - diffusivity in self-diffusion experiment 107
 - transport diffusivity 107
- MOF crystal 423, 747

- MOF-5 (IRMOF-1) material 734
- activation energies 735
 - PFG NMR spin echo attenuations 734
 - self-diffusion coefficients of *n*-alkanes in 735
- MOF ZIF-8 752, 800
- cage arrangement in 740
- MOF Zn(tbip) 423
- molecular diffusion 17, 19, 96, 347, 501, 808
- molecular displacements 114, 115
- probability distribution 353
- molecular dynamics (MD) 116–118, 235–272, 275
- equilibrium molecular dynamics simulations 235–265
 - extended ensemble molecular dynamics simulations 253–257
 - non-equilibrium molecular dynamics simulations 265–272
 - predictions 262
- molecular mechanics-type expression 204
- molecular migration, feature of 305
- molecular models construction 193–224
- coarse-graining and mean force potentials 222–224
 - Monte Carlo simulation methods 206–217
 - sorption equilibria, free energy methods for 217–222
 - zeolite–sorbate systems, models and force fields 194–206
- molecular orientation 245
- molecular relaxation time 231
- molecular sieve behavior 659
- molecular simulations 78
- effect of structural defects 78–80
- molecular traffic control (MTC) 130
- for CH₄ and CF₄ 130
 - conditions, to be fulfilled by 131
- molecule–molecule interactions 520
- molecule–wall collisions 91
- moments, method of 21, 378, 444–445
- momentum transfer (in neutron scattering) 5, 271
- in gas distribution 94
- Monte Carlo (MC) simulation methods 44, 134, 206–217, 370, 371
- adapting analysis for normal diffusion 123–125
 - canonical Monte Carlo 207–210
 - Gibbs ensemble and gage cell Monte Carlo 215–217
 - grand canonical Monte Carlo 210–214
 - metropolis Monte Carlo algorithm 206, 207
 - of random walk 588
- morphology, influence on diffusion 193, 541
- Mulliken population analysis 200
- multicomponent systems, self-diffusion in 67, 73, 185, 361, 441, 637, 640, 645, 784
- evolving during catalytic conversion 645
 - cyclopropane into propene 645–647
 - isopropanol into acetone and propene 647, 648
 - hydrocarbons 640–643
 - benzene–perfluorobenzene 641
 - ethane–ethene 642, 643
 - *n*-butane–perfluoromethane 641, 642
 - *n*-heptane–benzene 640, 641
 - under influence of co-adsorption and carrier gases 643
 - effect of inert carrier gas 644, 645
 - effect of moisture 643
 - water and ammonia 643, 644
- multidimensional transition state theory 283–289
- multi-region approach 374
- multistate multidimensional systems 290, 291
- n**
- NaCaA crystals 402 (see also LTA)
- nanoporous host materials
- bulk phase of 422
 - host–guest systems 35
- nanoporous materials, deviations from normal diffusion in 55–57
- nanoporous particles 305
- two-dimensional model bed of 372
- nanoporous sol–gel glass, single-particle trajectories 386
- Nath, Escobedo, de Pablo (NERD) force fields parameters 200
- NaX, diffusion in 607–648
- NaX–methanol, transient temperature response 437
- self and transport diffusivities 78
- NaX zeolite crystals 165, 187, 205
- gravimetrically measured transient sorption curves 432
 - model bed 205
- neutron scattering 305, 326, 327, 336, 337
- diffusion measurements 326–336
 - evidence on elementary steps of diffusion 334
 - experimental procedure 326, 327
 - fundamental relations 330, 331
 - intermediate scattering function 334, 335
 - measurements 520

