

Index

a

- [*n*]acenes 194, 195
peri-acenes 268–275, 278, 284, 415, 417, 483
 acenoacene family 411–414, 416
peri-acenoacenes 268, 278–279, 284
 ACID 16, 333–334
 activated carbon 390
 additional reactions 372
 aggregation induced emission (AIE) 182
 air–water interface 248
 annulative π -extension (APEX) reactions 127, 198
 [*N*]annulenes 4–6
 anthene 269
 anthracene 59, 65, 203, 205, 206, 230, 247–248, 254–255, 309, 346–349, 352, 355, 356, 391, 409, 411, 412, 415
 Ar-ion laser 45
 arm-chair (AGNR) 405, 409, 413, 415–420
 armchair CNBs 154
 armchair-edged nanographenes (A-NGs) 267
 armchair-type CNT 153
 aromatic 10,15-diaza[10]helicene 119
 aromatic enantiopure helicenes 107
 aromatic fluctuation index (FLU) 9
 aromaticity
 definition of 1
 global and local 2–6
 nanographene systems 20–24
 quantification methods
 electronic descriptors 9–13
 energetic descriptors 7–9
 geometric descriptors 13–14
 magnetic descriptors 14–20
 aromatic nanobelts 150, 154–158
 aromatic saddle 177, 325
 aromatic stabilization energy (ASE) 4, 6–8, 13, 269
 aromatic triyne 112
 atomic force microscopy (AFM) 5, 36, 37, 75, 152, 346, 363–366, 490, 500
 atropisomerism 94, 95
 Au ethynylene-anthracene wires 347, 348
 Au-mediated synthesis 306
 axially extended (long) helicenes 123
 azabora[7]helicene 123
 azacorannulenes 211, 212, 337, 338
 azacorannulenophane 211, 213
 aza[5]helicene cyclodimer 136
 aza[6]helicene 109, 119, 120, 122
 azahelicenes 108, 114, 119
 aza monkey saddle 331–335, 337, 339
 azaoxa[6]helicene 116, 122
 azapentabenzocorannulene 459
 (aza)sumanene 331, 335
 azoniahelicenes 114, 115
- ### **b**
- Beckmann rearrangement 432
 belt-shaped CPPs 156
 belt-shaped cyclonaphthylenes 254

- benzannulated [2.2]paracyclophane-1,9-diene 194
- benzofulvene 201
- benzyne Stevens rearrangement 204
- (bi)cyclic oligoarylene 196
- bifurcation value (BV) 11
- bilayer nanographenes 130, 224–226, 230–236, 238, 239, 436, 468–470
- bisanthene 269, 270, 353, 355, 356, 415–417
- bis(hydroxymethyl)pyrenes 208
- bisphenalenylenes 406–407, 411
- Bleaney–Bowers' equation 216, 271, 283
- (BO)₂-doped tetrathia[7]helicenes 109
- bonding/antibonding 403, 405, 406, 414, 416–418, 420
- bond length alternation (BLA) 6, 14, 467
- bond-resolved scanning tunneling microscopy (BR-STM) 497
- borahelicenes 123
- boraoxathia[7]helicene 110
- bottom-up synthesis 98, 150, 156, 248, 254, 316–317, 456, 459, 505
- bowl-shaped nanographenes 68, 371
- 2,9,14-and 4,9,14 brominated truxenes 328
- para*-bromo-benzoyl peroxide (BBPO) 49, 50
- 9-bromo[7]helicene 108
- buckycatcher 460, 461
- bulky imide substituents 229
- tert*-butyl groups 60, 91, 95, 271, 297, 339, 433, 489
- tert*-butyl substituents 269
- C**
- carbohelicenes 68, 108, 113, 428, 437
- (6,6)carbon nanobelts 203
- carbon nanobelts (CNBs) 70, 86, 149–154, 159, 203, 253, 262
- carbon nanorings (CNRs)
- CPP-based oligomers and polymers 258–261
- with π -extensions strategies 244
- PAHs solely
- anthracenes, pyrenes or chrysenes 254–255
- naphthalene 253–254
- six-membered ring-based PAHs
- anthracene and phenanthrene 247–248
- larger PAHs 249–251
- naphthalene 244–247
- pyrene and perylene 248–249
- carbon nanosolenoid 131, 132
- carbon nanotubes (CNTs)
- bottom-up synthesis 316–317
- chirality 316
- cyclacenes 151–152
- mass spectroscopy 152
- and nanographene 150
- synthesis of 153–157
- top-down approach 152–153
- carbon-carbon bond formation 252
- carbon schwarzites 163, 164, 184–188
- cationic dioxa[6]helicene 122
- cationic triarylcarbenium helicenes 120
- Chichibabin's hydrocarbon 215
- chiral amplification 392–393
- chirality 68, 83–87, 89–90, 95, 98, 106, 110, 116, 137, 215, 216, 231, 232, 234, 235, 239, 243, 244, 246, 254, 255, 311, 317, 318, 331, 334, 340, 381, 392, 426, 432, 435, 439, 440, 449, 457
- chiral molecular NGs
- flexible nanographenes 87–89
- inherent stability 84
- isolable nanographenes 90–93
- NGs with spectroscopically detectable chirality 89–90
- racemization barriers 84
- rigid nanographenes 93–95
- chiral nanographenes 427–444
- chiral nanomaterials 83
- chiral stationary phase HPLC (CSP-HPLC) 432, 434, 435, 438
- 1-chloro-1,2-benziodoxol-3(1*H*)-one (ClBO) 46
- chromophores 63

