

## Index

### a

- approximation
  - adiabatic 310
  - BORN–OPPENHEIMER 310
- augmented matrix 25

### b

- band gap
  - photonic 254
- band structure
  - Cu 199
- basis
  - function 107, 114
  - of group 36
  - rank of 36
  - reciprocal 135, 136
- binary rotation 15
- BLOCH
  - ansatz 135, 142
  - function 198, 201, 205, 206, 210, 217, 227, 231
  - theorem 135
  - wave 135

- block diagonal 88, 89
- BORN–OPPENHEIMER approximation 310
- boundary condition
  - BORN–VON KÁRMÁN 134
  - periodic 134
- BRAGG grating 253
- BRAVAIS lattice 311
- BRILLOUIN zone 138

### c

- character 94
  - projection operator 107
  - system 94, 98, 115
  - table 98, 187
- chiral
  - angle 76
  - vector 76

- cif-files 64, 66
- class 40, 98
  - multiplication 41
- CLEBSCH–GORDAN
  - coefficients 89, 112, 115, 117, 119, 120, 123, 155, 160, 172, 173
  - sum 88–90, 92, 114, 117, 192
- compatibility relation 201
- conical transformation 19
- coset 43
  - representatives 43, 126
- crystal
  - photonic 253, 254
- crystal field 98, 156
  - expansion 160, 161
  - Hamiltonian 160
  - operators 164
  - operators (BUCKMASTER–SMITH–THORNLEY) 165
  - operators (STEVENS) 166
  - operators (WYBOURNE) 165
  - parameter 161

### d

- degeneracy 156
- density functional theory 310
- dielectric atom 261
- direct product 48
- dynamical matrix 311
  - FOURIER transform 312
- dynamical symmetry 3

### e

- element
  - conjugate 40
  - self-adjoint 41
- empty lattice test 270
- endomorphism 38
- equivalence relation 39
- Euclidian group 25

- EULER angles 16
- EULER–RODRIGUES parameter 20
- f**
- factor
  - group 46
- FERMAT’s theorem 36
- FERMI
  - energy 231
  - surface 236
- filling factor 262
- FINDSYM 64
- force constant matrix 311
- form factor
  - pseudopotential 228
- g**
- generator 36
- GIBBS free energy 322
- graphene nanoribbon 238
- group 34
  - center of 41
  - composite 45
  - conjugate 66
  - continuous 34
  - covering 41
  - direct product 48
  - double 183, 186
  - finite 34
  - infinite 34
  - LIE 35
  - little 125, 142, 145
  - normalizer of 41
  - of  $\mathbf{k}$  138
  - of SCHRÖDINGER equation 154
  - order 35
  - semidirect product 49
  - semisimple 45
  - simple 45
  - space 62
  - super- 41
  - translation 59
- GTPack
  - GO XII
  - GODiagonal 115
  - GOHarmonics→“Real” 336
  - GOIrepNotation 101, 102, 157
  - GOPhotonic 312
  - GOProjection 204
  - GOReality 194, 195
  - GOREpresentation 183, 185
  - GOSpecMode 308
  - GOTable 62
  - GOTbLattice 215
  - GOVectorFields 291
  - GSMPBBands2D 341
  - GSMPBBands3D 341
  - GT XII
  - GTAbelianQ 34–36
  - GTAdjacencyMatrix 236, 242, 243
  - GTAllSymbols 52, 54
  - GTAngularMomentumChars 154, 156, 158, 334
  - GTAngularMomentumRep 84, 85, 334
  - GTBandsPlot 341
  - GTBandsPlotImprove 230, 234, 276, 292
  - GTBandStructure 210, 215, 216, 230, 312, 314, 315
  - GTBravaisLattice 137, 141, 146
  - GTBSTOperator 157, 166
  - GTBSTOperatorElement 157, 166
  - GTBuckyBall 75, 80
  - GTBZMPBPointMesh 342
  - GTBZPath 137, 141, 199, 215, 230
  - GTBZPointMesh 342
  - GTCartesianSphericalHarmonicY 333
  - GTCartesianTesseralHarmonicY 108, 296, 298, 336
  - GTCenter 39, 41, 42
  - GTCFDatabaseInfo 157, 167
  - GTCFDatabaseRetrieve 157, 167
  - GTCFDatabaseUpdate 157, 167
  - GTChangeRepresentation 183–186
  - GTCharacterTable 94, 98, 99, 101, 105, 115, 119, 157, 187, 188, 193–195, 200
  - GTCharacterTableOfk 143, 146, 147
  - GTCharProjectionOperator 105, 108, 109, 112, 283, 284, 288, 292
  - GTClasses 39–42, 104
  - GTClassMult 39
  - GTClassMultTable 39, 41, 42
  - GTClebschGordanCoefficients 112, 117–120, 173
  - GTClebschGordanSum 88, 90, 92
  - GTClebschGordanTable 112, 117, 119
  - GTCluster 210, 215, 219, 230, 248, 321
  - GTCompatibility 198, 202, 203, 279, 283, 284
  - GTConjugacyClass 39
  - GTConjugateElement 39, 40
  - GTCrystalField 162, 163
  - GTCrystalFieldExpansion 157
  - GTCrystalFieldParameter 157, 163
  - GTCrystalFieldSplitting 154, 157, 158
  - GTCrystalSystem 59
  - GTCyclicQ 36

