

Index

a

AHE *see* Anomalous Hall effect (AHE)

Angle resolved photoemission spectroscopy (ARPES) 7, 8, 162, 175, 186

- copper-doped bismuth selenide 94
 - crystal momentum 66
 - and energy distribution curve (EDC) 218
 - Fermi surface (FS) 68, 73, 91
 - Fermi velocity 84
 - intensity maps 60
 - laser-based 70
 - momentum-dependent electronic structure, solids 219
 - and momentum distribution curve (MDC) 218
 - photoemission intensity 218
 - photon energy 59, 70
 - resistivity-temperature profile 71
 - SnTe 86
 - spectral intensity 70
 - synchrotron based 73
 - topological protection 68
- Anomalous Hall effect (AHE)
- Chern insulator 360
 - Cr doped Sb_2Te_3 film 369
 - electrical gate 370, 371
 - ferromagnetic order 362, 363
 - mechanism 359
- ARPES *see* Angle-resolved photoemission spectroscopy (ARPES)

b

band inversion analysis

- DFT identification 170
- orbital motion coupling 170
- quasiparticle wave functions 169

- TI 170

Bi bilayer

- bandstructure 113
- Bi (111) bilayer and graphene 112
- conduction band 114, 115
- properties 115–117
- rhombohedral A7 structure 112
- scanning tunneling 120
- spin polarization 115

Bismuth chalcogenide, TIs

- bulk band structures 144
- high-index surfaces 155
- non-stoichiometric and functionalized terminations 151

- topologically protected states 148

bismuth-based TI materials

- carrier concentration and surface band bending 253, 254
- carrier density 251
- chalcogenides 245
- characteristics 255
- counter-doping 254
- crystal growth 254
- defect properties 253
- electrical resistivity 250, 251
- electronic and thermodynamic phase, Bi_2Se_3 247
- Fermi surfaces 251, 252
- magnetoresistance 246
- metallic and non-metallic specimens 255, 256
- post-synthesis treatment 255
- room temperature 248
- SdH oscillations, magnetoresistance 251
- stoichiometric Bi_2Te_3 ratio 246
- tetradymite *see* tetradymite
- thermoelectric materials 246

c

- conductance map analysis, TIs
 - atomic scale disorder 232
 - 2D electron systems 229
 - Fourier-transformed conductance map 232
 - magnetically doped 233
 - Majorana zero mode 235
 - spin-dependent scattering probability (SSP) 230
 - superconductor 235

d

- Density-functional theory (DFT)
 - accuracy and computational cost 131
 - atomic wave functions 137
 - auxiliary noninteracting system 134
 - electron density gradient 136
 - electronic-structure codes 136
 - electrostatic interaction energy of nuclei 133
 - exchange-correlation energy density 135
 - and generalized-gradient approximation (GGA) 132
 - Hohenberg-Kohn theorems 134
 - ionic pseudopotentials 138
 - many-electron wave function 133
 - plane-wave pseudopotential approach 132
 - pseudopotential method 137
 - quantum-mechanical many-body problems 131
 - topological materials 131
 - ultrasoft pseudopotentials 139
- DFT calculations, TIs
 - electronic band structure parameters 136
 - electronic-structure methods 131
- Dilute magnetic semiconductors (DMS) 335, 363
- DMS *see* Dilute magnetic semiconductors (DMS)
- 2D-TIs *see* Two-dimensional TIs (2D-TIs)

e

- Electron energy loss spectroscopy (EELS) 317
- electronic structure, TIs
 - band inversion 163, 179
 - band-structure concept 164
 - bulk projected band structures 174, 175
 - conduction-band minimum (CBM) 162