- chrysene 203, 254–255, 305, 311, 485
 circular dichroism (CD) 69, 83, 95, 183,
 235, 246, 255, 311, 326, 383, 426,
 427
 circularly polarized light (CPL) 110, 137,
 425–427, 440
 circularly polarized luminescence (CPL)
 83, 235, 237, 255, 315, 425–445
 (1 × HBC)-based chiral nanographenes
 428–434
 (1 × HBC)-based heteroatom-doped
 chiral nanographenes 431
 2 × HBC-based chiral nanographenes
 434–436
 3 × HBC-based chiral nanographenes
 436–438
 4 × HBCs-based chiral nanographenes
 438–439
 photophysical properties 441
 [5]circulene (corannulene) 85, 323
 [7]circulene 85, 89, 90, 169, 170, 172,
 181, 182, 450
 [8]circulene 85, 89, 91, 175–177, 179,
 181–183, 185, 186, 323, 324, 456,
 466
 [12]circulene 72, 137, 203
 circulene 72, 85, 89, 90, 169, 170, 172,
 175–177, 179, 181–183, 185, 186,
 323, 324, 450, 454, 456, 466
 circumacene family 417–419
 circumarenes 268, 279–284
 circumcoronene 2–4, 21, 279–281, 367
 circumpentacene 280, 282, 283, 418, 419
 Clar's aromatic sextet 176
 Clar's hydrocarbon 492
 Clar's π -sextet rule 2–4, 21
 Clar's sextets 268, 271, 282
 concealed non-Kekulé nanographenes
 486–488
 conformationally locked
 dithia[5]helicenes 120
 conformationally locked [4]helicene
 systems 120–122
 conjugated nano-hoops
 applications
 biological fluorophores 317
 CNTs, bottom-up synthesis
 316–317
 organic electronics 314–316
 properties
 chirality 311
 host-guest chemistry 311–313
 optoelectronic properties 309–311
 solid-state structures 313–314
 synthetic strategies 303–309
 Pt-, Ni- or Au-mediated
 macrocyclizations 304–307
 π -system panels 307–309
 π -conjugated polymers 345–360
 contact-ion products (CIPs) 452
 contorted nanographene
 bilayer 468–470
 corannulene 457–463
 cyclooctatetraene 463–467
 contractive annulation 198
 corannulene 8, 23, 66, 85, 89, 90, 95, 130,
 133, 134, 169–171, 323–325, 327,
 338, 430, 450, 451, 457–464
 corannulene-based nanographenes
 457–463
 corannulene-[6]helicene hybrid 130
 coronene 19, 87, 229, 230, 279, 280, 282,
 290, 293, 323–325, 340, 431, 454,
 455, 497
 coumarins 63
 covalently linked bilayers 232–238
 CPP-based polymers
 π -extended 260
 Jasti's synthesis 261
 and oligomers 258–260
 Tovar and Jasti's synthesis 261
 cross couplings 371
 C_2 -symmetric hexabenzotriphenylene
 133
 cumulene-linked periacene polymers
 352, 354
 curved nanographenes 66, 88, 90, 91,
 163–188, 205, 457, 464, 467
 cyanodiyne 115
 [12]cyclacene 151, 152, 203