- principle of method 326, 327
 - range of measurement 335, 336
 - scattering patterns and molecular motion 330–336
 - theory 327–330
 - thermodynamic factor 331–334
 - neutron spin echo
 - applications 335
 - experiments 334
 - Newton–Raphson method 252
 - Newton’s second law of motion 196
 - nitrogen 639, 640
 - 4A micropores 476
 - curves for 522
 - experimental pore diffusivities 89
 - experimental studies 421
 - gyromagnetic ratio 639
 - kinetic selectivity 522
 - long-range diffusivity of 369
 - permeation properties of 717
 - sorption isotherms 213
 - in zeolite NaCaA 369, 572–573
 - non-adsorbing carrier. *See* inert carrier
 - non-equilibrium molecular dynamics (NEMD)
 - approaches 227, 265–272
 - dual control volume grand canonical molecular dynamics 269–272
 - external field NEMD 266–269
 - gradient relaxation method 265, 266
 - simulations 267
 - trajectory 266
 - non-isothermal systems 5, 179–185, 430, 451, 470, 815–817
 - experimental non-isothermal uptake curves 183–185
 - intraparticle diffusion control 181–183
 - nonisotropic system 10
 - nonlinear system, transient behavior 506
 - Nosé MD method 256
 - nuclear magnetic resonance spectroscopy (NMR) 305, 306–326, 307, 446
 - anisotropy of the chemical shift 320
 - basic principles, behavior of isolated spins 306–309
 - behavior of nuclear spins in compact material 309–318
 - classical treatment 306–308
 - experiments 204, 310
 - field gradient method 379
 - fundamentals of line shape 311
 - imaging 481
 - impact 323–326
 - molecular motion effect on line shape 311–314
 - pulse measurements fundamentals 314–318
 - quadrupole NMR 320–323
 - quantum mechanical treatment 308, 309
 - resonance shifts by different surroundings 318–323
 - schematic representation of 314
 - self-diffusion measurements 352
 - signal intensity 356
 - spin echo 327, 335
 - spin-mapping 348
 - spins in different chemical surroundings 318–320
 - tracer desorption curves 376, 380
 - tracer desorption experiment 377
 - tracer exchange measurements 383
 - zeugmatography 348, 402
 - nuclear spin 306, 308, 309, 348, 380, 400, 402
- o**
- n*-octane 223
 - diffusion in NaY, USY and NaX 618, 619
 - extrapolation of 619
 - intracrystalline diffusivities of 619
 - in NaX 621
 - NMR self-diffusivity 610
 - PFG NMR measurements 618
 - Ohm’s law 61
 - olefins
 - in AgNaX 623
 - C₃/C₂, equilibrium ratio of 832
 - crystal size on 833
 - higher 831
 - light 623
 - methanol to 831
 - reduction in diffusivity 623
 - translational mobility of 623
 - yield, influence of crystal size on 833
 - one-component sorbate system 214
 - one-dimensional system 153
 - one-dimensional transport 112
 - Onsager coefficients 61, 230, 234, 264
 - Onsager reciprocity relations 61, 234
 - Onsager’s regression theorem 339
 - open micropore systems 106, 527, 528
 - estimating loading dependence 108
 - mobile phase model 106, 107
 - sinusoidal field 107, 108
 - organic linkers 731
 - oxygen
 - in Bergbau-Forschung sieve 522
 - bridges in zeolites 739
 - centers of 608
 - zeolite crystal structure 201