- DFT band gap, insulators and semiconductors 161
 - Dyson equation 163
 - full-potential linearized augmented-plane-wave (FLAPW) formalism 166
 - GW approach 164
 - GWSOC 172
 - LDA and GGA functionals 161
 - many-body renormalization effects 163
 - orbital analysis 174
 - photoemission spectroscopy experiments 163
 - plasmon-pole model 167
 - quasiparticle band structures 163
 - relativistic effects 166
 - room-temperature spintronics applications 162
 - topological invariants 167
 - valence-band maximum (VBM) 162
 - zeroth-order Green function 165
- electronic transport, TIs
 - Aharonov-Bohm (AB) effect 283–285
 - 1D electronic modes 285
 - description 279
 - Shubnikov-de Haas (SdH) oscillations 280, 282
 - superconducting proximity effect 286
 - ultrathin 283
 - weak anti-localization (WAL) 280, 281

f

- Ferromagnetic (FM) insulator
 - Bi-chalcogenide heterostructures 316
 - BS magnetization measurements 315
 - electrical transport measurements 320
 - hall measurements 318
 - magnetic domain switching 320
 - magnetic scattering 319
 - magnetization reversal 316
 - proximity-induced magnetism 315
 - reactive sputtering 316
 - secondary magnetic phase transition 317
 - spin-disorder scattering 316
 - time-reversal symmetry 321
 - transport devices 317
- ferromagnetism
 - conduction and valence bands 368
 - Cr doped $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin films 368, 370
 - Cr doped Sb_2Te_3 368
 - Sb_2Te_3 and Bi_2Te_3 368
 - van Vleck mechanism 367

g

graphene

- bandstructure 107
- 2D electron gas 107
- electronic structure 104
- Majorana fermions 107
- nearest-neighbor (NN) hopping 106
- pseudo-spin 104, 105
- spin-orbit gap 107
- types of hoppings 105

GW approach

- Bloch functions 166
- exchange-correlation (XC) effects 164
- Hedin's equations 165
- nontrivial functional derivatives 165
- optical measurements 180
- perturbative approach 167
- spin-independent screened interaction 165
- spline interpolation 167

h

Hall voltage 357

i

inversion-asymmetric systems 15, 16

k

Kitaev's model 378

'Klein-Majorana fusion' procedure 395

Kohn-Sham theory 134

l

LDA valence-band dispersion 176

Local density of states (LDOS)

- Friedel oscillations 229
- energy-momentum dispersion 224
- and STM 218

m

magnetic and superconducting doped TIs

- copper-doped bismuth selenide 94
- $\text{Cu}_x\text{Bi}_2\text{Se}_3$ 95
- ferromagnetism 89
- photoemission 89
- spin-resolved measurements 92
- surface adsorption method 92
- topological order 92
- magnetic doping, transition metal atoms 301
- magneto-transport experiments, HgTe quantum wells
 - magnetic-field induced phase transition 38
 - sample fabrication 36
 - transition, n-p conductance 37
- Majorana nanowires

- characteristic power-law scaling 380

- charging effects 379

- Coulomb interactions 378

- gapless surface modes 377

- interferometric detection 379

- nontrivial topological invariants 377

- quantum transport properties 378

- single-charge transistor 379

- spin-orbit coupling 378, 379

- zero-energy states 380

Majorana single-charge transistor

- charging energy contribution charf 383

- charging-induced correlations 385

- Coulomb oscillations, linear conductance 388

- finite bias sidepeaks 389

- functional integral approach 385

- gauge transformation 385

- inelastic cotunneling processes 387

- Josephson coupling, superconducting lead 391

- Majorana–Meir–Wingreen expression 385

- master equation approach 386

- noninteracting Majorana device 386

- power-law dependence 385

- resonant Andreev reflection to electron teleportation 389

- sequential tunneling rates 387

- superconducting phase fluctuations 385

- zero-bandwidth model 386

Majorana–Meir–Wingreen formula 381

MBE growth, TIs

- Bi- and Sb- Chalcogenides 300

- Bi_2Se_3 (BS) 303

- BST 305

- BT 303

- bulk HgTe 299

- carrier concentrations 298

- film growth, quality and stability 305

- ST 304

Metal-organic chemical vapor deposition (MOCVD) 272, 299

Molecular beam epitaxy (MBE)

- chalcogenides 296

- exfoliation process 298

- massless Dirac dispersion 297

- thermoelectric materials 296, 297

- transport measurements 297

p

probing TI surface states, STM

- and band structure, TIs 223

- Landau quantization 225

probing TI surface states, STM (*contd.*)