- cyclacenes 151–152, 154, 156, 184, 203, 323, 324
- cyclic oligoarylene 194–197
- cyclic paraphenyleneacetylenes (CPPA) 194
- cyclic voltammetry (CV) 234, 387, 450, 464
- [4]cycloanthracenes 256
- cyclobutadiene molecule (CBD) 398, 400–403, 416
- [4]cyclochrysenylenes 255, 256
- cyclocondensation reaction 289–291, 297, 300
- ortho-diamines vs. ortho-quinones 289, 290
- cyclodehydrogenation (CDH) 59, 74–76, 85, 107–112, 126, 130, 131, 133, 135, 167, 170, 177, 179, 205, 208, 233, 253, 275, 325, 326, 353, 367–369, 371, 373, 374, 430, 433, 464, 468, 495, 497
- cyclometalated helicenes 122
- cyclometalated platina[6]helicene 123
- [6]cyclo-*meta*-phenylene (CMP) 306
- cyclooctatetraene 95, 174, 175, 326, 330, 331, 333, 460, 463–467
- cyclooctatetraene-based nanographenes 463–467
- [6]cycloparaphenylene 194
- cycloparaphenylenes (CPPs) 154, 156, 194, 243, 245, 246, 249, 258, 260, 303, 305–307, 309–317, 450
- [2.2]cyclophane 204
- [2.2.2](1,3,5)cyclophane 215
- cyclophanediene 204, 213
- [2.2]cyclophanediene 204
- cyclophane-like nanographenes 233
- cyclophanes
- dibenzo[*c,l*]chrysenophanes (C₂₆) 203–205
- dibenzo[*f,j*]picenophanes (C₃₀) 205–207
- π -extended azacorannulenophane (C₃₆) 211–213
- hept*-hexabenzocoronophanes (C₄₃) 217–218
- hexabenzocoronophanes (C₄₂) 213–217
- indeno[2,3-*b*]triphenylenophanes 201–203
- pentacenophanes (C₂₂) 199–201
- synthetic considerations 197
- teropyrenophanes (C₃₆) 207–211
- tetrabenz[*a,c,h,j*]anthracenes (C₃₀) 205–207
- cyclophanetriene 194
- cyclophanetriyne 194
- [8]cyclophenacene 152
- [4]cyclopyrenylenes 256
- cyclothiophenes 154
- CYTOP 45, 46
- d**
- decamethylcobaltocene 387
- dehydrobenzannulenes 194
- dehydrogenations 36, 76, 151, 157, 179, 201, 205, 208, 212, 215, 271, 275, 277–279, 345, 367, 368, 371, 489
- delocalization index (DI) 9, 10
- density functional theory (DFT) 5, 88–94, 107, 152, 180, 182, 183, 212, 230, 237, 330, 331, 333, 335, 339, 346, 349, 350, 352, 353, 390, 431, 434, 453–455, 468, 495, 497, 501
- diaza[6]helicene 122
- diaza[7]helicene 109
- diaza[10]helicene 119, 120
- dibenzo[6]helicene 112, 113, 116, 430
- dibenzo[7]helicene 94, 111, 112, 116, 117
- dibenzo[*c,l*]chrysenophanes (C₂₆) 203–205
- dibenzo[*f,j*]picene 205, 206
- dibenzo[*f,j*]picenophanes (C₃₀) 205–207
- dibenzopyrrolo[7]helicene 111, 112
- dibenzotetrathio[7]helicene 111, 112
- α,ω -dibromides 201
- 7,8-dibromo[5]helicene 133
- 2,6-dibromopyridine 210

