

Index

a

- A₂BB'O₆ double perovskites
 - B-site cation order patterns 229
- ab initio calculations 6, 111, 272
- ab initio methods 297
- A³⁺B³⁺O²⁻₃ compounds
 - classification of 226
- ABX₃ perovskite
 - cubic crystal structure of 224
 - schematic drawing of 225
- acid–base reactions 62, 674
- acoustic phonons (overdamping) 656
- actinide hydrides 500
- activation energies 494, 496, 514, 601
- adiabatic temperature 400
- AeH₂ cotunnite structure 486
- AeH_x polyhedra 486
- Ae–H coordination 486
- Ae₂[ZnN₂]
 - crystal structures of 291
- Ag–Ag interactions 43
- AgPb₁₈SbTe₂₀ 456
- AgTaN₂ 293
- A- and B-site cation
 - ferrimagnetic spin structure of 237
- A- and B-site cation-ordered perovskite
 - crystal structure of 236
- A-type-La₂O₃ structure 262
- A-site cation ordered perovskite
 - crystal structure of 234
- A-site deficient perovskites 206
- A-site lanthanide ions 227
- AlB₂-structure type 444
- AlB₂-type borides 441
- Al₁₃(Co,Ni)₄ structure 77
- Al–Cu–Fe–Si system 83
- Al–Fe–Si system 83
- alkali borate glasses 122
 - Mayenite with 505
- alkali halide crystals 487
- alkali hydride, cubic lattice parameters 485
- alkali hydrides 487, 488
- alkali-metal based 1/1 Bergman phases 47
- alkali metal antimonides
 - photoemissivity of 457
- alkali metal halide layers 581
- alkali metal hydrides 484
- alkali metals 3, 139, 140, 141, 525
- alkali metal suboxides 140, 147, 149, 150, 157
- alkaline earth hydride crystal structures 486
- alkaline earth hydrides 479, 485, 486, 487, 488, 493
- alkaline earth ions 486
- alkaline earth metal containing compounds 317
- alkaline earth metal halides 257
- alkaline earth metal-rich systems 291
- alkaline earth metal nitrides, of transition metals 326
- alkaline earth metal nitridocuprates 292
- alkaline earth metal nitridometalates 300
- alkaline earth metals 140, 158, 443, 477, 525, 535, 537
 - subnitrides of 150
- alkaline earth subnitrides 157
- alkali silicate 122
- allotropes 436
 - of Ge 529
- Al–Mn–Fe–Si system 83
- Al–Mn–Si system 83
- Al–Cu network
- Al–O–P linkages 117
- Al–Pd–Mn–Si system 83
- α-Mg₃Sb₂
 - crystal structure of 457
- α-NaFeO₂-type structure 325, 574

- α -PbO₂ structure 269
- AlPO₄ segregation scenario 117
- Al-Re-Si system 83
- Al-Rh-Si system 83
- aluminum 440, 479
- aluminum-cobalt system 76
- ambient temperature VO₂ structure 183
- ambipolar conductivity 685
- amine intercalation 589
- ammonia catalysis 505
- ammonium Rochelle salt 653
- ammonolysis 370
 - preparation of 371
 - reactions 255, 371
- amorphous–crystalline transition 742
- amorphous phase-change materials (PCMs)
 - characteristics 740
 - microscopic complexity 741
- amorphous phases 740
 - experimental probes 742
 - first-principles simulations 742
- AMRO. *See* angular magnetoresistance oscillation (AMRO)
- angular dependence 610
- angular magnetoresistance oscillation (AMRO) 610
- angular momentum 4
- anionic conduction 364
- anionic formal charge 361
- anionic lattice 362
- anionic p-phenylene derivative
 - chemical formula of 547
- anionic poly(p-phenylene) derivative 546
- anionic tetrahedral networks
 - dimensionalities of 317
- anion vacancy order 233
- anisotropic magnetic properties 447
- anisotropic magnetothermal properties, of
 - HoAlO₃ single crystals 631
- anisotropy 571, 630
- anomalous Hall conductivity
 - scaling 608
- antibonding (destabilizing) cation–anion interactions 744
- antibonding interactions 41
- antibonding orbitals 20, 62
- antibonding peak 37
- antibonding states 37
- antiferroelectric PbZrO₃
 - displacement pattern of Pb²⁺ ions 652
- antiferromagnet 412, 415, 619
- antiferromagnetic
 - arrangement 598
 - correlations 633
 - coupling 716
 - hexagonal spin cluster 629
 - interaction 414, 513
- antiferromagnetic order 269, 628, 708
- antiferromagnetic spin clusters 628
- antiferromagnetic state 39, 501
- antiferromagnetic transition temperature 502
- antiferromagnetic triangle 619
- antiferromagnetic V–O–V superexchange interaction 512
- antiferromagnetism 231
- antiferromagnets 619
- anti-Frenkel disorder 678
- anti-2H-BaNiO₃ 274
- antimonides 456, 471
 - semiconductance of 465
 - for thermoelectric energy conversion 471
- antimony telluride (Sb₂Te₃) 737
- antimony, toxicity of 472
- antiperovskite 243, 503
- antipolar structure 651
- antiprisms 460
- aperiodic crystals 73
- 2/1 approximant structure 84
- aqueous chemistry 672
- aristotype Li₄SrN₂ 294
- arrangement of truncated icosahedra in the 1/1 Tsai-type approximant 88
- Arrhenius law 675
- arsenides 456
- arsenopyrite 463
- artificial ion conductors 687
- artificial synapses 746
- atom, composition 643
- atomic hydrogen 478, 479
- atomic orbital (AO) 2, 3, 5, 6, 7, 52
- atomic positions and symmetry information for the CCP lattice 165
- atomic positions and symmetry information for the HCP lattice 166
- atomic radii ratio 525
- atomic size effects 57
- atomistic simulation 741
- Au–Sn and K–Sn COHP curves 16
- Au₂O₃, structure 178
- aurivillius compounds 634
- aurivillius-type structure 657
- aurivillius series members, structures 576
- avalanche effect 681
- average magnetic moment per Fe ion 415
- avian magnetic compass 722

- avian magnetoreception 722
- A_2X_3 bixbyite
– structures of 366
- AX_2 fluorite
– structures of 366
- azide-ligand 715
– end-on bridge 715
– end-to-end bridge 715
- azide (N^{3-}) ligand 715
- azido bridge 715
- b**
- Ba_3AlO_4H crystal structure 504
- $BaAl_4$ type structure 535
- $Ba_{14}(Ca,Sr)N_6$ clusters 153
- back reaction rate 683
- $Ba_{16}[CuN]_8[Cu_2N_3][Cu_3N_4]$ 297
- baddeleyite ($P2_1/c$) unit cell for ZrO_2 and HfO_2 188
- $Ba_3[FeN_3]$ 301
- $BaGa_2Sb_2$ 467
– crystal structure of 467
- Ba^{2+} ions 180
- $Ba_{14}LiN_6$ cluster 153
- ball milling 385
- $Ba_4[Mn_3N_6]$ 320
- $Ba_6Mn_{20}N_{21.5-d}$ 307
- Ba_5Na_{12} polyhedra 156
- $Ba_{16}[NbN_4]_3[Nb_2N_7]$ 319
- band ferromagnetism 705
- bandgap 8, 16, 546, 744
- band insulators 426
- $Ba_2[Ni_3N_2]$ 298
– crystal structure of 298
- $Ba_2[Ni_2(Ni_{1-x}Li_x)N_2]$ 298
- $Ba_8[NiN]_6N$
– crystal structure 297
- barium cations 504
- barium hydride 493
- bar magnets 721
- Barret formula 657
- $Ba_8Sb_4OH_2$ crystal structures 505
- $BaTiO_3$ 644, 649
– temperature dependent polarization directions 649
- $BaTi^{4+}O_{2.4}N_{0.4}$ structure 511
- Bärnighausen formalism 533
- B–O–Al linkages 118
- B–O(1) sublattice consists of corner sharing B–O(1) octahedra 194
- bcc Jones zone 30
- bcc solid solution 267
- Bergman-type clusters 81
- Bergman 1/1 quasi-crystalline approximants 45
- Berthollet'sches Knallsilber 272
- β -Mn nitrides
– Al_2Mo_3C type 280
- β -Mn structure 76
- β -rhombohedral boron 435
– crystal structure 436
– type borides 449
- β - Zn_4Sb_3
– crystal structure of 464
- B-site cation
– crystal structure B-site cation in perovskite of 233, 238
- B-site cation orders 230
- B-site-deficient perovskites 207
- B-sublattice of spinel structure 627
- B-sublattice structure (pyrochlore lattice) 627
- Bifidobacteria breve 721
- bifunctional molecular magnets 720
- bimetallic/alloy catalysts 551
- bimolecular rate law 682
- binary antimonides 456–464
– early transition metal antimonides 459
– late transition metal antimonides 462
– main group antimonides 457
- binary borides
– group elements 437
– lanthanides 437
– main group metals 436
- binary hydrogen compounds 497
- binary intermetallic phases 56
- binary IV–VI compounds
– structure map 743
- binary model glasses, medium-range order effects in 118
– cation next-nearest neighbor environments and spatial distributions 118
– ring-size distributions and “super-structural units” 124
- binary nitrides
– chemical bonding 252
– crystal structures 264, 268
– enthalpies of 259
– idealized crystal structures 263
- binary phase diagrams 24
- binary P_2O_5 – GeO_2 glass system 115
- binary system B_2O_3 – SiO_2 114
- binary TaN 285
- binary TMO with ideal rutile structure 182
- binary TM oxides
– MO, with NaCl structure 170
- binary transition metal nitrides 251

- binary transition metals 252, 464
 - nitrides, synthesis of 251, 252, 258, 260
 - binary Zn_3N_2 272
 - biogenic magnetism 720–723
 - magnetotactic bacteria 721
 - biogenic magnetite 722
 - biomineralization 721
 - bioplatfoms 721
 - $Bi_{95}Sb_5$ 458
 - Bi_2SiO_5 657
 - ferrielectric-like arrangement of dipole moments 657
 - vs. Bi_2WO_6 657
 - bismuth Aurivillius phases 244
 - bismuthides 456
 - Bi_2Te_3
 - superlattices of 456
 - $Bi_4Ti_3O_{12}$ structure 574
 - Bi_2WO_6 657
 - bixbyites 190, 365
 - Bloch states 609
 - boat-like conformation 445
 - body-centered tetragonal structure 38
 - Bohr magneton 597
 - Boltzmann conditions 673
 - Boltzmann constant 661
 - Boltzmann equations 596, 598
 - Boltzmann statistics 672
 - bond angle distribution 112
 - bond angles 27
 - bond valence sums (BVS) 488
 - borate glasses 95, 120
 - boric acid 438
 - boride
 - synthesis 439
 - boride crystals 440
 - boride materials 439
 - borides 435, 442
 - icosahedra 448
 - synthesis 439
 - – nanomaterials 440
 - – powder preparation 439
 - – single-crystal growth 439
 - Born-Mayer potentials 146
 - boron 435
 - allotropes 435
 - atom arrangement, in metallic borides 438
 - icosahedron atom 436
 - structural arrangement of atoms 441
 - boron halides 439
 - boron hydrides 479
 - boron-rich borides 449
 - boron-rich materials 438
 - boron-rich metal borides 436
 - boron-rich solids 446
 - boron–oxygen compounds 438
 - boron nitride 443
 - boron oxide 113, 439
 - bottom of conducting band (BCB) 546
 - Bragg reflections 633
 - Bravais lattice 30, 32
 - bridging ligands 704
 - bridging oxygen atoms 544
 - Bridgman methods 256
 - Brillouin zone 656
 - brittleness 500
 - brookite (TiO_2) showing channels 186
 - Brønsted acid–base picture 671
 - Brønsted acids 577, 587
 - Brønsted concept 668
 - Brønsted-type basic sites 549
 - Brønsted level 671
 - Brouwer approximation 673
 - brownmillerite, $A_2BB'O_5$, structure 209
 - brownmillerite-type $A_2B_2O_5$
 - crystal structure of 239
 - brownmillerites 207
 - structure 210
 - type 239
 - brucite 584
 - distortion of 542
 - structure of 542
 - B/Si ratio 116
 - bulk defects 686
 - bulk sensors 715
 - Butler–Volmer equation 685
- C**
- $Ca_7Ag_{2.72}N_4$ 330
 - $Ca@Ag_{18}$ polyhedra
 - chemical pressure 59
 - $CaAgSb$ 466
 - crystal structures of 466
 - Ca_3AlSb_3 468
 - crystal structures of 468
 - $Ca_5Al_2Sb_6$
 - crystal structures of 470
 - $Ca_{14}AlSb_{11}$ 470
 - $CaAl_2Si_2$ 466
 - Ca_2AuN 330
 - $Ca_2B_2C_2$ 17
 - $Ca_4[Cr_2N_6]$
 - edge-sharing double tetrahedra 319
 - $Ca_6[Cr_2N_6]H$ 304
 - $CaCu_5$ -type phase $SrAg_5$ 26
 - $CaCu_5$ -type structure 283