p

- paraffins
 - HZSM-5 824
 - selectoforming process 825
 - solubility of 696
- paramagnetic centers 312
- Parrinello–Rahman extended ensemble algorithm 210
- particle–particle interaction 127
- partition function 197, 255
- n*-pentane
 - cracking of 826
 - diffusion in silicalite/HZSM-5 660, 661, 663
 - experimental uptake curves 183
 - in porous Vycor glass 555
 - QENS diffusion studies 612
 - supercritical transition 555
- periodically continuous model systems 200
- permeabilities 411, 774
- permeability–diffusivity ratio 760
- permeability measurement, through silicalite 506
- permeation efficiency 760
- permeation, zeolite layer 792
- perm-porosimetry 793
- perturbation theory 309
- PFG NMR. *See* pulsed field gradient NMR (PFG NMR)
- phase-space probability density 285
- phenomenological transport coefficients 230
- piezometric method 156, 433, 435
- piezometric system 435
 - components of 433
 - theoretical response curves for 435
- Planck’s relation 309, 317, 318
- Poiseuille flow (see also viscous flow) 90, 94, 501, 532, 793, 501, 792
- Poisson process 294
- polar angle 96
- polycrystalline membranes 773
- polyethylene oxide 527
- polymer–zeolite interface 801
- polypropylene oxide 527
- polystyrene particles
 - in controlled porous glasses (CPG) 339
 - diffusion measurements by light scattering 340
- pore network, diffusion in 94
 - capillary condensation 97, 98
 - dusty gas model 94, 95
 - effective medium approximation 95
 - parallel pore model 96, 97
 - random pore model 97
 - tortuosity factor 95, 96
- pore radius 86
- pore size 85, 87, 535
 - distribution 96
- porosity 525
- porous adsorbent particles, diffusion 159
- porous catalyst particle
 - diffusion and reaction 809
 - direct measurement of tortuosity in 525, 526
- porous coordination polymers (PCPs) 730
- porous glasses 518
- porous Vycor glass, diffusion in 553–555
- positron emission profiling (PEP) 397, 481
- potential of mean force 222, 223, 278
- pre-exponential factor 105, 107, 288, 584–587
- probability density 214, 282
- probability distribution function (PDF) 47, 48, 276
- probability ratios 293
- propagator function 29–31, 114
- propane
 - comparison of diffusion in NaX, 5A and silicalite 666
 - diffusion in LTA 582
 - diffusion in silicalite 662
 - transient concentration profiles 748
 - transient intracrystalline concentration profiles of 749
- propene 645
 - conversion of cyclopropane 645, 646
 - conversion of isopropanol in NaX 647
 - cyclopropane 645–647
 - isopropanol 647, 648
 - in NaX 646
 - transport inhibition of 648
- propylene polymerization 831
- Pt/H-mordenite 139
- Pt/SiO₂ catalysts 139
- pulsed field gradient NMR (PFG NMR) 347, 348, 353, 358, 497
 - application of 365
 - Arrhenius plot of 373
 - attenuation curve 376
 - complete evidence of
 - diffusivity, concept of 354–355
 - mean propagator, concept 352–355
 - consistency, experimental tests of 379
 - crystal size, determination of 381–382
 - crystal size, variation of 379
 - diffusion measurements with different nuclei 379–380
 - external magnetic field, influence of 380