- GTDensityOfStates 210, 314, 342
- GTDensityOfStatesPlot 342
- GTDensityOfStatesRS 236, 243
- GTDirectProductChars 112, 115, 117, 119, 190, 330
- GTDirectProductRep 112, 113, 115, 116, 120
- GTEulerAnglesQ 11, 16, 17
- GTFermiSurface 236
- GTFermiSurfaceCut 236, 237
- GTFermiSurfaceXSF 236, 237
- GTFindStateNumbers 236, 244
- GTGauntCoefficient 157, 163, 164
- GTGenerators 33, 36, 37, 58
- GTGetEulerAngles 11, 18
- GTGetIrep 88, 90, 91, 93, 108, 111, 115, 209
- GTGetIrepMatrix 221
- GTGetMatrix 13, 185, 186
- GTGetStructure 210, 228
- GTGetSU2Matrix 25, 30, 31
- GTGetSubGroups 34, 36, 42, 43
- GTGetSymbol 80
- GTGroupConnection 52, 59, 61
- GTGroupFromGenerators 33, 36, 37, 58, 78, 184, 186
- GTGroupGlp 210, 220
- GTGroupHierarchy 52, 59
- GTGroupNotation 52, 59
- GTGroupOfK 137–140
- GTGroupOrder 34, 35
- GTGroupQ XII, 34, 35
- GTHamiltonianList 210
- GTHamiltonianPlot 210, 215, 245, 248
- GTIcosahedronAxes 75, 80, 81
- GTImportCIF 67, 68, 339
- GTInstallAxis 52, 54, 55, 78
- GTInstallGroup 33–36, 56, 64, 65, 85, 87, 139, 146, 183, 185–188
- GTInstallStructure 339
- GTInvSubGroupQ 39, 45
- GTInvSubGroups 39, 45, 70
- GTIrep 94, 103, 104, 115, 119, 156, 158, 173, 190, 191, 203
- GTIrepDimension 88, 90, 91
- GTLatCluster 69, 288
- GTLatShells 69, 288
- GTLeftCosets 39, 44, 45
- GTLoadStructures 210, 228
- GTMagnetic 69, 70, 72
- GTMolChemicalData 301, 302, 339
- GTMolDatabaseInfo 301, 303
- GTMolDatabaseUpdate 301
- GTMolGetMolecule 203, 208, 301
- GTMolPermutationRep 203, 207, 208, 303
- GTMolToCluster 301, 339
- GTMPBBands 273
- GTMultTable 34–36
- GTNormalizer 39, 41, 43
- GTNumberOfIreps 88, 90, 91, 93
- GTOrderOfElement 34, 35
- GTPhBandsObjects 292
- GTPhCuboid 260
- GTPhDCObjects 260
- GTPhDCPixel 260
- GTPhEllipticRod 260
- GTPhFields 276
- GTPhMaster 270
- GTPhMasterObjects 270, 275
- GTPhMasterPixel 270, 275
- GTPhMPBBands 270, 341
- GTPhMPBFields 276, 277, 281, 282, 343
- GTPhPermittivityMatrix 260, 270
- GTPhPixelSmooth 260
- GTPhPixelStructure 260, 263, 264, 266
- GTPhPrismaticRod 260
- GTPhRodSmooth 260, 266
- GTPhShowStructure 260, 263, 264
- GTPhSlab 260
- GTPhSlabSmooth 260, 266
- GTPhSphere 260
- GTPhSymmetryAnalysis 292
- GTPhSymmetryBands 276–278
- GTPhSymmetryField 276, 277, 281, 282
- GTPhSymmetryPoint 276, 277
- GTPhUncoupledBands 283, 285
- GTPlotStateWeights 236, 244
- GTPlotStructure2D 210, 215
- GTPointGroups 52, 59, 61
- GTPProductGroup 48, 49
- GTPProductGroupQ 48, 49
- GTPProjectionOperator 105, 108, 109, 209
- GTPwDatabaseInfo 227, 228
- GTPwDatabaseRetrieve 227, 228
- GTPwDatabaseUpdate 227, 228
- GTPwDatasetRetrieve 229
- GTPwEmptyLattice 291
- GTPwEmptyLatticeIrep 270–273, 288
- GTPwHamiltonian 227, 229, 230
- GTPwPrintParmSet 227, 229
- GTPwSymmetrizePW 203–205
- GTQAbs 11, 23
- GTQConjugate 11, 23
- GTQInverse 11, 22, 23
- GTQMultiplication 11, 21, 22
- GTQPolar 11, 23