- sample preparation methods 219
- topography and defects 221
- TRS 217

Pulsed laser deposition (PLD) 299

q

QAHE *see* Quantum anomalous Hall effect (QAHE)

QPT *see* Quantum phase transitions (QPT)

QSHE *see* Quantum spin Hall effect (QSHE)

QSHE, HgTe quantum wells

- longitudinal resistance measurements 41
- non-local measurements 44
- spin polarization 45
- transport, helical edge states 43

Quantum anomalous Hall effect (QAHE)

111, 296, 315

- and AHE 359, 360
- ARPES band maps, Bi_2Se_3 365, 366
- band structure, TIs 360, 363
- $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ ternary compounds 366, 367
- challenges 375
- Cr doped $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ TI films 371
- crystal structure, Bi_2Se_3 364, 365
- electrical gate 370
- evolution, band structure and edge states 361, 362
- ferromagnetic (FM) order 362–364
- ferromagnetism *see* ferromagnetism
- Hall effect and QHE 357, 358
- magnetic field dependence 371, 373
- temperatures 373
- types 374

quantum-mechanical many-body effects 135

Quantum phase transitions (QPT)

- ARPES and spin-resolved ARPES 75
- bulk band inversion, BiTI 76, 77
- conventional band insulator 74
- energy dispersion and FS mapping 75
- photoemission measurements 75

Quantum spin Hall effect (QSH) 268

- backscattering, helical edge state 48
- Berry-phase effects 6
- description 3
- graphene 4
- HgTe/CdTe quantum wells 33
- in InAs/GaSb quantum wells 49
- in magnetic field 45
- probing, edge states 48
- quantized spin-Hall conductance 4
- in semiconductors 32

- semiconductor quantum well (QW) 31
- spin polarization 33
- system InAs/GaSb 35
- time-reversal (TR) invariant perturbations 32
- time-reversal (TR) symmetry 31
- and TIs *see* Topological insulators (TIs)
- topological phase transition 33
- transport measurement 32
- transverse conductivity 32

r

Reflection high energy electron diffraction (RHEED) oscillations 303

s

Scanning gate microscopy (SGM) 48

Scanning tunneling microscopy (STM)

- description 218
 - single atom imaging 218
 - scotch-tape method 247
- Screened-exchange LDA (sX-LDA) approach 179

SdH oscillations *see* Shubnikov–de Haas (SdH) oscillations

Shubnikov–de Haas (SdH) oscillations

- amplitude 343
- density of 2D carriers 343
- description 340
- 2D nature 340, 341
- Fourier analysis 342
- Landau-level (LL) fan diagram 341, 342

skyrmion 110

Spatially-resolved STS (SR-STs) 218

SPE *see* Superconducting proximity effect (SPE)

spin chirality, surface Dirac cones 19

Spin-orbit coupling (SOC)

- band gap region 161
- band inversion 169
- Hartree potential 164
- LDA calculations 171
- non-interacting reference system 163
- spin-orbit splittings 172
- treatment 170, 172

Spin-orbit interaction (SOI)

- computational requirements 142
- Dirac equations 140
- electronic and magnetic properties 139
- electronic-structure calculations 141
- first-order perturbation theory 141
- nonrelativistic pseudopotentials 140
- scalar-relativistic (SR) effects 139
- semilocal pseudopotentials 141