- extracrystalline space, blocking of 380–381
 - long-range diffusion 382
 - self-diffusion vs. tracer desorption measurements 380
 - tracer exchange measurements 382–383
 - diffusion anisotropy
 - host structure, evidence 364
 - measurements of 364
 - powder measurement 363–364
 - single-crystal measurements 362–363
 - diffusion measurements 151, 330, 335, 366, 371, 400
 - alternative approaches 362
 - application 325
 - data analysis 356–358
 - different regimes of 364–379
 - experimental conditions, limitations, and options for 355
 - extra-large stray-field gradients, benefit of 359
 - Fourier-transform 361–362
 - gradient pulse mismatch 358
 - impedance by contaminants 360
 - impedance by internal gradients 359–360
 - mechanical instabilities 358–359
 - multicomponent systems, self-diffusion measurement 361
 - performance 323
 - pitfalls 358
 - sample preparation 355–356
 - diffusivities 381, 384
 - ethane, long-range self-diffusion of
 - temperature dependence 370
 - fine-tuning 364
 - imaging techniques 353
 - long-range diffusivity measurements 365
 - measurement, principle 348
 - basic experiment 351–352
 - fundamentals 348–351
 - normal diffusion 356
 - pulse sequences 358
 - self-diffusivities 380
 - signal attenuation 357
 - in beds of zeolite crystallites 374
 - curves 371
 - signal-to-noise ratio 359
 - sine-shaped gradient pulses and eddy-current quench pulses 360
 - spin-echo attenuation 360, 364
 - curve 354
 - Fourier transform of 352
 - surface barriers, observation 377–379
 - tracer desorption technique 376–377, 382
 - two-dimensional Monte-Carlo simulation 371–374
 - two-region model 374–376
 - zeolite crystallites, molecular transport 355
 - zeolitic diffusion 379
 - pyridine, blocking effect 835
 - pyrolysis 520
- q**
- quadrupole moment 321
 - quantum mechanics/molecular mechanics (QM/MM) 194, 200
 - quartz crystal balance 432–433
 - quasi-classical approximation 310
 - quasi-elastic neutron scattering (QENS) 41, 347
 - diffusivities for pentane isomers 616
 - intermediate scattering function 339
 - measurements 223, 259
 - MIL-47, CO₂ diffusivities 753
 - qualitatively similar dependencies 754
 - self-diffusion data 754
 - quasi-Newton algorithms 292
 - quaternions 246
- r**
- radiofrequency pulse programs 317
 - random walk 5
 - diffusion path for 36
 - rapid recirculation systems 440, 441
 - model
 - Fick's equations, correspondence with 32, 33
 - mean square displacement 27–29
 - propagator 29–31
 - RATTLE algorithm 252
 - Reed–Ehrlich model 104, 636, 748
 - for surface diffusion 101
 - Rees, magnetically driven frequency response system 453
 - refractive index (RI) 343, 470
 - resistor network model 94
 - resonance line broadening
 - schematic representation 312
 - reversible reference system propagator algorithm (rRESPA) 240
 - pseudo-code implementing 240
 - Reynolds number 21
 - axial dispersion 473, 474
 - region 471, 478, 817
 - rigid zeolite framework 299
 - 12-ring zeolites 607. *See also* saturated hydrocarbons, diffusion of
 - fluorine compounds 637, 638

- hydrogen 636
 - methanol 635
 - PFG NMR diffusion measurements
 - with different probe nuclei 636–640
 - triethylamine 635, 636
 - water in NaX and NaY 633–635
 - X and Y zeolites, structure of 607–609
 - Rosenbluth weight 222
 - Rubotherm balance system 428
 - Runners model 315
- S**
- Saddle point calculation algorithms 292
 - SAPO-34 catalysts 835
 - SAPO-34 membranes 802
 - permeation 791
 - SAPO STA-7 crystals, pore structure 419
 - saturated hydrocarbons, diffusion of 659
 - cyclohexane 616–618
 - diffusion in NaCaX 619, 620
 - diffusion measurements as evidence of structural imperfection 621–623
 - diffusion of branched and cyclic paraffins 666–676
 - summary of diffusivity data 667
 - evidence from NMR 609–615
 - isoparaffins 616–618
 - linear alkanes 659–666
 - NMR and ZLC data for NaX, comparison of 615, 616
 - *n*-octane diffusion in NaY, USY and NaX 618, 619
 - SBA-15 material 528, 539
 - PFG NMR diffusion studies 540, 541
 - scattering experiments 327
 - application of neutrons 326
 - Schmidt number 478
 - Schrödinger equation 327
 - scintillation cocktail 447
 - selective surface flow 86
 - selectivity, mutual diffusion effect 790
 - selectoforming process 825
 - self-diffusion 7, 8, 16, 32, 65, 227–229, 258, 293, 299, 338, 360
 - coefficient 45, 233, 338, 350, 351
 - corrected diffusivity (D_0) 66
 - cross coefficients 67
 - entropy production by internal processes 66
 - experiments 407
 - at high occupancy 300
 - loading dependence 75–77
 - MD simulation 79
 - at low occupancies 296–300
 - phenomenological equations 65
 - relationship
 - between coefficients 65
 - between self- and corrected transport diffusivities 66, 77
 - of water 521
 - SHAKE procedure 252
 - shallow bed kinetic measurements, schematic diagram 442
 - Sherwood number 817
 - shielding effect 318
 - shrinking core model 173–176
 - Si/Al ratio 653, 654
 - Sierpinski gasket 50, 51
 - diffusion in 55
 - signal-to-noise ratio 439
 - silicalite (HZSM-5),
 - anisotropy 703–706
 - diffusion in 653–722
 - structure 654–657
 - sub-structure 696–700, 821
 - surface resistance 693, 694
 - surface etching 695
 - silicalite membranes 686, 772, 781
 - methane–ethane permeation 785
 - *n*-butane–isobutane in 781
 - single-component fluxes 780
 - temperature dependence 775
 - simple point charge (SPC) model 200
 - simulation box 266
 - simulations, of multicomponent adsorption and diffusion 738
 - single-component diffusion equation 186
 - single-file systems, infinitely extended 112
 - molecular dynamics 116–118
 - random walk considerations 112–115
 - single-particle tracking (SPT) 383, 387
 - single-resistance diffusion model 156
 - single-step frequency response method 436
 - singlet density distribution 208
 - sinusoidal channel segment 223, 297
 - sinusoidal field, diffusion in 107, 108
 - approximation 107
 - self-diffusivity 107
 - sinusoidal perturbation 452
 - size-selective molecular sieving 85–87
 - sodium borosilicate glasses 518
 - solid-sorbed fluid systems 253
 - sorbate-sorbate interactions 258, 269
 - sorbate-sorbate potentials 200
 - sorbate-zeolite systems 203
 - sorption/desorption curve 442
 - sorption isotherms 263
 - of nitrogen and carbon dioxide 213