- GTQuaternionQ 11, 21, 22
  - GTQuotientGroup 46, 47
  - GTQuotientGroupQ 46, 47
  - GTReadFromFile 210
  - GTReality 193, 194
  - GTReciprocalBasis 136, 137, 139, 146
  - GTRegularRepresentation 84–87, 96
  - GTReinstallAxes 13, 14
  - GTReinstallAxes 11
  - GTReorderMatrix 245
  - GTRightCosets 39, 44, 45
  - GTShells 210, 215, 219, 230, 240, 248
  - GTShellVectorsQlp 210, 220
  - GTShowSymmetryElements 52, 58, 320
  - GTSOCSplitting 189, 191, 192, 246
  - GTSpaceGroups 62, 64, 65
  - GTSpinCharacters 189–191
  - GTStarOfK 137–140
  - GTStevensOperator 157, 166, 169
  - GTStevensOperatorElement 157, 166, 169
  - GTStevensTheta 157, 166
  - GTSU2Matrix 25, 29, 30
  - GTSubGroupQ 34, 36
  - GTSymmetrizedProductChars 327, 328, 330
  - GTSymmetryBasisFunctions 210, 218, 296–298, 326
  - GTSymmetryElementQ 75, 77, 80, 320, 321
  - GTSymmetrySingleBand 230
  - GTTableToGroup 33, 36–38, 85
  - GTTbDatabaseInfo 210, 337
  - GTTbDatabaseRetrieve 210
  - GTTbHamiltonian 210, 215
  - GTTbHamiltonian3C 224
  - GTTbHamiltonianOnsite 230
  - GTTbHamiltonianRS 236, 243
  - GTTbIntegralRules 210, 221–223
  - GTTbMatrixElement 210, 212, 213, 338
  - GTTbMatrixElement3C 210, 221–223
  - GTTbNumberOfIntegrals 210, 220
  - GTTbParmToRule 210, 230, 231, 241
  - GTTbReadWannier90 210, 226
  - GTTbRealSpaceMatrix 236, 242
  - GTTbSpinMatrix 225
  - GTTbSpinOrbit 210, 225
  - GTTbSymbol3C 222, 223
  - GTTbSymmetryBands 230, 232, 235
  - GTTbSymmetryPoint 230, 232
  - GTTbSymmetrySingleBand 232
  - GTTbTubeBands 236
  - GTTbWannier90Hamiltonian 210, 226
  - GTTesseralHarmonicY 335
  - GTTPhMasterObjects 270
  - GTTTransformationOperator 111
  - GTTTransformQlp 210
  - GTTTransformToQlp 221
  - GTTubeBands 239
  - GTTubeParameters 75, 76, 239
  - GTTubeStructure 75, 77, 78, 238
  - GTVarList 221
  - GTVectorRep 302
  - GTVibDisplacementRep 302, 303
  - GTVibDynamicalMatrix 310, 312–314
  - GTVibLatticeModes 310, 316, 317
  - GTVibModeSymmetry 302, 305, 306, 309, 316
  - GTVibSetParameters 310, 312, 313, 315, 316
  - GTVibSpectroscopy 302, 308, 309
  - GTVibTbToPhonon 310, 315, 316
  - GTVibTbToPhononRule 310, 315, 316
  - GTVoronoiCell 68, 69, 137, 139, 141, 236
  - GTWavefunctionPlot 210
  - GTWhichAxes 11, 13
  - GTWhichRepresentation 183
  - GTWignerCharProjectionOperator 334
  - GTWignerProjectionOperator 105, 206, 334, 336
  - GTWriteToFile 210
- h**
- H<sub>2</sub>O 308
  - HAMILTON operator 152–154, 156, 159, 161, 196
  - Hamiltonian 152, 153
  - high symmetry
    - lines 139
    - points 139
  - holohedry 59
  - homomorphism 38, 178
- i**
- improper rotation 13
  - index 43
  - induced dipole moment 307
  - infrared activity 307
  - integral
    - on-site 212
    - three-center 212
    - two-center 212
  - invariant polynomial 326
  - inversion 6
  - irreducible tensor operator 121
  - isomorphism 38