- spinor plane-wave matrix element 142
- spinor wave functions 142
- spintronics applications 164
- Superconducting proximity effect (SPE)
 - Al-Bi₂Se₃-Al junction 349, 351
 - Bi₂Se₃-(Bi-2212) junctions 352, 353
 - differential resistance dV/dI 346
 - Josephson effect, Nb-Bi₂Te₃-Nb junctions 348
 - Majorana fermions 344
 - Nb-HgTe-Nb junction 350
 - Sn-Bi₂Se₃ and Pb-Bi₂Se₃ junctions 346
 - temperatures, Sn-Bi₂Se₃ 344, 345
 - W-Bi₂Se₃-W junction 347
- surface electronic structure, TIs and TCIs
 - ARPES and STM techniques 191
 - bismuth and antimony 200, 202
 - chalcogenites 198, 200
 - Fermi energy 198
 - mirror symmetry 204, 206
 - PbTe and SnTe 204, 205
 - scattering 207, 208
 - spin-degeneration 197
 - stability, surface states' existence 208, 209, 211
 - topological predictions 196
 - TRIMs *see* Time-reversal invariant momenta (TRIMs)
- t**
- TDS *see* Topological Dirac semimetals (TDS)
- tetradymite
 - chemical substitution and defects 249
 - melting powder 248
 - polycrystalline masses 246
 - rhombohedral crystal structure 247
 - SdH oscillations 250
 - transport measurements 250
- thin-film synthesis techniques 249
- TI nanostructures
 - applications 286, 288
 - description 267
 - doping and alloy 275, 276
 - exfoliation 273
 - fermi level modulation and bulk carrier control 276, 278
 - heterostructures 274
 - opportunities enabled 270
 - solution phase growth 273
 - vapor phase growth 271, 272
- Time-reversal invariant momenta (TRIMs) 170
 - definition 192
 - Fermi contours 195
 - inversion symmetry 193
 - parity invariants 193, 194
 - surface Brillouin zone (SBZ) 194, 195
 - surface state topology 194
- Time reversal symmetry (TRS) 217
- TIs *see* Topological insulators (TIs)
- TIs, magnetism
 - bulk ferromagnetism 313
 - FM/TI heterostructures 315
- TKI *see* Topological Kondo insulator (TKI)
- Topological crystalline insulator (TCI)
 - band inversion transition 86
 - GeBi₂Te₄ 87
 - Pb_xSn_{1-x}Te 85
 - protection, time-reversal symmetry 85
 - scanning tunneling spectroscopies 89
 - spin polarization 85
 - spin-resolved ARPES measurements 87
 - surface band dispersion 88
 - van Hove singularity (VHS) 87
- Topological Dirac semimetals (TDS)
 - arsenic ions 80
 - bulk conduction and valence bands 84
 - chemical composition delta 84
 - constant energy contour maps 82
 - Fermi level 80
 - graphene 76
 - mobility 84
 - Pauli matrices 79
 - spin-orbit coupling 80
 - surface electronic structure of 2D and 3D 83
 - tetragonal structure 81
 - topological phase transition 79
 - Weyl fermions 79
- Topological insulators (TIs)
 - ARPES 295
 - band structures 257
 - band structures, materials 61
 - bismuth *see* bismuth-based TI materials
 - bismuth-antimony alloy system 58, 59
 - bismuth selenide (Bi₂Se₃) 268
 - CdTe/HgTe/CdTe quantum 4, 5
 - chalcogenide 257
 - chalcogenide materials 269
 - chemical potential, Dirac point 67
 - crystals of SmB₆ 259
 - density, helical Dirac electrons 68
 - 2D HgTe quantum wells 245
 - discovery 8
 - dispersion, interface 23
 - electrical/optical method 353
 - electron transport 268
 - electronic phases 3