- sorption kinetics 143–188, 441, 501
 - adsorption/desorption curves 161
 - for binary mixtures 185–188
 - co-diffusion 187, 188
 - counter-diffusion 186, 187
 - isothermal linear dual-resistance systems 151–160
 - isothermal linear single-resistance systems 145–151
 - isothermal nonlinear systems 160–179
 - mass and heat transfer, resistances to 143, 144
 - mathematical modeling of 145–185
 - non-isothermal systems 179–185
- sorption/tracer exchange rates, direct
 - macroscopic measurement 427–428
 - differential adsorption bed 441–443
 - frequency response measurements 447
 - experimental systems 452–454
 - in flow system 455–456
 - measurement limits 451–452
 - results 454–455
 - temperature frequency response 451
 - theoretical model 448–451
 - gravimetric methods 427
 - bed diffusional resistance, intrusion of 431–432
 - experimental checks 432
 - experimental system 428–429
 - heat effects, intrusion of 429–430
 - negligible thermal effects, criterion for 430–431
 - response curves analysis 429
 - macro FTIR sorption rate measurements 437–440
 - piezometric method 433
 - mathematical model 434–436
 - single-step frequency response 436
 - single-step temperature response 436–437
 - quartz crystal balance 432–433
 - rapid recirculation systems 440
 - liquid phase systems 441
 - tapered element oscillating microbalance (TEOM) 432–433
 - tracer exchange measurements 445
 - experimental procedure 447
 - radioisotopes detectors 446–447
 - transient uptake rate data, analysis
 - method of moments 444–445
 - time domain matching 443–444
- spin-echo attenuation 363, 367
 - curves 376
- spin–lattice relaxation 311
- spin quantum number 320
- STA-7 (30) crystal
 - methanol, concentration profiles 420
- static structure factor 333
- statistical mechanics
 - of diffusion 227–235
 - of infrequent events 276–292
- statistical mechanics-based simulation techniques 202
- steady-state diffusivity 832
- Stefan–Maxwell diffusivity (see also Maxwell–Stefan diffusivity) 13, 45, 68–71, 781–791
- Stefan–Maxwell formulation 13
- steric effects 17
 - in larger pores 521
- steric hindrance 521, 524
- stiff orthorhombic model 297
- stochastic simulation algorithms 206
- Stokes' law 60
- straight cylindrical pore, diffusion in 87
 - combination of diffusional resistances 93, 94
 - different mechanisms, relative importance of 92
 - Knudsen mechanism 88–90
 - molecular diffusion 91
 - self-diffusion/tracer diffusion 92
 - surface diffusion 92, 93
 - transition region 91, 92
 - viscous flow 90, 91
- stray field gradient 359
- string-of-beads system 478
- supercritical transition, in adsorbed phase 555, 556
- surface diffusion 92, 506, 534
 - concentration dependence 535–538
 - determination of surface diffusivities 534, 535
 - mechanisms 100
 - by cage-to-cage jumps 104–106
 - Reed–Ehrlich model 101–104
 - vacancy diffusion 100, 101
 - of propane on silica gel 535
- surface permeability 756
 - bulk diffusivity 762
 - diffusivity 749
 - simulated concentration profiles 759
- surface resistances 19, 152, 411, 692, 693
 - control, concentration profiles during desorption 496
 - effect 153
 - external resistance to mass transfer 19–21
 - macroscopic rate measurements 693, 694
 - surface effects 696