- Diels–Alder cycloaddition 117–118, 130, 131, 133, 135, 167, 175, 233, 248, 271, 364, 464, 468
 aromatic vinyl ethers with
p-benzoquinone 117–118
- Diels–Alder reaction 4, 36–38, 107, 151, 152, 154, 165, 167, 176, 179, 245–279, 326, 371, 436
- Diels–Alder-type polymerization 59
- dihydrocumarin 328, 330
- 1,3-dihydro-1-hydroxy-3,3-dimethyl-1,2-benziodoxole (HOBQ) 46
- 1,4-dihydropyrrolo[3,2-*b*]pyrroles 65, 72
- dimers and trimers 501
- dimethoxyethane (DME) 129, 454
- 3,3-dimethyl-1-(trifluoromethyl)-1,2-benziodoxole (MFBO) 46
- diradical character 62, 215, 216, 230, 231, 268–271, 274, 282–284, 398–401, 403–407, 410, 413–420, 485, 486
- diradical molecules 398, 399, 420
- diradical state 398, 400–403, 405, 407, 410–420
- distributed feedback (DFB) 279
- 2,7-di-*t*-butylpyrene 209
- dithiacyclophane 203
- [3.3]dithiacyclophane 203
- dibenzo[*f,j*]picene system 206
- diverse carbohelicenes 108
- donor-acceptor π -systems 230, 315
- double Sonogashira coupling 233
- D_3 -symmetric perylene diimide-based twelve-fold [5]helicene nanocarbon 135
- e**
- eight-membered ring
 early stage 175–179
 final stage 179–181
- electric dipole moments 427
- electrochemical reduction 449, 450, 452, 454, 459, 461, 466, 468
- electron beam lithography (EBL) 38–43
- electron delocalization 2, 5, 6, 8–14, 16, 18, 20, 23, 24, 243, 416
- electron density of delocalized bonds (EDDB) method 12, 13, 22, 23
- electron density of localized atoms (EDLA) 13
- electron density of localized bonds (EDLB) 13
- electronic circular dichroism (ECD) 107, 203, 237, 427, 430–432, 434, 438
- electronic descriptors of aromaticity 9–13
- electron localization function (ELF _{π}) 11, 12
- electron paramagnetic resonance (EPR) spectroscopy 209, 275, 387, 432, 451, 453–455, 489, 490, 492–494
- electron repulsion 402
- electrons delocalization 2, 5, 6, 8–14, 16, 18, 20, 23, 24, 243, 406, 416
- enantio- and diastereopure 2*H*-pyran oxahelicene derivatives 116
- enantioenriched dibenzohelicenes 117
- enantiomerically pure propeller-shaped multipole D_3 -symmetric helicene 133
- enantiomerization 84, 86, 89, 94, 95, 99, 182, 336
- enantiopure cyclootrimer 136, 137
- enantiopure dibenzo[7]helicene derivative 117
- enantiopure fully aromatic helicenes 116
- enantiopure (*M*)-9,10-dibromo[7]helicene 133
- enantiopure 2-*p*-tolylsulfinylquinone 118
- enantiopure σ -[4]helicene 126
- enantioselective synthesis, of rigid molecular nanographenes 95–98
- energetic descriptors of aromaticity 7–9
- ethynyl helicene 468
- expanded [23]helicene system 129, 131
- π -extended azacorannulenophane (C₃₆N) 211–213

π -extended double [6]helicene 134
 π -extended helicenes 95, 131, 132, 428
 π -extended pyrene-fused double
 [7]helicene 134