- CaCu₅ structure 59
 Cadmium 86
 CaF₂ fluorite structure 187
 CaIn₂ type structure 526
 calcination 369, 551
 calcination–reduction process 551
 Ca₂[Li(Fe_{1-x}Li_x)N₂] 293
 Ca₂[(Li_{1-y}Cu_y)(Cu_{1-x}Li_x)N₂] 293
 Ca(Li[Mn_{1-x}Li_xN])₂
 – crystal structures of 295
 Ca₉Mn₄Bi₉ 468
 Ca₃[MnN₃]
 – structural relationship 302
 Ca₁₂[Mn₁₉N₂₃]
 – crystal structures 307
 Ca[MnN]·Li₂[MnN] 295
 cancer phototherapy 713
 cancer therapy 710
 Ca–Ag phase diagram 59
 Ca–Ag system 59
 (Ca₃N)₂[MN₃]
 – isolated trigonal-planar nitridometalate anions 301
 capping agent 712
 carbon-containing nanocomposites 462
 carbon-like frameworks of boron atoms, in borides 449
 carbon nanorings (CNRs) 548, 556
 carbon nanotubes 462
 carbothermal reaction 365
 carlsbergite 267
 catalytic sites 548
 CaTiO₃ 656
 – structure parameters of 227
 cation clustering 120
 cation coordination polyhedra, for 8a site in bixbyite 190
 cation defects 677
 cationic conductors 687
 cation ion radii 166
 cation next-nearest environments and spatial distributions studied by dipolar NMR 120
 cation ordering 739
 cation vacancies 744
 Ca₂[VN₃]
 – one-dimensional chains 320
 Ca₅[VN₄]N
 – crystal structures of 318
 CaWO₄
 – Ca- and W-based polyhedra in –scheelite arrangement of 367
 – luminescent properties of 369
 CCP lattice 165
 Cd₅₈Ce₁₃ and Zn₅₈₊₆Ho₁₃, complex modulated behavior 89
 Cd-doping 684
 CdSe and ZnS, mechanically induced self-propagating reactions 399
 CdTiO₃ 656
 Ce₆Cr_{20-x}N₂₂ 306
 cellulose acetate (CA) 558
 Ce₂[MnN₃]
 – crystal structure 322
 cesium 140, 141, 143
 – atom 149
 – suboxides 148
 cetyltrimethylammonium bromide (CTAB) 712
 chalcogenide compounds 528
 chalcogenides 13, 383
 chalcogens 383
 charge compensation 711
 charge density wave 417
 charge disproportionation
 – schematic drawings of 235
 charge-transfer material
 – purely organic fullerene-based 706
 charge-transfer organic complexes 703
 chemical bonding 532
 chemical diffusion 684
 – coefficient 685, 689
 chemical hydrides 477
 chemical-bonding 737
 chemical kinetics 668
 chemically ordered region 660
 chemical potential of Ag 672
 chemical pressure 58, 225
 chemical reaction 693
 chemical reactions, simple 685
 chemical shielding 532
 chemical shift anisotropy (CSA) 532
 chemical transport process 689
 chemical vapor deposition (CVD) 253
 chemotaxis 721
 chimie douce-type process 371
 chiral organic fluids 427
 chiral proline 430
 chocolate-brown Hg₃N₂ 272
 chromium-containing steels
 – steel-hardening process 267
 chromium ions 167
 chromium oxides 167
 citrate complexation 369
 classical magnetoresistance 595
 classical spin liquid 622

- clathrates 529
 - type I and type II crystal structure, cut out 528
- ClayFF force field 544
- close packing (CP) 163
- clustering behavior 124
- clusters in primitive Mackay 1/1 approximant 85
- cobalt-rich disordered phase FeCo_3N orders 275
- cobalt(II) hexacyanoferrate(III) 713
- cobaltocene-doped derivative 706
- cobalt oxyhydrides 507
- Co_{23}B_6 crystal structure 442
- CO_2 effect on the defect chemistry in hydroxides 680
- coercive field 647
- Co(II)Cu(II)-based ferrimagnetic chains 710
- coloring problem 17
- colossal magnetoresistance (CM) 595, 604
- columbite structure of CoNb_2O_6 184
- compass magnetoreceptor 722
- complex anions $[\text{Fe}_2\text{N}_4]^{8-}$, 1D $[\text{Fe}_2\text{N}_3]^{5-}$ 303
- Complex Layered Oxides, structural diversity 571
- compositional complexity 571
- compositional gradient 397
- composition dependence 414
- compound $(\text{Au}_{12}\text{Sn}_9)^{23-}$ clusters 15
- computational models 545
- computed tomography (CT) 562
- Co_4N crystallizes 271
 - in perovskite structure 271
- conduction band 668
- conduction electrons 598, 610
- conductivities 478, 492, 493, 506, 514, 528, 680, 684, 693
 - isotherm for single crystalline and mesoscopic nanocrystalline 689
- connectivities
 - cation distributions, in glasses with multiple network formers 129
 - and cation distributions, in glasses with multiple network formers 126, 127
- connectivity distribution of the bridging oxygen atoms in $(\text{K}_2\text{O})_{0.33}((\text{B}_2\text{O}_3)_x(\text{P}_2\text{O}_5)_{1-x})_{0.67}$ glasses derived from NMR data and comparison with 128
- connectivity distribution of the bridging oxygen atoms in $(\text{Na}_2\text{O})_{0.33}((\text{Ge}_2\text{O}_4)_x(\text{P}_2\text{O}_5)_{1-x})_{0.67}$ glasses derived from NMR data and comparison with 128
- connectivity distribution of the bridging oxygen atoms in $(\text{Na}_2\text{O})_{0.33}((\text{Te}_2\text{O}_4)_x(\text{P}_2\text{O}_5)_{1-x})_{0.67}$ glasses derived from NMR data and comparison with 129
- consecutive shells of the Bergman cluster in the icosahedral 1/1 approximant 82
- continuous random network model 93
- contour plots of magnetic neutron scattering intensity 628
- cooling 406
- cooperative paramagnet 620
- cooperative paramagnetism 622
- coordination number (CN) 166
- coordination polyhedron of the A-site in pyrochlore 192
- coordination sphere of boron atoms 441
- coordinatively unsaturated ZnAl-LDH nanosheets 550
- copper 440
- copper chalcogenides, synthesis of
 - by ball milling 385
- copper dianion 708
- copper dianion precursors 708
- copper halides-based oxide 588
- copper hexacyanoferrate (CuHCF) 723
- copper-red crystals Rb_9O_2 141
- copper metal 385
- corrosion 692
- CORSee chemically ordered region 660
- corundum or Al_2O_3 177
 - binary oxides 178
 - ilmenite and other ordered corundum-like structures 180
 - structure 177
- CoSb_3
 - thermoelectric properties of 463
- Coulomb bonding 668
- Coulomb forces 668
- Coulombic interactions 544
- Coulomb interaction 681
- Coulomb repulsion 148, 605
- counterintuitive orbital mixing 6
- coupling of ionic excitation and electronic excitation 671
- covalent bond 477, 478
- covalent bonding 384
- covalent network glasses 93
- covalent network glasses, medium range order in 109
 - glassy silica and the binary system 109
 - network connectivity in 113
 - ring size distributions 112

- covalent nitrides 331
- covalent oxide glasses 96
- Coxeter-Boerdijk helices 76
- CrB₄ structure 450
- CrGa₄
 - 18-electron configurations 52
- CrGa₄'s stoichiometry 53
- Cr₃GaN
 - electronic structures 278
- CrGa₄ structure 51
- crocon
 - P–E loops 662
- croconic acid 662
- crocon polarization switching
 - structural change before and after 662
- cross-layer magnetoresistance 602
- cross-linking density 361
- cross-plane transfer energy 610
- Cr₃Se₄, magnetic structure of 412
- crucible materials 254
- cryocooling 713, 717
- cryogenic temperatures 717
- cryptochromes (CRY) 722
- crystal
 - orbitals 7, 8, 49
 - piezoelectric deformation 650
 - properties 643
 - structures 27, 362, 483, 681
 - – and compositions 498
 - – La₂Ni₂O₅ 240
 - – TMO, representation of 169
- crystal chemistry 478
 - TMO 163
 - – close packing and hole filling 163
- crystalline Ge–Sb–Te phases 737
 - metastable 737, 739
 - stable 737
 - – quasibinary phases 739
- crystalline-electric field (CEF) 631
- crystallinity 385
- crystallization 440
- crystallized thiophene nanowire 720
- Crystallographic Information File 163
- crystal orbital Hamilton populations (COHP) 1, 7, 9, 11
 - analysis 10, 15
 - curves 10
 - data 16
- crystal orbital overlap population (COOP) 1, 7, 9, 10
 - analysis 11, 13, 15
 - Hoffmann and Zheng's application 12
- crystal symmetry 643
- CsCl-type high-pressure modification 261
- CsCl structures 17, 64
- Cs/O ratio 141
- CsTi₂NbO₇ structure 585
- CTAB. *See* cetyltrimethylammonium bromide
- Cu₂AlMn-type 306
 - metal substructure 308
- CuAl₂ type structure 535
- cube-octahedra 446
- cubic Al₂Mo₃C structure type 279
- cubic Ca₁₉Ag₈N₇ 329
- cubic crystal structures 33
- cubic Cu₃N with ReO₃-type structure 277
- cubic η-carbide Fe₃W₃C structure 280
- cubic face-centered lattice 362
- cubic γ(-Fe₄N) 270
 - structure 273
- cubic high-temperature phase γ-Mo₂N 267
- cubic perovskite
 - Cartesian axes of 224
 - cubic (Pm-3m) perovskite structure 197
- cubic SrTiO₃
 - crystal structures of 226
- Cu ions 397
- Cu_{1-x}Al₂ crystal structure 533
- Cu–Al system 535
- Cu–Cd and Au–Cd binary phase diagrams 33
- Cu–Se system, partial phase diagram of 395
- Cu–Ti
 - binary phase diagrams 65
- Cu–Zn system 523
- Cu NMR signals 535
- Cu₃PdN 277
- Curie constant 413, 647
- Curie–Weiss behavior 300, 627
 - magnetic susceptibility 300
- Curie–Weiss law 6, 647
- Curie–Weiss temperature 622, 627, 658
- Curie temperatures 276, 283, 600, 609, 654
- Cu₃Se₂ by making α-CuSe and α-Cu₂Se, formation of 394
- Cu₁₅Si₄ 31
- CuTi structures 17, 65
- cyano bridge 712
- cyanogen, (CN)₂ 331
- cyano-nitrido-metalates 255
- cyanometallates 714
- cyclotron frequency 596
- cyclotron motion 610
- Czocharlski (Cz) technique 631

- d**
- data processing 735
 - data storage 735
 - applications 735
 - density 718
 - Debye frequency 661
 - Debye–Waller factors 30
 - Debye temperature 659
 - Debye wave vector 659
 - decagonal approximants 76
 - defect chemical treatment, shown for an oxide
 - with dominant anti-Frenkel-disorder in oxygen sublattice 676
 - defect chemical variations
 - within homogeneity range of oxide 677
 - in homogeneity ranges of, PbO and 678
 - defect chemistry 665, 667, 668, 671, 675
 - at boundaries and heterogeneous electrolytes 686
 - defect concentration, as function of temperature 682
 - defect fluorite-type
 - structures of 364
 - defect fluorites
 - vacancies, role of 378
 - defect-fluorite solid solutions
 - R–Ta–O–N system 376
 - R–W–O–N system 373
 - degeneracy 619
 - degree of anisotropy 488
 - de Haas–van Alphen effect 610
 - dehydration–rehydration process 710
 - Delafossite-type nitrides CuNbN_2 293, 328
 - deltahedra 446
 - δ -MoN, hexagonal modifications 267
 - δ -NbN in nitrogen atmosphere 265
 - dendrites 722
 - density functional theory (DFT) 4, 105, 543, 544, 742
 - calculations 15, 26
 - calibrated Hückel model 63
 - calibrated simple Hückel DOS 8
 - density of states (DOS) 7
 - curves 9, 13
 - distribution 62
 - desintercalation 364
 - deuterides 485
 - deuterium 477, 484
 - DFT. *See* density functional theory
 - 3d-transition metal chalcogenides, structural relation between 403
 - diamond 46
 - diantimonides 462
 - diatomic covalent bond 3
 - diborides 442, 443
 - dielectrics 643
 - classification 643
 - constants, effect of oxygen isotope exchange 658
 - materials, classification 644
 - properties 232
 - diffraction 73
 - techniques 533
 - diffuse scattering pattern 632, 633
 - diffusion barriers 251
 - diffusion coefficient 545, 683
 - dilute magnetic semiconductor (DMS) 595, 608, 609
 - 3+1 dimensional direct space 74
 - Dion–Jacobson phases 243, 579
 - crystal structures of 244
 - Dion–Jacobson series members, structures of 578
 - dipolar second moments in sodium ultraphosphate glasses 125
 - dipolar second moment values, measured via spin echo decay method 121
 - dipole glass 660
 - dipole interaction 660
 - dipole magnets 721
 - dipole–dipole interactions 114, 120
 - Dirac cone 611
 - disproportionation, between light Li and heavy Ag sites 42
 - DMS. *See* dilute magnetic semiconductor (DMS)
 - $3d^4$ – $3d^7$ coordination 714
 - dodecaborides, icosahedra 448
 - dodecagonal approximants 80
 - donor/acceptor impurities 609
 - dopant anions 557
 - doping effect 223, 493, 638, 680, 692, 705
 - double-exchange ferromagnetic phase 606
 - double-exchange interaction 602, 603
 - double-exchange mechanism 600, 601
 - double-layer Ruddlesden–Popper perovskite structure 508
 - double hysteresis loop 651
 - double perovskite $\text{A}_2\text{BB}'\text{O}_6$
 - spin glass magnetic structure of 232
 - double perovskites
 - charge differences of 230
 - group–subgroup relationships of space groups 231
 - doxorubicin (DOX) 563
 - Dreiding force field 544