- surface etching 694, 695
 - theoretical frequency response 450
 - transient concentration profiles, measurement of 695, 696
- t**
- tapered element oscillating microbalance (TEOM) 433
 - Taylor–Golay model 480
 - temporal analysis of products (TAP) system 500–501
 - test particle insertion method 218
 - thermal conductivity 470, 484, 817
 - thermal wavelength 197, 211
 - thermodynamic correction factors (see also chemical potential) 257, 333
 - thermodynamic forces and fluxes 60, 61
 - Thiele concept 124, 125
 - Thiele moduli 123–125, 808, 810, 811, 818, 823, 833
 - effectiveness factor, variation of 810
 - for first-order isothermal system 810
 - time scale separation 275, 276–281
 - tortuosity factors 96, 525
 - total pore diffusivity 90
 - tracer diffusion, basic principle 447
 - tracer exchange measurements 445
 - experimental procedure 447
 - radioisotopes detectors 446–447
 - tracer permeabilities 417
 - tracking temporal evolution
 - in network of states 292–296
 - transferable potentials for phase equilibrium calculations (TraPPE) parameters 200
 - transformation matrix 246
 - transient adsorption/desorption curves, macroscopic measurement 445
 - transient concentration profiles imaging 395
 - observation options 396
 - IR microscopy 399–400
 - magnetic resonance imaging (MRI) 400–403
 - optical microscopy 398–399
 - positron emission tomography (PET) 397
 - X-ray monitoring 397–398
 - surface barriers, direct measurement of 415
 - sticking probabilities to nanoporous particles 421–423
 - surface permeability, concentration dependence 415–417
 - surface permeability through crystal faces 417–421
 - transition state theory (TST) 105, 277, 281
 - application 277
 - approximation 281–283, 290
 - transport diffusivities 7, 8, 15, 16, 32, 41, 65, 232, 268, 271, 329, 339, 742
 - loading dependence 77, 78, 409
 - MD simulation 79
 - and self-diffusivity, relation between 71, 72
 - using thermodynamic factors 520
 - transport resistances 111
 - assessment by micro-imaging 699, 700
 - transverse nuclear magnetization 313, 325
 - transverse relaxation times 325
 - Trotter theorem 239
 - tubular membrane module, construction of 801
 - two-component diffusion 716
 - co- and counter-diffusion of benzene and toluene 718–720
 - counter-current desorption of *p*-xylene–benzene 717, 718
 - counter-diffusion of isobutane and *n*-butane 720, 721
 - methane and ammonia 717
 - methane and *n*-butane 259–262
 - methane and tetrafluoromethane 716
 - methane and xenon 716, 717
 - permeation properties of nitrogen and carbon dioxide 717
 - type A zeolites, general patterns of behavior in 582–584
 - activation energies
 - and pre-exponential factors 584–587
 - variation, for diffusion on 4A and 5A with molecular diameter 585
 - Arrhenius plot 583
 - TZLC desorption curves 497
 - experimental vs. theoretical 498
- u**
- ultraviolet absorption (UV) detection 470
 - unit bond vector 244
 - united-atom representation 195
 - unsaturated, and aromatic hydrocarbons in NaX 623
 - benzene 627–632
 - hysteresis 631, 632
 - macroscopic and microscopic measurements, comparison of 627, 628
 - mechanism, diffusion in zeolites NaX and NaY 628–631
 - C₈ aromatics 624–627
 - discrepancy in measurements 632, 633
 - light olefins 623
 - uptake curve approaches 147–149, 152, 174