**k**

- kinetic energy 152
- KORRINGA–KOHN–ROSTOKER method 294
- k-space 133

**l**

- LAGRANGE's theorem 36
- lattice 59
  - real-space 136
  - reciprocal 136
- LEGENDRE polynomial 160
- lemmas of SCHUR 91
- LIE group 35
- LÖWDIN transformation 211

**m**

- master equation 254, 256, 270, 293
- materials equations 255
- Mathematica
  - \$BaseDirectory 347
  - Import 343
  - MatrixPower 32
  - Method 111
  - MonomialList 326
  - PauliMatrix 32
  - Q XII
  - RotationMatrix 30, 87
  - SphericalHarmonicY 332
  - SphericalPlot3D 335
  - ThreeJSymbol 166
  - \$UserBaseDirectory 347
  - WignerD 333
- matrix
  - representation 88, 89
- matrix element
  - reduced 122
  - theorem 156
- MAXWELL's equations 254, 256, 257
- method
  - of induction 123
  - pseudopotential 227
- MIE scattering problem 294
- multiplication table 35

**n**

- nanotube
  - armchair 77, 238
  - chiral 240
  - chiral angle 76
  - chiral vector 76
  - single-walled 75
  - translational vector 76
  - zigzag 238

## notation

- BETHE 99
- BOUCKAERT 99
- international 64
- MULLIKEN 99, 100
- SCHÖNFLIES 52, 64

**o**

- OPECHOWSKI theorem 186
- orbit 144
- order
  - of group 35
  - of group element 35
- order parameter 323
- orthogonality theorem 92, 107
  - characters 97

**p**

- PAULI
  - equation 28, 178, 183, 196, 253, 257
  - matrices 28, 178
  - vector of matrices 28
- PBS 270
- perturbation theory
  - time dependent 169
  - time independent 157
- photonic band gap 274
- photonic crystal 253
- point
  - charge model 161
  - defect 279
- potential
  - external 152
- product
  - direct 48, 113
  - KRONECKER 113
  - semidirect 49, 142
- projection operator 107, 108
- proper rotation 13
- pseudopotential 227
  - empty core 228
  - form factor 228
  - HEINE–ABARENKOV 228
- pseudo-wave function 227

**q**

- quaternion 20
  - pure 20
  - real 20
  - unit 21
- quotient
  - group 46
  - set 46

*r*

## RAMAN

- activity 307
- polarisability tensor 307

## reflection 15

- lines 6

## representation 84

- allowed 146
- direct product 113, 114, 116–118
- displacement 304
- equivalent 89
- extra- 187
- faithful 85
- induced 123
- irreducible 89, 98, 103, 107, 108, 115, 121–123, 127, 142, 143, 154, 156, 159, 186
- matrix 84
- permutation 302
- reducible 89
- regular 103
- similar 89
- theory 84
- unitary 84
- vector 304

## rotation 6

- binary 15
- improper 13
- pole 18
- proper 13

## rotoreflexion 15

*s*

## SALC 206

## SCHÖNFLIES, A.M. 52

## SCHRÖDINGER

- equation 133, 134, 136, 151, 152, 154–156, 159, 161, 170, 177, 178, 183, 189, 195–198, 203, 210, 211, 219, 254, 257
- equation, group of 154

## SCHRÖDINGER equation

- stationary 152

## selection rules 169

## semidirect product 49, 124

## single-walled carbon nanotubes 238

## site symmetry 66

## SO(3) 178

## space group 62

- irreducible representations 230
- nonsymmorphic 62, 77, 143
- symmorphic 62, 77, 142

## spherical harmonics 294

## spin space 178

## spin-orbit coupling 178, 180, 182, 189

star of  $k$  138

## structure

- perovskite 248
- zinc blende 240

## SU(2) 178

## subgroup 6, 36

- conjugate 41, 66
- diagonal 113
- invariant 44, 63

## subspace 114

## supergroup 41

## symmetry

- adapted linear combination 206
- group 6
- time-reversal 196

*t*

## tight-binding

- real-space approximation 240
- two-center approximation 212

## transformation matrix 89

*u*

## uncoupled bands 283

## unit cell 61

- nonprimitive 61
- primitive 61

*v*

## VAN HOVE singularity 285

## vector

- field 254
- spherical harmonics 294

## VORONOI cell 68

*w*

## WANNIER

- function 226
- transformation 226

## wannier90 226

## water 308

WIGNER 3/*J*-symbol 166

## WIGNER-ECKART theorem 120–123, 155, 160, 172, 203, 307, 308

## WIGNER-SEITZ cell 65

*x*

## XCrysDen 237

XeF<sub>4</sub> 308

## xenontetrafluoride 308