- Drosophila melanogaster* 722
 Drude model 596
 3D ThCr₂Si₂ structure 13
 3d transition metal chalcogenides 403
 duralumin 521
 DVD-RAM 735
 Dyaloshinski–Moriya (DM) interaction 634, 637
 dye–alkylsulfonate/LDH system 545
- e**
- effective Bohr magnetons 413
 eH orbitals 41
 eHtuner 6
 elastic effects 688
 electrical conductivity 438, 443, 444, 528, 603, 609, 675, 684
 electrical data storage devices 530
 electrical driving forces 685
 electrical gradients 683
 electrical potential 683
 electrical resistivity 385, 418, 420, 741
 – β -Cu_{2-x}Se 386
 – In_xNb₃Te₄ 421
 – measurements 288
 – temperature variations of 423, 424
 electric dipole 643
 electric energy 528
 electric field gradient (EFG) 104, 114, 532, 643
 electric polarization 643, 644
 electric potential 682
 electric quadrupole moment eQ 104
 electric susceptibilities 650
 electrocatalysis 691, 692
 electrocatalytic oxidation 557
 electrochemical applications 693
 electrochemical devices, for energy research 694
 electrochemical energy applications 665
 electrochemical energy technology 669
 electrochemical potentials 479, 672
 electrochemical reactors 685
 electrochemistry 494
 – functional materials for 669
 electrode/electrolyte interfaces 685
 electromotive force (EMF) 398
 – α -Cu₂Se | β -CuSe system 399
 electron affinity 6
 electron beam lithography 448
 electron density 2, 479, 483
 – antimony atom 74
 electron diffraction 421, 739
 electron doping 510
 electronegative elements 18
 electronegative metals 61
 electronegativity differences 60
 electron energy DOS 32
 electroneutrality 365
 electroneutrality equation 672
 electron-mediated magnetic interaction 600
 electronic carriers 685
 electronic charge density 417
 electronic conduction 500, 506, 675, 684
 electronic conductors 686
 – current collectors or taguchi sensors 696
 – fuel cells and batteries 696
 – sensors 696
 electronic defects 668, 684
 electronic disorder 668
 electronic DOS pseudogaps 51
 electronic energy 20
 electronic influences on site symmetry 168
 electronic materials 687
 electronic occupation 714
 electronic properties determination
 – disorder, role of 745
 electronic stability 13
 electronic structure 7
 electronic wavefunction 746
 electron localization function (ELF) 315
 electron microscopy 77, 389
 electron–electron repulsion 608
 electron–hole separation 549
 electron probe microanalysis (EPMA) 390
 electron spin polarizer 719
 electron tunneling 606
 electrophilicity 1
 electropositive elements 525
 electropositive metal 14, 61
 electrostatic interactions 552
 electrostatic lattice energy 230
 electrostriction coupling 650
 electrostriction effect 650
 elemental mixture in methanol 391
 elementary plaquette of a triangular lattice 621
 elements of frustration 620
 elements that accommodated on A-site and B-site of perovskite structure oxides 198
 EMF. *See* electromotive force
 enantiomeric secondary alcohols 428
 enantioselective crystallization 428, 430
 – amorphous Se 427
 energy-band structure 420

- energy level diagrams for water, AgCl, and Si) 670
 - energy resolution 632
 - enhanced permeability and retention (EPR) 562
 - measurements 306
 - enthalpy 115, 478, 482, 483, 673
 - entries in Shannon Tables of Effective Ionic Radii (Å), example 167
 - entropies 483
 - entropy 682
 - enzyme immobilization 710
 - EPMA. *See* electron probe microanalysis
 - electron probe microanalysis (EPMA)
 - ϵ -Fe₂CoN 279
 - ϵ -Fe₂NiN 279
 - ϵ -Fe₃N_{1+x} 269
 - ϵ -Mn₄N crystallizes 268
 - ϵ -phase 270
 - ϵ -TaN 266
 - ϵ -TaN transforms 265
 - ϵ -Ti₂N 262
 - equiatomic antimonide 466
 - equilibrium conditions 668
 - essentially discrete diffraction diagram 73
 - EuB₆ crystals 447
 - (Eu₃N)In 278
 - Eu₄[TaMgN₅]
 - crystal structures 321
 - EXAFS. *See* extended X-ray fine structure
 - absorption spectroscopy (EXAFS)
 - extended Hückel (eH) 5
 - methods 18, 297
 - extended X-ray absorption fine structure 94
 - extended X-ray fine structure absorption spectroscopy (EXAFS) 742
 - extracellular matrix (ECM) 710
- f**
- fabrication of an (LDH/PSS)_n-PVA film
 - schematic illustration of 561
 - face-centered cubic (fcc) compounds 39
 - face-centered cubic (fcc) symmetry 712
 - face-centered cubic (fcc) 164, 618
 - Fe_{3.1}Ga_{0.9}N 275
 - Fe-containing phase 293
 - Fe-phthalocyanine 604
 - Fe(II)Cu(II)-based magnets 709
 - [Fe^{III}N₃]⁶⁻ anions 303
 - FeMoN₂
 - crystal structures of 327
 - Fe₃Nb₃N 281
 - Fe–Fe bond distances 37
 - Fe–N phase diagram 270
 - FeNiN 285
 - Fe³⁺ oxides 584
 - fergusonite 377
 - fermi energy 8, 52
 - fermi level 671
 - fermi liquid behavior 603
 - fermi sphere 31
 - fermi surface 422, 595
 - Nb₃Te₄ 420
 - fermi wavenumber 608
 - fermi wave vectors 417
 - ferrelectric
 - first-order phase transition 648
 - ferrielectric 651
 - ferrimagnet 412, 705, 720
 - ferrimagnetic building-blocks 706
 - ferrimagnetic chains
 - assembly of 707
 - ferrimagnetic interactions 707
 - ferrimagnetic octacyanate 710
 - ferrimagnetic ordering 708
 - ferrimagnetism 415
 - ferroaxial coupling 236
 - ferroelectric 579, 720
 - definition 644
 - displacive-type 656
 - first-order phase transitions 648
 - free energy 649
 - optical soft mode 644
 - phenomenological considerations 653
 - polarization 236, 637
 - second-order phase transition 647
 - soft mode frequency 644
 - successive phase transition 649
 - ferroelectric Aurivillius phases
 - crystal structure of 246
 - ferroelectric transition temperatures 653, 657, 662
 - ferromagnet 705
 - ferromagnetic and antiferromagnetic interactions 634
 - ferromagnetic coupling 527, 630
 - ferromagnetic interaction 235, 414, 714
 - ferromagnetic interactions 712
 - ferromagnetic itinerant state 606
 - ferromagnetic magnetic semiconductors 608
 - ferromagnetic metal 509
 - ferromagnetic nanoparticles 722
 - ferromagnetic phases 606
 - ferromagnetic phase transition 600
 - ferromagnetic semiconductor 608

- ferromagnetism 35, 232, 509, 608, 635, 720
 - Fe, Co, and Ni 37
 - Fe₃Se₄ and FeTi₂Se₄, magnetic structures of 415
 - FeSe_x, phase diagram of 406
 - Fick's law 683
 - field-cooled magnetization 713
 - filiation 362
 - filled skutterudites 463
 - semiconductance in 463
 - thermoelectric properties of 463
 - first-order J–T (FOJT) 168
 - first-order or higher order phase transformation 682
 - fluctuations of the spins in a spin liquid–
 - classical or quantum, spin vice 619
 - fluoride 501
 - fluoride ion, ionic radius 479
 - fluorite 362
 - composition 363
 - structure of 363
 - structures, other defect 196
 - fluorite, CaF₂, and related structures 188
 - binary oxides 188
 - ordered defect fluorite structures; bixbyite, pyrochlore, and weberite 189
 - fluorite-type structures
 - defect fluorites 365
 - – bixbyite and antibixbyite 366
 - – pyrochlore 369
 - – scheelite 367
 - – zirconium-based oxynitrides 365
 - from diamond to fluorite; antiferrofluorite 364
 - structural filiation to 362
 - fluorspar 363
 - Frank-Kasper polyhedra 524
 - free crystal
 - susceptibility 650
 - free electric susceptibility 651
 - free electron concepts 45
 - free electron model 32
 - free energy 647
 - Frenkel disorder 680
 - Frenkel enthalpy 680
 - Frenkel level 671
 - frustrated lattices 625
 - frustrated magnetism 617, 618, 619
 - frustrated magnetism on 2D and 3D lattices 618
 - frustrated magnets 619
 - frustrated materials 619
 - frustrated systems 631
 - frustration 617
 - fullerene acceptor 720
 - fullerenes 703
 - fulminating silver 272
- g**
- Ga -hybrid orbitals 10
 - γ-AgCuS + Cu → Ag + Cu₂S 388
 - γ-AgCuS, decomposition of 388
 - γ'-Fe₄N 270
 - γ'-Fe₄N-type perovskite structure 268
 - γ'-Fe₄N structure 272
 - γ'-M₄N phases 275
 - γ-Mo₂N 267
 - Ga–Ga bonding interactions 9
 - Ga–Ga bonds 8
 - Ga–Ga curve 10
 - Ga–Ga interactions 9, 10
 - Ga NMR signal 537
 - Ga 4p orbitals 9
 - GaSb 458
 - gas barrier films
 - with brick–mortar–sand structure 558
 - with brick–mortar structure 558
 - with self-healing properties 560
 - gas barrier properties 558
 - gas-phase interstitial modification technique 253
 - GdFeO₃-type distortion 656
 - GdFeO₃-type orthorhombic structure 656
 - Ge–Sb–Te alloys 739, 744
 - Ge–Sb–Te based optical memory disks 746
 - Ge–Sb–Te system 735
 - Ge–Te binary phase diagram 738
 - GeO₂ glass 113
 - geometrical frustration 618, 622
 - in simple atomic systems 619
 - – curved-space approach 620
 - germanate 95
 - germanium chalcogenides 737
 - germanium telluride (GeTe) 737
 - GeSb₂Te₄
 - atomistic explanation 745
 - metal–insulator transition 745
 - GeSb₂Te₄ films 745
 - electrical properties 745
 - GeSbTe system
 - ternary phase diagram 529
 - GeTe–Sb₂Te₃ compounds
 - crystal structures 738
 - GeTe–Sb₂Te₃ system 530
 - GGA-DFT electronic structure of ScNi₂ 7
 - giant magnetoresistance 595
 - giant magnetoresistance (GMR) 599, 718

- giant magnetoresistance materials 599
 Gibbs free energy 503, 672, 681, 692
 glassy magnetic state 413
 Glazer tilt systems 199
 golden metallic rock salt-type δ -TiN_x 262
 Golden yellow metallic rock salt-type ZrN 262
 Goodenough–Kanamori rules 163
 grain boundaries 669
 graphene 595
 – microspheres (GMSs) 556
 – nanosheet 548
 – quantum dots 548
 – spintronics 719
 graphite 443
 greigite (Fe₃S₄) 721
 group V elements, structure map 743
 growth kinetics 693
- h**
- half-Heusler compounds 2, 527
 half-Heusler phases 51
 half-metallic electronic structure 232
 Hall angle 596, 609
 Hall resistivity 596
 Hall voltage 595
 Hamiltonian matrix 5
 hardness 448
 H₂/Ar gas mixtures 280
 Hartree–Fock-type mean-field approximation 608
 HCP lattice 165
 HDDR process (hydrogenation–decomposition–desorption–recombination) 253
 heat conduction 746
 heat-resistant alloys 252
 heavy alkali metals 141
 heavy alkaline earth (Ca, Sr, and Ba) hydrides 485
 heavy fermion 603
 heavy rare earth trihydrides 500
 HeI photoelectron spectra
 – of Cs, Cs₁₁O₃·Cs₁₀, and Cs₁₁O₃ 146
 Helical chains 297
 Helmholtz free energy 649
 heptacyanate anion 714
 hepta/octacyanates 714
 heterogeneous catalysis 455
 heterogeneous electrolytes 687
 Heusler-phase 306, 322
 Heusler phases 527
 hexaborides 447
 hexacyanometalates 710
 hexagonal bipyramidal 289
 hexagonal ϵ -NbN 265
 hexagonal-close-packed 618
 hexagonal lattice 403, 405
 hexagonal Mn₅Si₃ structure 285
 hexagonal Nb₅N₆ 265
 hexagonal perovskite compounds 241
 – tolerance factor 241
 hexagonal perovskite structures 212, 213, 241
 – projections, of octahedra network 241
 hexagonal single crystals 256
 hexagonal symmetry 542
 hexakaidecahedra 529
 Hf d orbitals 18
 Hf–Hf and Hf–P bond strengths 18
 Hg–In
 – binary phase diagrams 61
 [Hg₂N]⁺ in mercury-containing nitride phases 273
 4H–BaRuO₃-type structure 277
 high density metal nanoparticles
 – schematic illustration of 550
 higher borides 450
 higher moments 25
 highest occupied crystal orbital
 – isosurfaces encasing 745
 high-density information storage devices 717
 high-energy-resolution spectrum 633
 high-pressure behavior 489
 high-pressure phase 387
 – pyrite-type CuSe₂, 387
 – tetragonal Cu₂–xS 385
 high-pressure phase transitions 490, 491
 high-resolution transmission electron microscopy (HRTEM) 740
 high-spin state 169
 high-T_c superconducting copper oxides
 – crystal structure of 240, 246
 high-temperature centrifugation-aided filtration (HTCAF) 288
 highly frustrated magnetism in spinels 626
 high spin –low spin transitions 714
 H₂ molecular orbital diagram 3
 Ho₃Al₅O₁₂ garnet 634
 hollandite structure exemplified by Ba₂Mn₈O₁₆ 186
 homing 722
 homogeneity 371
 homogeneous catalysts 552
 homogeneous glasses 117
 homogeneous transition 606
 homonuclear pnictogen–pnictogen bond 462