f

Faraday's law 14
 FeCl₃-mediated intramolecular Scholl
 reactions 206
 flexible π -expanded [13]helicene 129
 flexible nanographenes 87–89
 9-fluorenyl-based cyclophanes 203
 fluorenyl-based cyclophanes 202
 1-fluoro-3,3-dimethylbenziodoxole
 (FMBO) 46
 fluorophores 260, 314, 316, 317
 Förster resonance energy transfer (FRET)
 436
 Friedel–Crafts acylation 126, 165, 166
 Friedel–Crafts alkylation 210, 278
 Friedel–Craft cyclization 85, 271, 278,
 282
 Friedel–Crafts reactions 152, 157, 271,
 275
 frontier molecular orbitals 310, 312, 401,
 404, 407–409, 411, 412, 414–416,
 418, 420, 430, 451
 fully π -extended [9]helicene 132
 functionalized (hetero)helicenes 115
 fused aromatic networks (FANs)
 aza-CMP synthesis 297
 aza-COF-1 synthesis 296
 C₂N synthesis 296
 C₅N and of [30]KL-FAN synthesis
 297, 298
 CS-COF synthesis 298, 299
 [90]KL-FAN synthesis 299, 300
 TIPS-CMP synthesis 297, 298
 2D FANs structure 299
 fused radicals, bilayers from 230–232

g

gauge-including magnetically induced
 currents (GIMIC) method 15, 22,
 23

Gaussian curvature 85, 92, 93, 98, 327,
 328
 geometric descriptors of aromaticity
 13–14
 Gibbs free energy 230
 Glaser alkyne coupling 167
 Glaser coupling 369
 Glidewell's rules 355
 graphene covalent function
 large-scale STM 44
 laser writing 44–50
 lithography-assisted molecular
 engineering 37–44
 molecular building blocks 42
 multiply pattern 41
 sp²-hybridized framework 31
 substrate-mediated chemical patter
 33–35
 tip-induced patterned function
 35–37
 graphene nanoribbons (GNRs)
 fused aromatic networks 293–300
 nanographenes 289–293
 NR-10, NR-20 and NR-30 291
 NR-13, NR-33 and NR-53 294
 NR-20, NR-40 and NR-60 292
 NR-27, NR-67 and NR-147 295
 SNG chemical structures 293
 graphene quantum dots (GQDs) 425,
 426

h

harmonic oscillator model of aromaticity
 (HOMA) 14, 21, 23, 281
 Hartree–Fock (HF) method 5, 6, 174,
 369
hept-HBC cyclophanes 218
 helical bilayer nanographenes (HBNGs)
 130, 234–236, 239, 468
 helical carbon nanohoops 246
 helical graphene nanoribbon 131, 132
 helically twisted [12]circulene 136, 137
 helical trilayer nanographenes 130, 237,
 238
 [4]helicene dicarboxylic acid 122

- [6]helicene derivative 109, 110, 119–121, 433
- [7]helicene ferrocene 122, 123
- [10]helicene derivative 119
- [11]helicene-based helical bilayer nanographene 132
- [16]helicene 108, 126, 131
- [24]helicene-related nanoribbon 132
- helicene 22, 72, 73, 85–86, 91–95, 98, 105–137, 170, 233–239, 381, 382, 391–393, 430, 438, 468–470
- advanced helicene architectures 123–137
- characteristics of 106–107
- chiral amplification 392–393
- Diels–Alder cycloaddition of aromatic vinyl ethers with *p*-benzoquinone 117–118
- with different number of ortho-fused benzene rings 86
- photocyclodehydrogenation of 1,2-diaryl olefins 107–111
- preparation 391–392
- Scholl reaction 111
- for simplicity 105
- transition metal-catalysed [2 + 2 + 2] cycloisomerization of π -electron systems 111–117
- transition metal-catalysed hydroarylation of alkynes 119–120
- helicene-based macrocycles 136, 137
- helicene cyclotrimers 136, 137
- helicene-derived macrocycles 135
- helicene macrocycles 126
- helicenoid twistacenes 123, 135
- [17]heliphene 129, 131
- helquats 107
- heptagon-embedded HBC 166
- (hetero)aromatic (bis)vinylethers 118
- heterocyclic compounds 73
- heterocyclic of non-planar nanographenes 71–74
- heterocyclic, planar nanographenes 63–66
- (hetero)helicene (bis)quinones 118
- (hetero)helicenes 108, 115, 116, 120
- hexaazacoronene derivative 230
- hexabenzocoronene (HBC) 2, 56, 131, 133, 135, 164, 165, 179, 213, 217, 224, 227–229, 233–235, 249, 279, 337, 367, 369, 373, 417, 418, 426, 428–439, 450, 455, 468
- hexabenzocoronenophanes (C₄₂) 213–217
- hept*-hexabenzocoronenophanes (C₄₃) 217–218
- hexabenzotriphenylene (HBT) 19, 133, 429
- hexa-*cata*-hexabenzocoronenes 337
- hexadehydro-Diels–Alder reaction 371
- hexa-*peri*-hexabenzocoronenophanes 213, 214, 216, 217
- hexa-*peri*-hexabenz[7]helicene 94
- hexapyrrolohexaazacoronene 63, 232
- high-pressure liquid chromatography (HPLC) 72, 92–95, 97, 121, 183, 186, 215, 231, 235, 237, 238, 248, 255, 311, 326, 432
- high spin non-Kekulé nanographenes 492–498
- homoaggregation 227
- homodesmotic reaction 4, 7, 8
- HOMO–LUMO gap 226, 383, 398, 403, 413, 418, 419, 431
- host-guest chemistry 150, 303, 311–313
- hPDIs 383, 388–391
- Hückel energy distribution 401
- Hückel molecular orbital method 408, 412, 414, 416, 418
- hybrid [7]cycloparaphenylene-[6]helicene Möbius-type figure-of-eight macrocycle 137
- hydroxyindanone 328
- i**
- indacenopicene pincers 461
- indeno[2,3-*b*]triphenylene system 201
- indeno[2,3-*b*]triphenylenophanes 201–203, 206