- comparison of solutions 150
- experimental 180
- details 176
- invariance 181
- for moisture 175
- expression for 181, 183
- theoretical 182
- vs. experimental 168
- transient, non-isothermal models for 180
- uptake vessel, pressure response 434

v

- vacancy diffusion 34, 100
- self-diffusion, in cubic lattice 34
- van Deemter equation 468, 480
- van der Laan's theorem 444, 464, 467
- van der Waals interactions 199
- van Hove correlation functions 329
- self-correlation function 347
- van't Hoff equation 795, 819
- Verlet algorithm 237, 251
- leapfrog algorithm 247
- pseudo-code implementing 237
- vibration frequency 100
- Vignes correlation 785, 787
- viscous flow 90, 94, 532, 793
- Vycor glass, diffusion in 319

w

- water
- adsorption 332
- anisotropic self-diffusion of 530
- elimination of 831
- hydrogen bonding of 521
- in MCM-41 539
- in MFI-type zeolite crystals 381
- O-H bond 250
- oxygen atom 250
- PFG NMR self-diffusion measurements for 602
- purification 143
- self-diffusivities of 521
- solubility of paraffins 696
- as solvent 687
- zeolite-sorbate system 249
- Wicke-Kallenbach method 534
- Widom's test particle insertion method 219
- Wiener-Khintchine relation 341, 508
- window blocking 587
- sorption cut-off 587
- variation of fraction of open windows, with degree of ion exchange 588

x

- X-ray computed tomography (XCT) 407
- X-ray diffraction (XRD) 202
- o*-xylene
- CCZLC curves 498
- gravimetric uptake curves 683
- in NaX zeolite 626
- permeance/selectivity, equimolar mixture of 782
- p*-xylene-benzene
- with benzene counter-adsorbing 718
- counter-current desorption of 717
- xylene isomers 826
- equilibrium mixture 827
- in NaX zeolite 627
- NMR PFG self-diffusivities 625
- p*-xylene spectra 827, 829
- co-diffusion of 440
- counter-diffusion of 439
- diffusion time constants, concentration dependence 624
- experimental uptake curves 624
- frequency response data 684
- gravimetric uptake curves 683
- permeance/selectivity, equimolar mixture of 782
- set of 439
- yield, in toluene disproportionation 829
- X zeolite membranes 802

z

- Zeolite A 562–601
- cation sites 562, 563
- deactivation 579, 596–601
- diffusion in 565–567, 571–596
- structure 562–564
- zeolite 4A, micropores of 476
- zeolite 5A, ZLC response curves for N₂ 488
- zeolite catalysts
- coking of 833
- information from fluorescence microscopy 835
- information from PFG NMR 834–835
- diffusional effects 807
- diffusional restrictions 822
- activation energies 825–826
- catalytic cracking over HZSM-5 824–825
- catalytic cracking over zeolite Y 823–824
- MTG reaction 830–831
- MTO Process 831–833
- size exclusion 822–823
- toluene, selective disproportionation of 828–830
- xylene isomerization 826–828