- homopolar Ge–Ge bonds 742
 - Hume-Rothery electron concentration
 - phases 1, 32, 35, 522
 - tight-binding energy 24
 - Hund's rules 499, 703
 - Hund coupling 600
 - Hückel approaches 6
 - Hückel calculations 25, 300
 - Hückel energy 25
 - Hückel-based model 7
 - Hückel methods 4
 - Hückel model 6
 - Hückel theory 4
 - Hückel tight-binding method 426
 - hybridization 500
 - hydride 507, 511
 - hydride anion 479, 504, 506, 510, 512
 - in oxides 501, 506
 - hydride compounds, thermodynamics of 480
 - hydride diffusion 511
 - hydride exchange reactions 511
 - hydride ions 488
 - mobility, in saline hydrides 478, 491
 - hydride phase 481
 - hydride species 477
 - hydroformylation 552
 - hydrogen 477, 481
 - hydrogen AO electron clouds, change in 2
 - hydrogenation reaction 502
 - hydrogen atom
 - electron affinity 479
 - hydrogen bond 477
 - hydrogen bonded system
 - potassium dihydrogen phosphor 653
 - hydrogen bonding 703
 - hydrogen chemistry 478
 - hydride compounds 479
 - hydrogen species 478
 - hydrogen impurities 255
 - hydrogen partial pressure 481
 - hydrogen storage 455, 478, 481
 - hydrogen sulfide 501
 - hydrotalcite-like compounds 541
 - hydrous oxides 572
 - hydroxyl hydrogen 544
 - 18-electron rule 51
 - μ_2 -Hückel chemical pressure analysis 58
 - Hückel model of SrAg₅ 26
 - scaled sH 27
 - μ_2 -scaling 25
 - hypothetical CaCu₅-type CaAg₅ phase 60
 - hysteresis loop 709, 716
- i*
 - icosahedra 446
 - icosahedral approximants 80
 - icosidodecahedral shells 85
 - icosidodecahedron 85
 - Imma* orthorhombic 239
 - Imma* structure 210
 - impurity phases 253
 - indium 440
 - industrial device fabrication 737
 - inelastic neutron scattering 628
 - inelastic scattering spectrum 632
 - infinite zigzag chain anions 296
 - infrared absorption 94
 - infrared spectroscopy 631
 - inorganic crystal structure database 163
 - insulator–metal transition 225
 - insulators 643
 - classification of materials 644
 - interatomic distances 25, 500
 - interatomic interactions 25, 59
 - intercalation 364, 589
 - interfacial charge 686
 - Intergrowths 211
 - inter-particle interactions 712
 - inter-spin interactions 632
 - interlayer reactions 587
 - intermediate-range order 94
 - intermetallic bonding 1, 2
 - intermetallic community 13
 - intermetallic compound (IMC) 8, 16, 17, 31, 51, 55, 521, 551
 - characteristic of 17
 - intermetallic phases 6, 33, 521
 - intermetallics, investigation of 532
 - intermetallic structures 27, 59
 - intermetallic systems 6
 - intermolecular exchange interactions 705
 - intermolecular interactions 703
 - interpolyhedral interaction 446
 - interstitial compounds 440
 - interstitial nitrides 331
 - Interstitial nitrogen 284
 - intrinsic magnetic anisotropy 718
 - inverse-Heusler compounds 527
 - inverse piezoelectricity 645
 - inverse piezoelectricity effect 653
 - iodine 440
 - ion conduction, mechanism of 683

- ion conductivities 684
 - solid electrolytes, as function of temperature 685
 - ion conductors 684
 - solid electrolytes 693, 695
 - ion exchange 587
 - ion-exchange materials 584
 - ionic and electronic defects, as acid–base and redox particles in equilibrium 669
 - C-rule 674
 - P-rule 674
 - T-rule 674
 - ionic and electronic diagrams 671
 - ionic bonding 477
 - ionic bonds 477, 478
 - ionic compounds 478
 - ionic conductivity for Cu ions 398
 - ionic conductors 584, 684
 - ionic crystal 680
 - ionic crystals 665, 669
 - concept 222
 - ionic defects 687
 - ionic disorder 668, 671, 673
 - ionic gap 670
 - ionic liquids 522
 - ionic materials 479
 - ionic mobile species 693
 - ionic model 488
 - ionic nitrides 330
 - ionic radius 479
 - of large halides 479
 - ionic redistribution effects at contacts 688
 - ionization energy 6, 479
 - Ir DOS distribution 64
 - Iron (Fe) deficiency 327
 - iron-based nitrides 275
 - iron-based superconductor 406
 - Ising systems 717
 - isolated double tetrahedra $[M_2N_6]^{8-}$ 319
 - isolated dumbbell anions 290
 - isolated nonplanar anions 304
 - isolated planar anions 300
 - isolated tetrahedra $[MN_4]$ 318
 - isolobal T–T bonds 55
 - isostructural compounds
 - semiconductance of 462
 - isostructural oxides 512
 - isotropic chemical shift 104
 - isotypic $Ba[Mg_{3.33}Nb_{0.67}N_4]$ 321
 - isotypic high-temperature phases
 - $Ba_3[MoN_4]$ 319
 - isotypic phase $Ba_2[NNiCN]$ 291
 - isotypic phase $Sr_2[Ni_2(Ni_{1-x}Li_x)N_2]$ 298
 - isotypic quaternary nitridorhenates 315
 - isotypic $Sr_3[CrN_4]$ 318
 - isotypic structures $Li_3Ba_2[NbN_4]$ 314
 - itinerant ferromagnetic state 606
- j**
- Jahn–Teller distortion 223, 231, 300
 - Jahn–Teller effect 27
 - Jahn–Teller J–T phenomena 168
 - Jahn–Teller transition 627
 - Jahn–Teller type, symmetry breaking 40
 - $J_1 - J_2$ model, showing ground state spin configurations for 621
 - Jones model 33
 - Jones reflections 35
 - Jones theory 32, 41
 - Jones zones 31, 34
 - for γ -brass (Cu_5Zn_8 -type) Cu_5Cd_8 and Cd_3Cu_4 32
- k**
- Kanamori–Goodenough rule 232
 - κ -space 34
 - $K_{23}Au_{12}Sn_9$
 - electronic structure analysis 16
 - $K[CoO_2]$ -type structure 323
 - K-edge XANES 290
 - k-space 27
 - K-values 675
 - kinetic energies 2, 3
 - $KNbO_3$ 654
 - K–Au interactions 16
 - Knight shift 532
 - Kohler’s law 597
 - Kohler’s rule 596
 - Kohn–Sham Ansatz 4
 - Kohn–Sham equation 4, 6
 - Kondo effect 603
 - $KOsO_3N$ monocrystals 368
 - K_5Pb_{24}
 - eH bonding analysis 15
 - Kröger–Vink diagram 675
 - Kröger–Vink nomenclature 668
 - Kröger–Vink notation 480
 - $KTaO_3$
 - temperature dependence of dielectric constant 658
 - $K_3Ti_5NbO_{14}$ structure 585
 - $KTiNbO_5$ structure 585

I

- La₃[Cr₂N₆]
 - crystal structures 324
- Lactobacillus fermentum 721
- LaHO crystal structure 503
- La₂LiO₃H-Sr₂LiOH₃ system 514
- Landau levels 598, 609
- Landau phenomenological equation 649
- Landau theory 227, 647
- lanthanide 4f orbitals 8
- lanthanides 448
 - Ce–Lu 259
- lanthanoides 140, 435
- lanthanum hexaboride 448
- laser-heated diamond-anvil cells 262
- LaSrCoO₃H_{0.7} crystal structures 508
- LaSrCoO₃H_{0.7} QENS data 509
- La_{1.4}Sr_{1.6}Mn₂O₇
 - resistivity of 602
- latent heat 426
- lattice constants 225
- lattice thermal conductivity 462, 468
- Laves phases 2, 523
 - AB₂, MgCu₂, crystal structures 524
- layered cobalt oxide Ca₃Co₄O₉
 - magnetoresistance scaling 604
- layered double hydroxide (LDH) 541, 584
 - active species-intercalated nanocatalysts 552
 - based materials
 - biorelated applications of 563
 - overpotentials of 557
 - basic structural features 542
 - biological and medical properties 561
 - in bioapplications 562
 - in drug delivery and treatment 562
 - drug-delivery performance 563
 - synthesis of LDH-Based biomaterials 561
 - brucite-like layers 542
 - catalytic properties of 548
 - confinement effect 546
 - on electron distribution of guest molecules 546
 - on hybrid materials 546
 - construction of 543
 - density functional theory calculations of 545
 - electrochemical catalysis 556
 - electrochemical energy storage properties 553
 - electronic properties 545
 - fabrication of 554
 - facile exfoliation of 553
 - formula 541
 - general structure 584
 - host layer structure of 543
 - host–guest interaction of 546
 - interlayer galleries of 552
 - interlayer structure of 543
 - metal-based catalysts 550
 - microspheres 555
 - microstructure and property of 544
 - molecular dynamics simulations of 544
 - photocatalysis of 549
 - properties and applications of 546
 - rearranged geometric configuration 547
 - solid base catalysis of 549
 - for stoichiometries 543
 - structural characteristic of 543
 - structural properties of 545
 - supercapacitors (SC) 554
 - theoretical studies of 544
- layered oxides 571
 - containing metal-oxygen octahedra 573
 - made up of edge- and/or corner-shared metal-oxygen octahedra 584
 - miscellaneous 586
 - possessing rocksalt superstructures 581, 582
 - rocksalt superstructure family, structures of 583
 - types 572
- layered oxyhalides 587
- layered oxynitrides 587
- layered oxysulphides 587
- layered perovskites 573
- layered perovskites A_mB_{m-1}O_{3m}, structure 580
- LDA-DFT
 - eH-fitted band structure of γ -brass 42
- LDA-DFT band calculations 41 (LDH/CA)_n multilayer film
 - schematic representation of 559
- “spintronicmaterials 161
- leak currents 646
- LED industries 331
- Lennard-Jones 6– α 12 potential 25
- Li_{52.0}Al_{88.7}Cu_{19.3} 46
- Lewis acid 479
 - Lewis acid–base reaction 62
- Lewis bases 63, 478, 479
- Lewis notation 139
- Lewis structure 1
- Lewis theory 62
- L-proline intercalated LDHs
 - schematic model of 553

- Li₈Ag₅
 - γ -brass structure 44
 - Li₃₂Ag₂₀
 - DOS and COOP for Ag framework 44
 - Li₃₃Ag₁₉ 43
 - Li_{52,0}Al_{88,7}Cu_{19,3}
 - DOS and COOP 48
 - Jones zones 45
 - Li_{54,0}Al_{89,2}Cu_{19,0} powder 47
 - Li atoms 44
 - Li₆C a metal-rich species 139
 - Li₆(Ca_{1-x}Sr_x)₂[Mn₂N₆] 304
 - Li₆Ca₂[Mn₂N₆]
 - crystal structures 306
 - Li₁₅[Cr^{VI}N₄]₂N
 - crystal structures of 313
 - LIESST. *See* light induced excited state trapping (LIESST)
 - ligand field favoring 714
 - ligand holes, localization of 235
 - light-switchable materials 715
 - light induced excited-spin state trapping 715
 - light irradiation 714
 - Li-ion batteries
 - transition metal as anode material in 364
 - Li-ion batteries (LIB) 556
 - coulombic efficiency 556
 - degree of dispersion 556
 - performance of 556
 - use of, carbon materials 556
 - Li-ion conduction 684
 - lithium nitrides for 455
 - Li-Mg-Zn-Al Bergman phases
 - using Mulliken populations 19
 - Li-storage 688
 - Li⁺ ions 19
 - Li₂[(Li_{0.5}Co_{0.5})N]
 - DC magnetization 288
 - Li₂[(Li_{1-x}Cu_x)N] 290
 - Li₂[(Li_{1-x}Fe_x)N] 288
 - Li₅[(Li_{1-x}Mn_x)N]₃ 295
 - Li₂[(Li_{1-x}M_x)N] 290
 - Li₅[(Li_{1-x}M_x)N]₃
 - crystal structures 289
 - Li(2)₂[Li(1)N] 287
 - Li₂[LiN] crystal structure 289
 - Li₂[LiN]-type structure 288
 - Li₂₄[Mn^{III}N₃]₃N₂ 305
 - [LiN] chains 295
 - Li–Ga curve 10
 - Li–Ga interactions 9, 10
 - Li–Ga overlap 10
 - Li–Ge–thiophosphates 684
 - Li–Hg and In–Hg phase diagrams 61
 - linear combination of atomic orbitals (LCAO) 4, 42
 - linearly coordinated Li 287
 - linear magnetoresistance (LMR) 393
 - Linear Muffin Tin Orbital-Atomic Sphere Approximation-Tight-Binding (LMTO-ASA-TB) 15
 - Li₂N layers 289
 - Li₃N substitution variants 290
 - Li₃N superstructures 287
 - Li₂O-type defect and order variants 304
 - Li₂O structure 310
 - liquid crystallinity 719
 - Li₃[ScN₂] 310
 - Li₂Sr₅[MoN₄]₂ 314
 - Li₃Sr₃[NiN]₄
 - predominant structural features 295
 - Li₂Ta₃N₅ 326
 - Li₁₆[TaN₄]₂O
 - LiTaO₃ 654
 - lithium alkaline earth metal nitridometalates
 - linear chains 294
 - lithium battery cathodes 163
 - lithium clustering 122
 - lithium extraction 313
 - lithium ion conductor 287
 - lithium ions 120, 586
 - lithium salts (LiMO₂) 588
 - lithium silicate glasses 120, 122
 - Li₇[VN₄] 312
 - Li_x[Mn_{2-x}N] 304
 - LiZrN₂ 328
 - LMR. *See* linear magnetoresistance
 - localized bonding models 48
 - local modes 626
 - Lorentz field 597
 - Lorentz force 596, 609
 - LT-SrCeN₂ 325
- m**
- MA. *See* mechanical alloying (MA)
 - 2/1 Mackay approximant, shells of cluster 86
 - magnesium borides 443
 - magnesium hydride (MgH₂) 488
 - magnetic abnormality 636
 - magnetic anisotropy 716
 - magnetic centers 703
 - magnetic diffuse scattering pattern 633
 - magnetic dipole–dipole coupling 115
 - magnetic dynamics 718
 - magnetic entropy change 713