- inelastic electron tunneling spectroscopy (IETS) 500, 501
- infinite 157, 158, 203–205
- inter-system crossing (ISC) 433
- intramolecular McMurry reaction 169, 185, 207, 208
- intramolecular Scholl reaction 55, 57, 63, 64, 66, 68, 76, 206, 207, 367
- intramolecular Wurtz coupling 208
- isodesmic reactions 7
- isolable nanographenes 90–93
- isomerization stabilization energies (ISEs) 7
- j**
- Jahn Teller effect 353
- k**
- Kekulé
- diradical 399
 - NGs 483–505
 - and non-Kekulé NGs 483–505
- kekulene 129, 203, 365–367
- Kondo effect 419, 488
- Kumada coupling of dibromide 213
- l**
- Lambert–Beer law 427
- laterally π -extended dithia[6]helicene 131
- laterally extended (wide) helicenes 123
- Lieb's theorem 484
- lithium diisopropylamide (LDA) 124, 167, 307, 387
- lithography-assisted molecular engineering 32, 37–44
- Lloyd's rule 4
- localized orbital locator (LOL) 12, 13
- Lucas' synthesis 184
- luminescent solar concentrators (LSCs) 316
- LUMOs 452
- m**
- Mackay crystals 163, 323
- magic-angle twisted 223
- magnetic descriptors of aromaticity 14–20
- Mallory reaction 107, 196, 204
- mass spectroscopy 152
- McMurry coupling 108, 129, 169, 184, 185
- metallohelicenes 120, 122
- methylene-bridged [6]CPP ([6]MCP) 156
- Mitsunobu reaction 40
- Möbius belt-shaped CPP 157
- Moiré pattern formation 33
- molecular nanographenes 83–99, 224–230, 239, 409, 439, 449, 450, 456, 457, 470
- contorted nanographene 456–470
 - planar nanographene fragments 452–456
 - 2D and 3D 450
 - van der Waals 225–230
- π -molecular orbitals (MOs) 5
- monkey saddle PAH 328, 331–340
- inversion barriers and chiroptical properties 334–337
 - NICS and ACID plots 333–334
 - and related systems 337–339
 - synthesis 328–331
 - X-ray crystal structures of 331–333
- monkey-saddle shape NGs 90, 92
- Mulliken charge density 111
- multicenter index (MCI) 10, 11, 23
- multiple helicenes 68, 95, 98, 123, 132–134, 428, 433
- n**
- nanobelt 86, 136, 137, 149–159, 184, 185, 187, 323
- nanocarbon infinite 203
- nanographenes (NGs)
- aromaticity 20–23
 - and carbon nanotube 150
 - Csp² framework 83
 - diradical 403–410
 - representative edge structures of 268
 - structural motifs for chirality
 - Gaussian curvature 85