- diffusion and reaction 807
- diffusion-controlled catalytic reaction
 - concentration profiles, direct measurement 819–820
- HZSM-5 crystal, furfuryl alcohol reaction 820–821
- mesoporous MCM-41 reaction 821–822
- diffusion limitation 813, 815
- effectiveness factor 808–811
- external mass transfer resistance 811
- internal and external resistances 816–817
- intracrystalline diffusivity, determination of 817–819
- effective diffusivity, temperature dependence of 819
- non-isothermal systems 815–816
- pressure dependence 814–815
- reaction order 814
- temperature dependence 812–814
- zeolite crystals 43, 145, 181
 - diffusion 398
- zeolite frameworks 197, 254
 - reliable flexible models for 256
- zeolite membranes 771–803
 - behavior of 779
 - binary mixtures, modeling permeation of
 - concentration profile 785–789
 - Maxwell–Stefan model 784–785
 - membrane thickness 791
 - mutual diffusion, importance of 789
 - support resistance 791–792
 - cracks/defects 779
 - gas mixtures, separation of 779
 - diffusion-controlled permeation 781–783
 - equilibrium-controlled permeation 783–784
 - size-selective molecular sieving 779–780
 - membrane characterization
 - bypass flow 792–793
 - isotherm determination 795–796
 - perm-porosimetry 793–794
 - transient response analysis 797
 - membrane separation processes
 - alcohols dehydration, pervaporation process 797–798
 - amorphous silica membranes 800
 - barriers to commercialization 802–803
 - butene isomers, separation of 799
 - CO₂–CH₄ separation 798
 - H₂ separation, MOF membranes 799–800
 - membrane modules 801–802
 - membrane reactors 802
 - stuffed membranes 801
 - polymeric membrane 773
 - porosimetry characterization, apparatus 794
 - separations 775, 797
 - single-component permeation 773
 - permeation, modeling of 776–778
 - selectivity/separation factor 774–776
 - synthesis 772–773
 - transport 773
 - zeolite NaCaA (see also LTA)
 - ethane, molecular selfdiffusion 353
 - long-range diffusivities for nitrogen 369
 - zeolite–sorbate interactions 197, 201
 - zeolite-sorbate systems 193, 194, 227, 249, 265
 - *ab initio* molecular dynamics 203, 204
 - meso/macroporous structure, computer reconstruction 204–206
 - models and force fields 194–206
 - molecular model and potential energy function 194–203
 - zeolite theta, frequency response spectrum 454, 455
 - Zeolite X (and Y)
 - cation sites 609
 - diffusion in 609–648
 - hysteresis 631
 - structure 607–609
 - zeolite Y (see also Ch 17)
 - catalytic cracking 823
 - equilibrium isotherm 437
 - zeolitic imidazolate frameworks (ZIFs) 731, 739, 799
 - analogies in building blocks 739
 - ethane-ethene mixtures in 745
 - membrane
 - permeance with kinetic diameter for light gases 800
 - methanol, ethane, and ethanol 741
 - self- and transport diffusion 740
 - ZIF-8 membranes 744, 746
 - zero-length column (ZLC) method 459, 483
 - counter-current ZLC (CCZLC) 498
 - curves, for benzene–silicalite 499
 - desorption curves 495, 496, 499
 - for benzene–*n*-hexane, experimental liquid 500
 - for propane 497
 - desorption, for *n*-hexadecane 488
 - deviations 489
 - extensions of 497–500
 - fluid phase hold-up 490–491
 - heat effects 492–493
 - intraparticle diffusion control, theory 485–486

- isotherm nonlinearity, effect of 491–492
- liquid phase measurements 498–500
- macroporous particles, diffusion 488–489
- practical considerations 493–497
- principle of 483–485
- response curves 489, 490
 - for benzene–NaX 491, 492
 - for CO₂ desorbing 486, 487
 - isothermal criterion, validity 493
 - for N₂ 488
- schematic diagram 484
- short-time behavior 486–488
- surface resistance
 - fluid film resistance 489
 - measurement 489–490
- tracer ZLC 497–498
- ZLC curves for benzene–silicalite 499
- Zn(tbip) crystal 418, 761
 - boundary and equilibrium concentrations 755
 - 1D-arrangement of 757
 - mass transfer, structure model 758
 - MOF 755
 - MOF specimen of 747
 - pore system of 757
 - transport diffusion and self-diffusion 750
- ZSM-5 (see also silicalite), 2,2-dimethylbutane 824