- magnetic field 598, 710
- magnetic field (MF) 710
- magnetic frustrated materials 625
- magnetic frustration 619
 - in multiferroic materials 634
- magnetic hydrogels 710
- magnetic-ion density 609
- magnetic hysteresis 716
- magnetic information 722
- magnetic interaction 413, 631
- magnetic ion doping 634
- magnetic MAX phases 282
- magnetic moment 703
- magnetic ordering 720
 - temperature 712, 713
- magnetic particles 722
- magnetic properties 412
 - of BTFO film 634
- magnetic random access memory (MRAM) 718
- magnetic relaxations 716, 717
- magnetic resonance imaging (MRI) 562
- magnetic sensor 720
- magnetic spin ordering 720
- magnetic susceptibility 413, 425, 628
 - data 306
- magnetic tunnel junctions 719
- magnetic zeolitic structures 720
- magnetism 512, 617, 704
- magnetite (Fe_3O_4) 161, 721
 - crystals 721
- magnetization 704
 - relaxation time 716
- magnetocaloric effect 713, 717
- magnetocaloric effect (MCE) 713, 717
- magnetocaloric refrigeration 438
- magnetocrystalline anisotropy 443
- magnetoelectric coupling 637, 720
 - in BTFO film 637
- magnetoelectric effect 634
- magnetopolarization measurements 637
- magnetoreception 722
- magnetoresistance (MR) 595, 719
 - classification of 598
 - effect 223, 719
 - types of 599
- magnetostrictive semiconductor 609
- magnetsensitive system
 - cryptochrome-based 722
- magnetsome 721
- magnetotactic bacteria 720, 721
- magnetotactic bacteria (MTB) 721
- magnetotaxis 721
- magnets 716
 - molecule-based 704
 - rare earth-based 723
- manganese borides 438
- manganese hexacyanoferrate (MFCN) 723
- manganese-rich $\text{Ca}_{12}[\text{Mn}_{19}\text{N}_{23}]$ 305
- manganese oxides 602
- MAS-NMR spectrum of glassy B_2O_3 104
- mass action constant 673
- mass action laws 674
- mass-market devices 735
- mass spectrometry 510
- MAX-phases $\text{M}_{n+1}\text{AN}_n$
 - crystal structures 282
- maximally localized Wannier function 49
- MAX phases 272, 278, 281, 282
- Maxwell equations 713
- mayenite 505
- MB_4 variants 447
- McConnell's model 706
- MCE. *See* magnetocaloric effect
- MD. *See* molecular dynamics
- MD simulations 113, 120
- mechanical alloying (MA) 384
- mechanical energy 401
- mechanochemical reactions 384
- mechanochemical synthesis 384
- ME coupling versus magnetic field of BTFO15 film 635
- medium-range order 94
 - experimental characterization of 99
- medium-range order, experimental characterization of
 - solid-state NMR 103
 - dipolar NMR methods 105
 - magic-angle spinning NMR 104
 - vibrational spectroscopy 101
 - X-ray and neutron diffraction techniques 99
- memory effect 709
- metal atom coordination, in diborides 443
- metal atom matrix 139
- metal atoms 403
- metal borides 435, 438, 439, 441
- metal cations 544
- metal chalcogenides 383, 384, 402
 - preparation methods of 383
- metal diborides 445
- metal film 692
- metal fluxes 257
- metal halides 439
- metal hydrides 478, 501
- metal-like electrical resistivities 326
- metal-organic magnets

- Ni₂A-based 723
- metal-oxygen octahedra 573
- metal-rich borides 440
- metal-rich compounds
 - multinary derivatives of 272
 - β-Mn derivatives 279
 - ε-Fe₃N derivatives 278
 - η-carbide derivatives 280
 - γ'-Fe₄N derivatives 273
- metal-rich Rb₆O 143
- metal ions 572, 586, 588, 590
- metallic bond 478
- metallic compounds La₃[Cr₂N₆] 324
- metallic conductivity 509, 526
- metallic η-carbide-type compounds 280
- metallic glasses 93
- metallic hydrides 477, 479, 487, 496, 500
 - structural information for 498
- metallic lattice 501
- metallide nitrides 258, 328
- metal ligand 507
- metallization 490
- metal-metal bonds 139, 140, 159
- metal-metal-bonded clusters 159, 160
- metal–boron interactions 445
- metal–insulator transition 604, 605, 745
 - field-induced 606
- metal–metal hydride phase diagram 481
- metal–metal multibond 450
- metal–nonmetal arrays 588
- metal–nonmetal layered structures 581
- metal oxides 93, 383, 439, 692
- metal vacancies 405
- metastable oxides 587, 590
- metastable semiconducting Cu₃N 271
- metastable ternaries 739
- metathesis product 439
- methylammonium cation 223
- methylammonium lead halides 223
- methyl–ammonium–lead iodide 685
- MF. *See* magnetic field (MF)
- MFCN. *See* manganese hexacyanoferrate (MFCN)
- Mg₂Al–benzoate LDH 544
- Mg₃₂(Al,Zn)₄₉ phase 19
- MgCu₂
 - tight-binding energies of 23
- MgCu₂ structure 57
- MgEu₄[TaN₄]N 320
- MgH₂ rutile structure 488
- Mg/Mg²⁺ couple 479
- Mg₃Sb₂ 457
 - thermoelectric properties of 457
- m-Co₄Al₁₁ structure of two layers 78
- microcrystalline samples 271
- microscopic probes 606
- microwave communication devices 233
- microwave irradiation 589
- migration energy 680
- migration of Cu⁺ ions 398
- milling 384
- Millon's base [Hg₂N]N₃ 272
- missing cations 744
- mixed conductors
 - as electrodes or absorbers 695
 - batteries 696
 - fuel cells 695
 - sensors, chemical storage and permeation devices 696
- mixed metal oxide (MMO) 549, 557
- MM'₃N phases
 - crystal structure types 274
- Mn-based perovskite nitrides 276
- Mn(II)Cu(II) molecular magnets 707
- Mn₄N
 - Curie temperature 276
- Mn₃SbN 276
- Mn₃ZnN exhibits antiferromagnetic order 276
- mobile carrier 600
- mobility 675, 684
- Mo–Mo bond 460
- modified oxide glasses 124
 - medium range order in 118
- modified random network (MRN) 119
- molecular building blocks 711
- molecular cluster 716
- molecular crystal lattice 709
- molecular dynamics (MD) 544, 742
 - simulations 95
- molecular magnet
 - design 704
- molecular magnetic sponges 709, 710
- molecular magnetic switches 715
- molecular magnets
 - design and synthesis strategies 704
- molecular magnets design
 - using azido bridge to mediate spin–spin couplings 715
- molecular materials 703
- molecular multication ferrimagnets 713
- molecular orbital theory 6
- molecular spintronics 718
- molecular wires 719
- molecule-based magnet
 - self-assembly 704

- molybdenum diboride 445
 moment analyses 20
 – higher moments 21
 monosilicides 525
 morphotropic phase boundary 646, 661
 morphotropic phase boundary (MPB) 646, 661
 Mo_3Sb_7 462
 – crystal structure of 461
 – density of states of 461
 Mössbauer spectra 290
 – for Fe atoms 288
 MoS_2 -type structure 327
 Mössbauer effects 631
 Mössbauer spectra
 – of BTFO ceramic sample 636
 – of BTFO15 ceramic sample 637
 motion sensors 645
 motivation 521
 Mo_3 triangles
 – in MoS_2 50
 Mott insulator 627
 Mott–Hubbard model 163
 MPB. *See* morphotropic phase boundary (MPB)
 MR. *See* magnetoresistance (MR)
 MRAM. *See* magnetic random access memory (MRAM)
 MRN hypothesis 120
 M_4Si_4 crystal structures, cut out 525
 MTB. *See* magnetotactic bacteria (MTB)
 multielectron wave function 49
 multiferroicity 236
 multiferroic materials 634
 multifunctional molecular magnetic materials 719
 multiple inhomogeneities 660
 multiple quantum well (MQW) 546
 muon spin rotation (μSR) spectroscopy 631
 M_2 values 120, 122, 123
- n**
- Na_2B_{29} structure 449
 Na_3B_{20} structure 448
 NaCl crystal structures of binary nitrides 261
 Na^+ conductivity 684
 $\text{Na}_3\text{Co}_2\text{SbO}_6$ oxide 583
 $\text{Na}_2\text{Co}_2\text{TeO}_6$ oxide 583
 $\text{Na}_2[\text{HgO}_2]$ -type 291
 nanocrystalline 688
 nanodomains 456, 464
 nanoionics 686
 nanomagnets 717
 nanomaterials 528
 nanoparticle systems
 – magnetic properties 712
 nanoporous molecular magnet 720
 nanostructuring 456, 466
 nanowires 528
 $\text{Na}_4[\text{Re}^{\text{V}}\text{N}_3]$ contains pyramidal anions $[\text{ReN}_3]^{5-}$ 304
 narrow-gap semiconductors 458, 462, 467
 narrow magnetic hysteresis loops 709
 $\text{Na}_2\text{Ti}_3\text{O}_7$ structure 585
 $\text{Na}_2\text{Ti}_4\text{O}_9$ structure 585
 N_2 atmosphere 252
 Nb–O bonds 184
 Nb–O octahedron in CoNb_2O_6 184
 NbSb_2 460
 – crystal structures of 459
 Nd–O coordination polyhedron with $\text{Nd}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$
 – magnetic diffraction 605
 – resistivity 605
 Néel temperature 269, 508, 632
 nearest-neighbor 618
 near-infrared 713
 near-infrared (NIR) 713
 nearly free electron model 29
 negative magnetization 713
 neodymium iron boride 438
 neodymium phase 369
 Nernst–Einstein equation 684
 nerve fibres 722
 nesting 422
 net reaction rate 683
 network formers 93
 neurodegenerative diseases
 – magnetic particles formation 723
 neuromorphic 746
 neutron diffractions 369, 377, 408, 445, 510, 602, 636, 737
 – data 446
 – experiments 120
 neutron diffuse scattering patterns of $\text{Ho}_3\text{Al}_5\text{O}_{12}$ garnet measured at 633
 neutron inelastic scattering spectra of $\text{Ho}_3\text{Al}_5\text{O}_{12}$ garnet measured at 632
 neutron powder diffraction 636
 – of BTFO ceramic sample and analysis of specific peak 636
 neutron scattering 656
 – experiments 632
 next-nearest neighbor correlations in tetrahedral network glasses 97
 N_2/H_2 gas mixture 280