- helicenes 85–86
 rolling 86
 strain 87
 top-down and bottom-up approaches 267
 two classes 483
 nanographenoid radical 230, 232
 nanographenophane 193–219
 naphthalene 133, 167, 172, 177, 230, 244–251, 253–254, 305, 309, 339, 385, 391, 413–415, 418, 452, 456, 457, 466
 naphthalenemonoimide units 230, 232
 naphtho-fused double[7]helicene 133, 134
 natural orbital occupation number (NOON) 216
 near-infrared (NIR) 70, 237, 271, 284, 387, 432, 439, 451, 494, 497
 negatively curved nanocarbons 163
 negatively curved nanographenes 88, 163–193, 464
 bottom-up approaches to carbon schwarzites 184–186
 eight-membered rings
 early stage 175–179
 final stage 179–181
 seven-membered rings
 early stage 165–168
 last stage 168–174
 stereochemical dynamics and properties 181–184
 negative curved nanographenes' racemization barriers 90
 negatively curved *N*-heteropolycyclic aromatics (*N*-PACs) 337–339
 NGs with spectroscopically detectable chirality 89–90
 Ni-mediated synthesis 307
 NICS2BC method 3, 21
 NICS-XY-scan method 18–20
 nonbenzoid [10]helicene 236, 237
 non-contact atomic force microscopy (nc-AFM) 347–349, 351–354, 356, 357, 359, 489–491, 494, 495, 498, 501
 non-Kekulé nanographenes
 spin $\frac{1}{2}$ dimers 498–501
 [3]triangulene ($S = 1$) based spin chains 501–504
 triangulene ($S = 1$) dimers and trimers 501
 non-Kekulé polyaromatic hydrocarbons 483
 nonplanarity 198, 212, 463
 nonplanar polyaromatics 132, 133
 norcorrolophane 197
 notable nanographenes 203
 NPDH 392
 nucleus independent chemical shift (NICS) 17–21, 23, 271, 273, 281, 333–334, 465
- O**
- obvious non-Kekulé NGs 484, 488–498
 octamethoxytetraphenylene (OMT) 464
 octaphenyltetrabenzocyclooctatetraene (OPTBCOT) 464–466
 octazethrene 404–406
 oligorylene family 413–415
 on-surface covalent synthesis 345
 on-surface diradicals 407–409
 on-surface synthesis
 diphenalanyl 500
 [3]triangulene 494
 [*n*]triangulene 496
 open-shell
 bilayer nanographene 230–234
 graphene radicaloids 487
 Kekulé nanographene 485–486
 nanographenes 410–415
 wavefunction 400
 optically pure S-shaped double oxahelicene 117
 orange-coloured teropyrenophanes 208
 organic chemistry 32, 164, 193, 345, 363–375
 organic electronics
 conjugated nano hoops 314–316
 NGs 267, 268
 organic field-effect transistors (OFETs) 183, 315