- Topological insulators (TIs) (*contd.*)
 - electronics applications 267
 - energy gaps 257
 - experimental discovery of 3D 57
 - fabrication process 298
 - gapless states, interface 22
 - half-Heusler *RTX* compounds 257
 - half-Heusler materials 257, 258
 - helical spin texture 64
 - heterostructures 315
 - Heusler materials 6
 - ionic liquid gating 298
 - IQH, FQH and QSH 55
 - Kondo insulator 259
 - magnetism/superconductivity 296
 - material quality 7
 - mirror symmetries, crystalline 67
 - nanostructures *see* TI nanostructures
 - non-metallic behavior 258
 - non-zero Berry's phase, Fermi surface (FS) 61
 - photo-induced band-gaps, graphene 8
 - photon energy 59
 - physical properties 63
 - quantized hall conductance 296
 - quantum oscillations 340, 341, 343
 - Rashba splitting, surface states 24
 - room temperature 64, 66
 - skipping orbits 56
 - SPE *see* Superconducting proximity effect (SPE)
 - spin-ARPES 58, 63
 - spin-momentum interlocking 267
 - spin-orbit coupling 7, 295
 - spin polarization 66
 - spin properties 61, 63
 - spin-resolved ARPES 331
 - spintronic device configurations 295
 - superlattice 25
 - surface energy bands 24
 - surface oxidation and mobility degradation 269
 - surface states and electronic band dispersion 59, 60
 - tetradymite *see* tetradymite
 - thermoelectric properties 8
 - thin film 20
 - three dimensional, graphene 5, 6
 - three-dimensional topological order 57
 - time-reversal invariant momenta (TRIM) 12
 - topological invariants 57
 - topological order 62
 - two dimensions (2D) *see* Quantum spin hall effect (QSHE)
 - WAL *see* Weak anti-localization (WAL)
 - and Weyl semimetals, phase transition 15
- topological invariants
 - deformation process 144
 - inversion symmetry 144
 - numerical approaches 144
 - time-reversal invariant momenta 143
- topological Kondo effect
 - bosonization approach 396
 - conductance tensor 396
 - fixed point 395
 - low-energy theory 393
 - Majorana spin 394
 - renormalization group analysis 394
- Topological Kondo insulator (TKI)
 - CsCl-type structure 70
 - Fermi surface map 73, 74
 - heavy fermion behavior 69
 - laser-based ARPES system 70
 - photon energy, laser-ARPES 73
 - surface-sensitive transport measurements 69
 - temperatures 70, 73
- topological phases 55
- topological phases and surface states
 - band structures 11
 - chirality 11
 - nontrivial transition 12
 - pair annihilation 18
 - Weyl semimetals 13
- Topological surface states (TSSs) 217
- transport studies, TI thin films
 - charged impurity disorder 307
 - hall effect 307
 - hybridization gaps, Ultrathin 3D TI films 311
 - lattice mismatch 307
 - mesoscopic transport, 3D TI films 310
 - QC, diffusive transport in 3D TI Films 309
 - QSH effect 306
 - Shubnikov-de Haas (SdH) oscillations 308
 - spin polarizations 307
- transport, Majorana nanowires
 - conductance, non-interacting 382
 - Majorana-Meir-Wingreen formula 381
 - Majorana single-charge transistor 380
- Troullier-Martins scheme 139
- Two-dimensional TIs (2D-TIs)
 - alloyed layers, Bi and Sb 118, 119
 - Bi bilayer *see* Bi bilayer
 - binary compounds 122, 123
 - bismuth and mercury compounds 104

- Chern number 111
- 2D Dirac equation 108
- Dresselhaus effect 112
- graphene and QSHE *see* grapheme
- Hamiltonian properties 110
- Luttinger-Kohn Model 109
- mass-velocity 109
- material-dependent parameters 110
- semiconductors 103
- skyrmion 110
- spin channel 109
- surface bands 103
- ternary compounds 124, 125
- topological description 111

v

- valence band dispersion 176
- Vapor liquid solid (VLS) methods 299

w

- WAL *see* Weak anti-localization (WAL)
- Weak anti-localization (WAL)
 - Cr-doped Bi_2Se_3 films,
 - magnetoconductivity curves 335, 336
 - gate voltage 337, 338
 - HLN equation 332

- impurity effect 333
- magnetoconductivity, 10 nm Bi_2Se_3 332
- magnetoresistance (MR) measurement 332
- monolayer (ML) Fe deposition 333, 335
- nanowires 339
- normalized magnetoresistance, Bi_2Te_3 333, 334
- phase coherent length 339
- SdH oscillation 336
- surface electron 331
- ultra-thin Bi_2Se_3 films 336
- Weyl semimetals
 - apex, Dirac cone 13
 - 2D Dirac semimetal 15
 - Fermi arc surface states 13
 - inversion symmetry 15
 - time-reversal symmetry 15
 - and topological insulators, phase transition 15
 - topological nature 13

x

- X-ray magnetic circular dichroism (XMCD) 314