- N-poor phase boundary 267
 - Ni_2Al_3 structure 57
 - NiAs-type structure 265
 - nickel hexacyanoferrate (NiHCF)
 - nanoparticles 712
 - $\text{Ni} \cdots \text{Ni}$ contacts 297
 - NiHCF–DODA films 712
 - Ni-based perovskites Ni_3MN 277
 - Ni membrane 255
 - $\text{Ni}_2\text{Mo}_3\text{N}$ antiferromagnetism 280
 - niobium chalcogenides 418
 - NITR, chemical structure 706
 - nitridation 366, 370, 373, 377
 - nitrided R_2WO_6 precursors
 - composition and unit cell parameter of 373
 - nitride ions 327
 - nitride–metalide phases 329
 - nitride oxides 251
 - nitrides 251
 - nitrides, non-main group elements
 - preparative aspects 252
 - nitridoferrates(II) $\text{Ca}_2[\text{FeN}_2]$ 303
 - nitridometalate-azide-nitride $\text{Ba}_9(\text{Ta}, \text{Nb})\text{N}_4)_2[\text{N}_3]\text{N}$ 255
 - nitridometalate oxide $\text{Ba}_3[\text{ZnN}_2]\text{O}$ 291
 - nitridometalates 251, 254, 286, 300, 309, 310, 323, 331
 - binary transition metal nitrides 253
 - chemistry 309
 - containing heavier alkali metals 306, 316
 - crystal structures of 305
 - planar zigzag chains 296
 - prototypes 325
 - synthesis 254
 - tetrahedra 316
 - nitridosilicates 251
 - nitridotungstates 257
 - nitrogen 253, 259
 - sensitizing effect 366
 - nitrogen/europium concentration ratio 366
 - nitrogen-rich tantalum nitride 266
 - NMR chemical shifts 507
 - NMR coupling parameters 533, 535
 - NMR crystallography 132
 - NMR methodology 94
 - NMR signals 533, 537
 - NMR spectroscopy 120, 535
 - noble metal chemical bond 42
 - noble metal γ -brass e^-/a ranges 33
 - noncoherently magnetic 1 : 3 transition metal species 29
 - nonconducting materials 532
 - non-Kramers garnets 632
 - non-spin polarized bcc Cr band structure 41
 - noninteracting paramagnet 622
 - nonmagnetic Cr Fermi energy 39
 - nonmagnetic Fe
 - DOS and COHP 37
 - nonmagnetic metals 412, 413
 - nonmagnetic probiotic bacteria 721
 - nonmagnetic transition metal compounds 38
 - nonmetallic impurities 254
 - Nowotny chimney ladder (NCL) 53
 - phases 2, 53, 54
 - $n = 1$ RP phase, Sr_2TiO_4 , as an intergrowth of one perovskite 211
 - nuclear Bragg reflection position 633
 - nuclear magnetic resonance (NMR) 94, 506, 522
 - nuclear quadrupole moment 532
 - nucleation 481, 689, 693
 - nucleophilicity 1
- O**
- occupancy rate (p_o) 404
 - octagonal approximants 75
 - octahedral 446
 - distortion 223
 - linkage pattern in anatase (TiO_2) 186
 - rotations 224
 - octahedral rotations
 - lattice connectivity 224
 - magnitude and phase of 224
 - octahedral site preference energies (OPSE) 168, 169
 - octahedral sites 543
 - octahedral tilting distortion 228
 - Ohm's law 596, 683
 - O holes 165
 - $o\text{-Al}_{13}\text{Co}_4$ structure of two layers 78
 - olefins 552
 - oligomeric anions 303
 - one-electron Schrödinger equation 5
 - opaque classical magnets 710
 - $o'\text{-Al}_{13}\text{Co}_4$ structure of two layers 79
 - optical data storage devices 530
 - optical micrographs of ZnSe 402
 - optical rotation 430
 - optical storage media 744
 - optimization process 228
 - optoelectronic displays 715
 - orange-red Ta_3N_5 266
 - orbital-ordered states 601
 - orbitals 5
 - degrees of freedom 601
 - ordered perovskite structures

- involving combinations of A- and B-site and oxygen vacancy ordering 211
 - order–disorder-type ferroelectrics 643, 653
 - order–disorder phenomena 617
 - order–disorder transition 493
 - organic chemistry 1
 - organic ferroelectric 662
 - organic-based material
 - iron-containing 705
 - organic–inorganic hybrids 590
 - organic polymeric structures 705
 - organic salts 607
 - organic spintronic device 719
 - organometallic compound 51
 - organophosphonic acids 590
 - orientation 693
 - orthorhombic approximant 81
 - orthorhombic $\text{Ba}_2[\text{Ni}_3\text{N}_2]$ 297
 - orthorhombic CaTiO_3 crystal structures 226
 - orthorhombic compounds 282
 - orthorhombic phase $o\text{-Co}_4\text{Al}_{13}$ 77
 - osmium atoms 446
 - O_2 system
 - darker contrast 36
 - overdoping 679
 - oxic–anoxic interface 721
 - oxidation 140, 148, 163
 - state 161, 166
 - of Mg atoms 444
 - oxide-based functional materials 571
 - oxides 581
 - ions 192
 - materials 572
 - oxonitridometalates 251
 - oxyfluorides 229, 503, 504
 - oxygen 140
 - atoms 142
 - crystal structure of 238
 - defect perovskites 207
 - evolution reaction (OER) 556
 - interaction 691
 - stoichiometry 689
 - profiles for Fe-doped 690
 - transmission rate (OTR) 558
 - vacancies 238, 693
 - oxygen isotope exchanged SrTiO_3
 - ϵ versus T^2 plot 659
 - oxyhydrides 477, 501, 502, 503, 514
 - high-pressure synthesis of 513
 - oxynitrides 229, 361, 511
 - crystal chemistry of 361
 - environmental applications 361
 - optical properties of 361
 - and oxides, comparison between 361
 - powders 375
 - preparation of
 - solid/gas reactions 370
 - with pyrochlore structure
 - preparation of 370
 - scheelite structure type 368
 - solid solutions
 - characterization of 376
 - synthesis 370
 - oxynitride tungstates
 - spectral selectivity of 376
- p**
- packing of characteristic, Li_{26} and $\text{Ba}_5\text{Na}_{12}$ units
 - in $\text{Li}_{13}\text{Na}_{29}\text{Ba}_{19}$ and central Li_4N unit 156
 - paraelectric KDP 643
 - crystal structure 654
 - paramagnetic centers 716
 - partial amorphization 401
 - partial electron transfer 27
 - particle diffusion 684
 - Pauling bond order function 18
 - Pauli paramagnets 412
 - PBA. *See* prussian blue analogues (PBA)
 - p block states 14
 - Pb–Pb interactions 14, 15
 - PB NPs. *See* Prussian blue nanoparticles
 - PbTiO_3 654
 - $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ system
 - phase diagram 661
 - PbZrO_3 651, 654, 661
 - $\text{PbZrO}_3\text{–PbTiO}_3$ (PZT) 646
 - PCM. *See* phase-change material (PCM)
 - PD_2 Al–Co–Ni structure of two layers 79
 - Pearson Crystal Database 75
 - Peierls-like distortion 737
 - Peierls-type distortion 450
 - Peltier effect 456
 - pentagondodecahedron 529
 - perfect and defective crystal situations
 - for compound M^+X^- 667
 - periodic table 139
 - with the transition elements identified 162
 - perovskite
 - X anion vacancy order 237
 - perovskite-related layered structure
 - compounds 243
 - perovskites 221
 - ABO_3 structure 574
 - A-site cation order 233
 - A-site cations and B-site cations 236
 - as ionic crystals 222

- B-site cation order 230
- Ca_3AuN 329
- chemical formula 221
- chemical variety of 222
- compositional flexibility 229
- crystal structure of 223
- electronic structure of 222
- ferroelectric soft modes 644
- hydrides, structural information for 495
- -type oxides 655
- – tolerance factor dependence of dielectric and ferroelectric properties 655
- ion order in 229
- mineral, of calcium titanium oxide 221
- nitrides 278
- phase 368, 369
- physical and chemical properties 221
- related compounds 654–656
- related compounds r R1_Start1 654
- related structures 202
- and related structures 197
- rock salt-type order 230
- solar cells 223
- structure 511
- – ideal 495
- phase
 - boundary 661
 - crystallize 323
 - separation 411
 - stability/flexibility 494
 - transformation 682
 - transition
 - – temperature 652
 - transitions 500
- phase-change material (PCM) 530, 735
 - origin and nature of vacancies 744
 - resonant bonding 743
- phase competition 606
- phase diagram 606
 - $\text{A}_2\text{BB}'\text{O}_6$ double perovskites showing existence range for ordered “rock salt” structures 203
 - ANiO_3 227
 - $(\text{Co}_x\text{Fe}_{1-x})_3\text{Se}_4$ 410
 - CrSe_x 406
 - Cs/O 140
 - $\text{Cs}_{11}\text{O}_3/\text{Rb}$ 142
 - FeSe_x 407
 - $(\text{Ni}_x\text{V}_{1-x})_3\text{Se}_4$ 411
 - Rb/O 142
 - TiSe_x 404
- phase-change data storage 746
 - functional principle 736
 - material requirements 736
- phase-change materials (PCM) 735
 - materials properties 743
 - property contrast 743
- phase-pure nitridometalates 255
- phenomenological theory 648
- phonon glass electron crystal (PGEC) 529
- phosphates 95, 572
- phosphides 18
- photoactive components 549
- photoactivity 378, 703
- photocatalysis 373, 455, 549
- photocatalysts 584
- photocatalytic
 - activity, for water splitting 549
 - performance 546
- photocathodes 457
 - Cs_3Sb as 457
 - Na_2KSb as 457
 - Na_3Sb as 457
- photoconductivity 427
- photodynamic therapy (PDT) 563
- photoelectrochemical (PEC) 557
- photoelectrochemical water splitting 557
- photoelectrodes 685
- photoelectron spectroscopy 146
- photoinduced magnetization 723
- photoluminescence 377
- photomagnetic switching 710
- photothermal ablation agents 713
- phototransformations 715
- phthalocyanine molecules 562
- p- and f-block oxyhydrides 503
- p- and f-block oxyhydrides
 - rare earth oxyhydride 503
- p-NPNN
 - chemical structure 706
- p-orbital-based spins 703
- P-rule 675
- p-type conductivity 744
- physical picture (energy level diagram)
 - for ionic and electronic disorder at interfaces 687
- piezoelectric (PZT) 579, 645, 661
- PMN structure
 - possible microscopic model 660
 - temperature dependence of dielectric constant 660
- pnictides 455
- pnictogens (Pn) 455
- Poisson’s equation 687
- polarizability 684
- polarization 637

- switching 663
 - polarization (P) versus electric field (E)
 - loop 645
 - pole reversal 713
 - polyacrylic acid (PAA) 559
 - polyantimonides
 - in lithium batteries 455
 - polycyanometallates 710–714
 - prussian blue and its hexacyanate analogues 710
 - polyethylene terephthalate (PET) 561
 - polyhedra 446
 - polyhedra in boron-rich borides 446
 - polyhedral connectivity 182
 - polyhedral distortion 166
 - polyhedral morphology 429
 - polymer consistent force field (PCFF) 544
 - polymeric anions
 - linear arrangement 293
 - polymer magnets
 - design 705
 - polymer spintronics 719
 - poly(p-phenylene) (APPP) 546
 - polypyrrole (PPy) core 555
 - poly(sodium styrene-4-sulfonate) (PSS) 560
 - poly(vinyl acetate) (PVA) 560
 - polyvinyl chloride (PVC) 140
 - polyvinylpyrrolidone (PVP) 712
 - porphyrin 562
 - post-perovskite
 - crystal structure of 242
 - post-perovskite compounds 243
 - crystal structure of 243
 - in geoscience research 243
 - postulated charge redistribution
 - occurring in alkali borophosphate glasses 130
 - potassium ion sensing 712
 - potential energies 2
 - Potts models 617
 - powder X-ray diffraction (PXRD) 577
 - premilling process 401
 - primary susceptibility 647
 - pristine polymer 558
 - (100) projections of CaF_2 and $\text{AA}'_2\text{BO}_7$
 - weberite unit cells 195
 - projections of crystal structures
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_7$ 152
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_8$ 152
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_{14}$ 152
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_{17}$ 152
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_{21}$ 152
 - $\text{Ba}_{14}\text{CaN}_6\text{Na}_{22}$ 152
 - Cs_{11}O_3 145
 - $\text{Cs}_{11}\text{O}_3\text{Cs}$ 145
 - $\text{Cs}_{11}\text{O}_3\text{Cs}_{10}$ 145
 - $\text{Cs}_{11}\text{O}_3\text{Rb}$ 145
 - $\text{Cs}_{11}\text{O}_3\text{Rb}_2$ 145
 - $\text{Cs}_{11}\text{O}_3\text{Rb}_7$ 145
 - Rb_9O_2 144
 - $\text{Rb}_9\text{O}_2\text{Rb}_3$ 144
 - projections of rod structures
 - Ba_2N 150
 - Ba_3N 150
 - $\text{Ba}_3\text{N Na}$ 150
 - $\text{Ba}_3\text{N Na}_5$ 150
 - protonated oxides 590
 - proton conductors 572
 - proton-assisted hydride diffusion 511
 - prototypical relaxor 659
 - Prussian blue analogues (PBA) 710, 711
 - fcc structure 711
 - Prussian blue nanoparticles (PB NPs) 713
 - Prussian blue salt 711
 - pseudobinary $\text{M}_3\text{X}_4\text{--M}'_3\text{X}_4$ system 408
 - pseudobinary $\text{M}_3\text{X}_4\text{--X}_4$ system, phase diagram
 - and site preference in 406
 - pseudobinary systems 410
 - pseudobrookite (Fe_2TiO_5)-type structure 266
 - pseudocapacitance performance 554
 - pseudocapacitors 554
 - pseudogap 8, 13, 14, 32, 46, 604
 - pseudopotentials 1, 34
 - theory 34, 35
 - PtN synthesis 271
 - purely organic magnets 705
 - pyramidal anion $[\text{Re}^{\text{V}}\text{N}_3]^{4-}$ 304
 - pyrochlore lattice 626
 - composed of corner-sharing tetrahedra 630
 - pyrochlores 191, 365
 - phase 370
 - structures 192, 369
- q**
- quadratic–pyramidal coordinated transition
 - metal sandwich 324
 - quadrupolar coupling
 - parameters 111
 - quadrupole coupling 532
 - qualitative treatments 29
 - quantization 598
 - quantum critical point 659
 - quantum mechanics 58
 - quantum paraelectricity 657
 - quantum spin liquid 623
 - quantum theory 1

- quantum theory of atoms in molecules (QTAIM) method 332
- quantum transport 595, 609
- phenomena 609
- quasibinary electroneutrality equation 677
- quasi-crystalline approximants 45, 75
- $\text{Li}_{52.0}\text{Al}_{88.7}\text{Cu}_{19.3}$ 46
- quasi-crystals 2, 45
- quasi-inelastic neutron scattering (QENS) 508
- quasi-one-dimensional compound NbSe, charge density wave instability in 417
- quaternary compounds 530
- quaternary hexanitridodichromate(V) $\text{Li}_4\text{Sr}_2[\text{Cr}_2\text{N}_6]$ 315
- quaternary nitrides $\text{Li}_3\text{Sr}_2[\text{NbN}_4]$ 313
- quaternary nitridometalates
- crystal structures of 315
- quaternary nitridometalates containing Li
- crystal structures of 314
- quaternary system Li-Sr-M-N 294
- quenching 141, 440
- r**
- radical pair mechanism 722
- radical pair mechanism (RPM) 722
- radius ratios 166
- Raman scattering 94
- Raman spectra 113
- $(\text{Na}_2\text{O})_x(\text{B}_2\text{O}_3)_{1-x}$ glasses 102
- Raman spectroscopy 741
- raMO analysis 54, 55
- rare earth elements 326, 368, 376, 435
- rare earth metal nitridometalates 317
- rare earth metals 140, 477, 478, 479, 499, 525
- rare earth–tungsten–oxygen system
- stoichiometries in 372
- rare earth oxyhydrides 503
- rare earth tantalates 370
- rate constant 683
- rate equations 668
- rattling effect 463
- $\text{Rb}_2\text{Ba}_6\text{Sb}_5\text{OH}$ crystal structures 505
- RbH_5
- interpretation 50
- Rb_{13} icosahedra 144
- Rb^+ ions 588
- Rb_9O_2 and Cs_{11}O_3 clusters
- in alkali metal suboxides 143
- Rb_9O_2 clusters 142, 143, 144
- Rb_6O octahedra 144
- Rb/O system 147
- reaction temperature 681
- reactive molecular nitrogen 253
- read-head devices 718
- real ferroelectric
- formula generalization 650
- ReB_2 -structure type 444
- ReB_2 -type crystallizing compounds 445
- rechargeable Ca-ion battery concept 723
- REDOR experiment
- on a borophosphate glass 109
 - principle 106
- REDOR pulse sequence timing and corresponding evolution of dipolar Hamiltonian 107
- reentrant phase transition 653
- refractory materials 254
- regioselective hydrogenation 552
- REHO compounds 503
- relaxors 659
- dielectric behavior 661
 - ferroelectric 659
- $\text{RE}_2\text{M}_{17}\text{N}_x$
- magnetic properties 284
- $\text{RE}_2\text{M}_{17}\text{N}_x$ compounds 284
- $\text{REM}_{12}\text{N}_x$ crystal structure 284
- repulsive forces 166
- residual acidities 64
- resistivity 388, 601
- resonant bonding 743
- low thermal conductivity, relation with 746
- resonant X-ray diffraction 605
- resonating-valence-bond (RVB) 617
- Restricted Hartree–Fock calculations on $(\text{OH})_3\text{Si}-\text{O}-\text{Si}(\text{OH})_3$ clusters 111
- reversed approximation molecular orbital (raMO) 51
- reverse Monte Carlo (RMC) 742
- analysis 713
 - fitting 119
 - modeling (RMC) 110
- reversible hydrogen electrode (RHE) 557
- rhenium arsenide 462
- isostructural with Mo_3Sb_7 462
- rhenium nitrides ReN_x 269
- rhodium 552
- rhombicosidodecahedron 85
- R-phase 45
- R-value 147
- Rietveld refined Ag-rich phase 45
- Rietveld refinement technique 713
- rigid band model 20, 21
- ring size distributions
- in glassy silica 112
 - in glassy SiO_2 , and binary sodium silicate glasses 126

- ring structures
 - motifs in tetrahedral network glasses 98
 - postulated for modified borate glasses 126
 - RKKY. *See* Ruderman Kasuya Yoshida (RKKY)
 - Rochelle salt
 - potassium sodium tartrate 653
 - rocksalt 484
 - -type group 3, 285
 - -type phase $\text{Mo}_{1-x}\text{Nb}_x\text{N}$ 285
 - -type UN 262
 - phase 741
 - structure 581
 - 3R (AgCrO_2) structure 586
 - $\text{R}_2\text{Ti}_2\text{O}_7$ 370
 - rubidium 141, 143
 - rubidium Rochelle salt 653
 - rubidium suboxides 141, 143
 - Ruddlesden–Popper phases
 - crystal structures of 245
 - Ruddlesden–Popper-type manganese oxides 599
 - Ruddlesden–Popper-type perovskite oxides 512
 - Ruddlesden–Popper oxide 590
 - Ruddlesden–Popper phases 244, 588
 - Ruddlesden–Popper phase $\text{Sr}_3\text{Ti}_2\text{O}_7$ 324
 - Ruddlesden–Popper series 602
 - members, structures of 577
 - Ruddlesden–Popper structures 512
 - Ruderman–Kittel–Kasuya–Yoshida (RKKY) interaction 603
 - Ru sublattice 176
 - rutile and related structures 181
 - binary oxides 181
 - other forms of TiO_2 and MnO_2 187
 - site-ordered rutiles, trirutile structure and columbite 183
 - structures compositionally related to rutile, hollandites, and others 184
 - rutile (TiO_2) structure 182
 - R_6WO_{12}
 - thermal ammonolysis reaction of 374
 - $\text{R}_{14}\text{W}_4\text{O}_{33}$
 - thermal ammonolysis reaction of 374
 - R_6WO_{12} tungstates
 - preparation of
 - – amorphous citrate method 372
- S**
- saline hydrides 477, 479, 480
 - sample size 680
 - satellite positions 74
 - saturated magnetization 415
 - Sb_2 – Sb_2 bonds 460
 - Sb_2Te_3
 - superlattices of 456
 - scanning probe spectroscopy 606
 - Sc DOS curve 64
 - scheelites 365, 368
 - schematic decomposition
 - of $\text{Li}_{80}\text{Ba}_{39}\text{N}_9$ structure into Li_{13} , Ba_4 , Ba_6N , and $\text{Ba}_5\text{N}_6\text{Li}_{12}$ fragments 154
 - Schrödinger equation 2, 4
 - Sc_3InN 278
 - ScIr formation 63
 - ScNbN_2 327
 - Sc–Cu system 61
 - ScTaN_2 327
 - secondary alcohols, enantiomeric configuration 428
 - second-order Jahn–Teller (SOJT) effect 509
 - second-order optical nonlinearity 719
 - second order J–T (SOJT) 168
 - Seebeck coefficients 425, 438, 448, 456
 - Seebeck effect 456
 - used in spacecrafts 456
 - selenide systems 408
 - self-propagating high-temperature synthesis 399
 - self-propagating high-temperature synthesis (SHS) 399
 - semiconducting behavior 530
 - semiconductive-to-metallic transition 424
 - semiconductors 455, 458, 532, 670
 - technology 608
 - semiempirical parameters 4
 - semi-empirical relation 111
 - SEM images of Cu particles 392
 - sensory organelles 722
 - shell of centered 1/1 Mackay-type approximant 84
 - Shubnikov–de Haas effect 610
 - Shubnikov–de Haas oscillation 598, 610
 - S-doping 680
 - Si–O–B linkages 115
 - Si–O–Si bond angle distribution 111
 - functions 110
 - signal-to-noise ratio 484
 - Si-variants 684
 - silica glass (amorphous SiO_2) 740
 - silicate 95
 - simple Hückel (sH) 5
 - simple perovskite oxides
 - typical charge combinations of 222
 - simple perovskites 230

- group–subgroup relationships of space groups 228
- single chain magnets (SCM) 716
- single crystal X-ray diffraction (SXRD) 577
- single-chain magnet behavior 717
- single-chain magnets 717
- single-crystal sample of $\text{SrCo}_{12}\text{O}_{19}$
 - resistivity 607
- single-crystal X-ray 737
- single-molecule spintronics 719
- single-walled carbon nanotube (SWNT)-array
 - double helices 550
- single molecule magnets 716
- single molecule magnets (SMM) 716
- single tetrahedron inscribed in a cube 630
- singlet–singlet ground state system 634
- singlet–singlet systems 633
- sintering 440
- sinter metal boride powders 439
- site-ordered double perovskites 203
- site-ordered perovskites 205
- site-selective values extracted from 124
- site preference and magnetic properties 412
- sketches of different bonding situations, with metal-rich compounds 158
- skewness 20
- Slater determinants 49
- Slater-type orbital (STO) 5
- Slater model 654
- smart paper 746
- sodium ion distributions 120
- sodium oxotungstate 268
- sodium silicate glasses 123
- soft actuators 710
- soft mode theory 655
- solid electrodes 669
- solid electrolyte 364
 - for fuel cells 365
 - for gas sensors 365
- solid electrolytes 669, 684
- solid-state chemistry 362, 665, 669, 685, 709
- solid-state metathesis 252
- solid-state metathesis 257
- solid-state NMR experiments 120
- Solid-state NMR results on B_2O_3 – SiO_2 glasses
 - as a function of glass composition 116
- solid-state NMR spectroscopies 132
- solid-state reactions 392, 398, 440, 502, 572, 668, 689, 692
- solid-state sciences 735
- solid-state structures 6
- solid–solid interfaces 689
- solid solution system 410
- solid state ionics 665
- sol–gel system 117
- sol–gel technique 117
- solubility 437, 494, 675
- sonochemical reactions 389
- sonochemical synthesis 385
 - of Cu and Ag chalcogenides 389
- sonochemistry 389
- space charge effects 688
- space group “family tree” for double perovskites $\text{A}_2\text{BB}'\text{O}_6$ 204
- space group “family tree” for perovskites with a single B-site ion based on Glazer’s octahedral tilt systems 200
- space group symmetry, dependence, of Brownmillerites on 208
- specific capacitance 554
- specific heat 631
- spectroscopic techniques 532
- sphalerite 362
- spin crossover (SCO) 714
- spin delocalization 705
- spin echo double resonance (SEDOR) 108
- spinel AB_2O_4
 - showing edge-sharing octahedra of B-sites and A-site tetrahedra 213
- spinel 213, 626
- spinel structure 627
- spin frustration 637
- spin-based electronics 718
- spin-glass-like behavior 636
- spin-liquid phase of ZnCr_2O_4 629
- spin-orbit-lattice coupling 637
- spin-Peierls transition 627
- spin-polarized conduction electrons 232
- spin-state switching
 - ultrafast light-induced 715
- spin-valve devices 719
- spin-valve-type magnetoresistance 603
- spin ice 624
- spin ice compounds 629
 - $\text{Ho}_2\text{Ti}_2\text{O}_7$ and $\text{Dy}_2\text{Ti}_2\text{O}_7$ 629
- spin injection 719
- spin liquid 620
- spin–lattice complex 628
- spin–lattice coupling 627, 628
- spin–spin interaction 704
- spinodal decomposition 406
- spin polarization 705
- spin quantum number 705
- spins, artificial magnetic fields and monopoles
 - in spin ice 618
- spin transitions 714

- spintronics 595, 609
- spontaneous polarization 650
- spontaneous strain 650
- square-planar coordination 322
- Sr($\text{Al}_{1-x}\text{Ga}_x$)₄ lattice parameter 534
- Sr_{0.53}Ba_{0.47}[CuN] 296
- Sr₆[CuN₂][Cu₂N₃]
 - crystal structures of 292
- Sr₈[Fe^{III}N₃]₂[Fe^{II}N₂] 299
- Sr₁₀[FeN₂][Fe₂N₄]₂
 - crystal structures 299
- Sr₃GaSb₃ 468
 - crystal structures of 468
- Sr₂[Li(M_{1-x}Li_x)N₂] 294
- Sr[LiN] 293
- Sr₂[LiNCoN] 293
- Sr₂(Li₄N₂[Li_{1-x}Ni_xN]) 295
- Sr_{1-x}Ba_xGa₂ lattice parameter 536
- Sr_{1-x}Ga_{2+3x}, crystal structure, cut out 526
- Sr₈[Mn^{III}N₃]₂[Mn^{II}N₂] 302
- Sr₈[Mn₃]₂[Mn₂] 299
- Sr₈[MnN₃]₂[FeN₂] 299, 300
- Sr–Fe–N system 299
- SrTe nanocrystals 456
- Sr[TiN₂]
 - crystal structures 324
- SrTiO₃ 658
 - structure parameters of 227
- SrTiO₃-based oxides 507
- Sr₄Ti₃O₁₀ structure 574
- SrVO₂H crystal structures 512
- stacking sequence for Li₂ReO₃ 176
- stacking sequence of O–Li–O–Li/Sn–O layers in β -Li₂SnO₃ structure 175
- stacking sequences 738
- steady-state electrical transport 683
- steric strain 57
- stoichiometric compounds 141
- stoichiometry 366, 373
- Stoner ferromagnetism 608
- Stoner theory 609
- STP transition metal element crystal structure type 22
- strain effects 637
- strong-emissive Au NCs 548
- strontium hydride 493
- structural complexity 571
- structural distortion angle 543
- structural energetic stabilization energy 34
- structural energy difference theorem 25
- structural families, derived from ABO₃ perovskites 202
- structural order in glasses, general concepts of 95
- structural transition temperature 502
- structure field map for brownmillerites 209
- structure field map for stability of pyrochlore structure
 - TMO with the A³⁺/B⁴⁺ combination 191
- structure-dependent energy of atomic arrangement 34
- structure maps 744
- structure–bonding–property relations 522
- structure prediction diagnostic software (SPuDS) 228
- structure types for TMO 169
 - binary oxides 169
 - NaCl or rock salt 169
 - ternary and more complex oxides, with ordered-rock salt structure 172
- μ_3 acidity model 62
- μ_3 -neutralization 64
- suboxide hydrides 504
- suboxides, and other low-valent species 139
- suboxides of lithium and sodium 141
- substitution center (SC) 537
- successive phase transitions
 - in quasi-one-dimensional sulfides ACu₇S₄ (A= T l, K, Rb) 423
- successive shells
 - of Tsai-type approximants 87
- sulfides 18
- sulfur 13
 - content 13
- supercapacitor (SC) 553
- superconducting copper oxides 161
- superconducting region 501
- superconducting temperature 420
- superconducting transition 420
 - temperature 502
- superconductivity 384, 385, 388, 420, 423, 501, 505, 571, 573, 590, 607
 - in quasi-one-dimensional compound InxNb₃Te₄ 418
- superconductor 438, 443, 501
- super-exchange interaction 605
- superionic conductors 670, 681, 684
- superionic dissociation 668
- superionic situation 682
- superionic transitions 681
- superlattice reflections 421
- superlattice structures 533, 537
- superparamagnet 716
- superparamagnetic
 - maghemite nanoparticles 721

- surface reaction kinetics, analysis of 691
 - surface spin-disorder 712
 - switching 735
 - symmetry-breaking 38
 - synchrotron-quality X-ray diffraction 739
 - synchrotron X-ray diffraction studies
 - on glassy P_2O_5 115
 - synergism 40
 - between the nearly free electron and tight-binding models 42
 - Cu_5Zn_8 40
 - Li_8Ag_5 42
 - system Mn-Si-V 80
- t**
- Ta–O octahedron in $CoTa_2O_6$ 184
 - Tamann's rule 680, 681
 - Ta_3N_5
 - crystal structure 266
 - Ta–B system 440
 - Ta–S compound 13
 - Ta–S phases 13
 - Ta–Ta antibonding states 13
 - Ta–Ta bonding 13
 - Ta–Ta interactions 13
 - Ta_3N_5 , $Na_xTa_3N_5$ 326
 - tantalum-centered tantalum hexagonal antiprisms 80
 - tantalum oxynitride 372, 376
 - Ta_6S_5 compound 13
 - Ta_6S_5 phase 14
 - Ta/V–Te quasicrystals 80
 - T–O–T bond angles 113
 - tellurides 456
 - tellurium
 - toxicity of 472
 - temperature dependences of electrical resistivity 424
 - temperature hysteresis 605, 606
 - temperature programmed desorption (TPD) 559
 - ternary antimonides 464–471
 - without Sb–Sb bonds 465
 - with Sb–Sb bonds 469
 - ternary azidometalates 251
 - ternary B_2O_3 – SiO_2 – GeO_2 glasses 115
 - ternary ionic hydrides 494
 - ternary nitridometalates
 - tetrahedral anions 318
 - ternary systems 87, 95
 - ternary transition metal 18
 - tetragonal Nb_4N_5 265
 - tetragonal phases 283
 - tetrahedral coordination 309
 - tetrahedral voids
 - order patterns of 312
 - tetrahydridoborates 440
 - tetrathiafulvalene (TTF) 659
 - ThB_4 (UB_4) structure 446
 - $ThCr_2Si_2$ structure 11
 - thermal ammonolysis 369
 - thermal analysis 140, 522, 589
 - thermal annealing 522, 739
 - thermal conductivities 438, 458, 466, 471, 528, 529
 - thermal destiny 680
 - thermal destiny, of an ionic crystal 681
 - thermal lattice conductivity 528
 - thermally regenerative electrochemical cycle 723
 - thermally regenerative electrochemical cycle (TREC) 723
 - thermal transport
 - vacancy disorder, effect of 746
 - thermodynamic stability 478, 481
 - thermoelectric materials 522, 528, 603
 - alkali metal antimonides 457
 - thermoelectrics 456
 - efficiency of 456
 - thermal conductivity of 456
 - θ - Mn_6N_5 269
 - thin films 456
 - 2H ($CuAlO_2$) structure 586
 - T holes 165
 - thorium 262
 - three-cation coordination polyhedra in AA'_2BO_7 weberites 196
 - Ti, binary perovskite nitride 278
 - $TiCoSb$
 - crystal structure of 465
 - tight binding-based structure maps 27
 - tight-binding bonding models 40
 - tight-binding energy eigenvalues 41
 - tight-binding-based energy 41
 - tight-binding theory 27
 - tight-binding theory, emerging directions in 48
 - tilt systems among known perovskites with a single B-site ion, distribution of 201
 - $Ti_{21}Mn_{25}$ structures 65
 - $TiSb_2$ 459
 - crystal structures of 459
 - $TiSe_x$ phase diagram of 404
 - titanate oxides 658

- titanate perovskites
 - temperature dependence of dielectric constant 658
 - titanium 438
 - diboride 443
 - titanium niobium containing oxides 589
 - titanium oxyhydrides 509
 - TiCu₇S₄, schematic crystal structure 423
 - TM ions 167
 - TMO catalysts 163
 - TMO with bixbyite structure 190
 - TMO with columbite structure 185
 - TMO with ilmenite structure 179
 - TMO with trirutile, *P4₂/mmm* structure 185
 - T–E bonding 54, 55
 - T–E compounds 55
 - T–E intermetallic compounds 51
 - T–T bonding 54
 - T–T contacts 54
 - tolerance factor 224, 514
 - toluene 551
 - top of the valence band (TVB) 546
 - topotactic oxidation 231
 - total energies 18, 25, 26, 58, 62
 - total number of P–O–Al linkages n_{P-O-Al} as extracted from 117
 - tracer diffusion 684
 - transition elements 45, 161
 - transition-metal phthalocyanines 719
 - transition metal 13, 54, 462, 502, 581
 - interact with the filled low-lying d orbitals 62
 - oxidation states and valence electron configurations 49
 - transition metal (T) 51
 - transition metal atoms 463
 - transition metal borides 449
 - transition metal cations 234, 581
 - transition metal chemistry 140
 - transition metal compounds
 - tight-binding derived energies 29
 - transition metal d orbitals 8
 - band 13
 - transition metal elements 13, 27, 39
 - transition metal (T) elements 61
 - transition metal-based CsCl-type phases 27
 - transition metal intermetallic phase formation 63
 - transition metal ions 166, 588, 645
 - transition metal MAX nitrides 281
 - transition metal oxide (TMO) 161, 506, 512
 - transition metal oxyhydrides 502, 507, 513
 - transition metal positions 77
 - transition metals 63, 326, 361, 435, 440
 - nitridometalates of 286, 332
 - structures 63
 - tight-binding energies 22
 - transition/rare earth metals
 - binary nitrides of 258
 - transition temperature 408, 420, 501, 590
 - transmission electron microscopy (TEM) 419, 606, 739
 - transparency 6
 - transparent phases Ca₂[ZnN₂] 290
 - transport and transfer 682
 - treasure map 746
 - triclinic Sr₁₀[FeN₂][Fe₂N₄] 299
 - triethylphosphine 590
 - triglycine sulfate 645
 - triglycine sulfate (TGS)
 - P–E loop 646
 - trigonal Li₂₄[Mn^{III}N₃]₃N₂ 304
 - Triple-quantum (TQ-) MAS-NMR spectrum of glassy B₂O₃ 105
 - triple perovskites 239
 - triplet state 703
 - trirutile structure, AB₂O₆ 184
 - tritium 477
 - truncated icosahedron 82, 87
 - Tsai-type approximant 87
 - 2/1 Tsai-type approximant, arrangement of truncated icosahedra in 88
 - Tsai-type cluster 86
 - T sublattice orbitals 55
 - tubular furnace
 - nitridation of 370
 - tunable metal ion 556
 - tungstates
 - thermal nitridation of 374
 - tunneling magnetoresistance (TMR) 606
 - two-phase mixture 606
 - two-step electrosynthesis method 555
- u**
- UB₄ structure 447
 - UB₁₂ structure 448
 - UB₁₂ with boron atom cube-octahedra structure 449
 - ultrathin film (UTF) 546
 - uniaxial ferroelectric 647
 - unit cell 527
 - 2/1 approximant 83
 - of Ba₆N·Na₁₀ 149
 - constants and cell volumes for binary TMO
 - – with Al₂O₃ structure 178

- constants, for binary TMO oxides with the CaF_2 structure 188
 - of doubly ordered double perovskite
 - NaLaMnWO_6 205
 - of FeTiO_3 179
 - of $\gamma\text{-LiFeO}_2$ 173
 - of $\text{La}_{0.33}\text{NbO}_3$ 206
 - of LiBa_2N , increasing sizes for N, Li, and Ba 153
 - $\text{Li}_8\text{Ba}_{12}\text{N}_6\text{-Na}_{15}$ with $\text{Li}_3\text{Ba}_{12}\text{N}_6$ clusters 155
 - $\text{Li}_4\text{MgReO}_6$ 176
 - $\text{Li}_3\text{Mg}_2\text{RuO}_6$ 176
 - $\text{Li}_2\text{Ti}_2\text{O}_4$ 173
 - NbO unexpected SQP coordination of $\text{Nb}^{2+}(4d^3)$ 171
 - NdTiO_3 (Pnma) $a^-b^+a^-$ 201
 - suboxometalate Cs_9InO_4 and coordination of InO_4^{5-} ion by Cs atoms 148
 - urea route
 - using halides ($\text{M}_x\text{Cl}_y+(\text{NH}_2)_2\text{CO}$)/oxides ($\text{M}_x\text{M}'_y\text{O}_z+(\text{NH}_2)_2\text{CO}$) 253
- v**
- vacancy 684
 - defects 741
 - vacancy-ordered rock salt-type Ta_4N_5 266
 - vacancy-ordered structures 406
 - in binary MX MX₂ system 402
 - vacancy-ordering 404
 - vacancy ordered brownmillerite structure (*I2mb*) 207
 - valence electron concentration (VEC) 18, 23, 51, 522, 523
 - valence electrons 547
 - valence states 222
 - vanadium octacyanoniobate ferrimagnet 724
 - vanadium oxyhydrides 512
 - Van't Hoff plot 483
 - van der Waals forces 738
 - van der Waals gap 268
 - van der Waals interactions 459, 544, 703
 - vaporization 140
 - V–V bond distances 183
 - Vector spins 617
 - versatile materials platform 746
 - vertex-sharing tetrahedra 309
 - infinite chains 316
 - vertex-sharing tetrahedral 317
 - vibrational spectroscopy 94
 - Villain model 618
 - virial theorem 3
 - Vogel Fulcher's formula 661
 - void volumes 741
 - $\text{V}^{2+}/\text{V}^{3+}$ ions 180
- w**
- Wannier analysis
 - of H-based bands 50
 - Wannier function 1, 48– 50
 - water
 - photooxidation 378
 - photoreduction 378
 - water-in-oil microemulsion technique 712
 - wave function 4
 - wave vector 421
 - WC-type structure 265
 - weak-emissive Au NCs 548
 - weak (Anderson) localization 598
 - weberites 195
 - Weiss temperature 413
 - $[\text{WN}_2\text{N}_{2/2}]$ tetrahedra build six-membered rings 316
 - Wolfsberg–Helmholz approximation 6
 - Woodward–Hoffmann rules 1
 - Wurtzite-type structures 285
 - Wyckoff symbols 189
- x**
- $(\text{XAl-LDH/PAA})_n\text{-CO}_2$:
 - schematic illustration of 560
 - X-ray and neutron diffraction 94
 - x-ray diffraction 404, 483, 522
 - analysis 426
 - data 259, 446
 - x-ray fluorescent holography experiment 609
 - X-ray machine collection factors 30
 - X-ray/neutron diffraction 132
 - X-ray photoelectron spectroscopy 94
 - X-ray scattering factors
 - of 1/1 quasi-crystalline Bergman phases and Jones zones 46
 - XMCD measurements 275
 - XRD method. 395
 - XRD pattern of
 - CuInSe_2 388
 - $\text{Cu}_{1.96}\text{S}$ 387
 - CuSe_2 387
 - tetragonal $\text{Cu}_{1.96}\text{S}$ 386
- y**
- YBa_2MnO_5 and $\text{YBa}_2\text{Cu}_3\text{O}_7$ structures 210
 - $\text{Yb}_5\text{In}_2\text{Sb}_6$
 - crystal structures of 470
 - $\text{Yb}_9\text{Mn}_{4+x}\text{Sb}_9$
 - crystal structure of 469

YCoC-type structure 293
ytterbium dihydride 499
yttrium–barium–copper oxide 675
 $Y_6WO_{12-3x}N_{2x}$ oxynitride powders
– diffuse reflectance spectra of 375

Z

Zeeman effect 598
zeolites 572
zero band gap 611
zero bits 741
zero-energy Landau levels 611
zero-field cooling (ZFC) 288
zero-field resistance 595
zero standard reaction free energy
682
 ζ -phase 270
 $\zeta(\zeta')$ - Mn_2N 268

ZFC–FC curves of BTFO films measured under
different magnetic fields 635
zigzag Au chains 330
zinc phthalocyanine (ZnPc) 562
Zintl concept 8
Zintl electropositive/electronegative atom
ratios 27
Zintl phases 2, 14, 525, 526
Zintl ZE_3 compounds 28
zirconium 159
– metal 500
– oxides 371
Zn corrosion 692
 $ZnCr_2O_4$, spin structure 628
Zr d orbitals 18
 $Zr_3Er_4O_{12}$
– nitridation 366
 Zr_2ON_2 366