- organic light-emitting diodes (OLEDs) 315, 316, 433
- organic photovoltaics (OPVs) 315, 388–389
- [2.2]orthocyclophane 215
- Ovchinnikov's rule 275, 484
- overcrowded triply fused C_2 -symmetric [7]helicene 133
- oxa[19]helicene-like system 129, 131
- oxahelicenes 114–116
- oxa[7]superhelicene 72, 130, 132, 234, 238, 438
- p**
- palladium-catalyzed cross-coupling 181
- pancake bonded nanographenes 230
- [2.2]paracyclophane 194, 199, 201, 215
- [2.2]paracyclophane-1,9-diene 194
- [2.2.2]paracyclophane 194
- partially hydrogenated [7]helicene bisquinone 118
- Peierls distortions 410, 411
- Penrose stairs 135
- pentaaza[10]-circulene 338, 339
- peri*-pentacene 274, 275, 284
- pentacene-based polymers 351–353
- pentacene-6,13-dione 200
- (1,4)pentacenophane 199
- pentacenophanes (C_{22}) 199–201
- pentadecabenz[9]helicene 131, 132, 439
- pentalene-linked π -conjugated polymers 356
- pericyclic reactions 371
- Perkin reaction 196
- peropyrene 195, 251, 430
- perylene 59, 62, 133, 179, 230, 244, 248–249, 269, 340, 364, 381, 382, 386, 389, 413–415, 429–431, 452
- perylene diimide (PDI) 109, 381–383, 389–393
- perylene diimide-embedded double [8]helicenes 109
- PHATN 389, 390
- [5]phenacene 195
- [*n*]phenacenes 194, 195
- phenanthrene 3, 107, 157, 200, 247–248, 391
- Kekulé resonance structures of 3
- six-membered ring-based PAHs 247
- phosphahelicenes 114, 115
- phospha[7]helicenes 115
- phosphonium salt 153
- photocyclodehydrogenation 1,2-diaryl olefins 107–111
- methodology 108
- photodetectors 388–389
- planar nanographenes 56–66, 452–456
- platina[6]helicene 122, 123
- Pt-mediated cyclization 251, 304, 305
- platinum-mediated synthesis 252, 305, 306
- Pt-, Ni- or Au-mediated macrocyclizations 304–307
- polycyclic aromatic framework 163, 165, 175, 179
- polycyclic aromatic hydrocarbons (PAHs) optoelectronic characteristics of 244
- six-membered ring-based 249
- anthracenes, pyrenes or chrysenes 254–255
- naphthalene 253–254
- other carbon nanorings 257
- polycyclic conjugated hydrocarbons (PCHs) 4, 6, 18, 410–415, 428, 435, 438
- poly(methyl methacrylate) (PMMA) 38, 43, 316
- poly(*para*-phenylene) (PPP) 258, 259, 309, 310
- poly(thiaheterohelicene) 132
- porphyrins 43, 55, 63, 64, 76, 197, 468
- potassium organometallic bilayers 236
- principal curvatures 327, 328
- projected density of states (PDOS) 348, 351
- pyrene 59, 129, 133, 134, 154, 203, 209–213, 230, 248–251, 254–255, 293, 297, 298, 389, 419, 452

- pyrene-fused double [7]helicene 133, 134
 pyreno[7]helicene 132
 (2,7)pyrenophane 205, 211, 212
 [8.2]pyrenophane 207
 pyrenophane 8, 208, 210–213
 [*n*.2]pyrenophanes 208
 pyridazinohelicenes 115
 pyridine-derived stilbene-type precursor 108
 pyridinophane 210
 pyridohelicenes 113
 pyrido-pyrrolo[6]helicene 109
 pyridotriyne 115
- q**
p-QDM 403, 406
 quantum computing 483, 485, 501
 quenching 42, 187, 228, 229, 270, 271
 quinoidal cyclophane 215
 quinoidization 413
 quintuple [6]helicene 133, 134
- r**
 racemic dibenzo[6]helicene derivative 112
 racemic figure-of-eight propellicene 135
 racemic helicene bisquinones 118
 racemic hexahelicene ([6]helicene) 105
 racemization energy barriers 88, 99
 reactive hydroaromatic (bis)dienes ((bis)vinylderivatives) 118
 rhodium-catalyzed intramolecular [2 + 2 + 2] cycloaddition chemistry 201, 203
 rhombenes 368, 419–420
 rigid molecular nanographenes, enantioselective synthesis 95–98
 rigid nanographenes 93–95
 ring-closure bifurcation value (RCBV) 11, 12
 ring-opening metathesis polymerization (ROMP) 260, 261
 rolled-up nanographenes 203
 rubicene 61
 rubidium organometallic bilayers 236
- S**
 saddle mathematics 327–328
 saddle-shaped π -molecules 183
 scanning probe microscope 363–366
 scanning tunneling spectroscopy (STS) 214, 348, 349, 351–354, 363, 365, 487, 489, 494, 495, 497, 498, 501
 scanning tunnelling microscopy (STM) 36, 44, 75, 152, 347, 348, 351, 352, 354, 356–359, 363, 365, 366, 368, 369, 420, 488, 490, 492, 494–498, 502–504
 Scholl reaction
 curved, non-planar nanographenes 66–71
 heterocyclic analogs of planar nanographenes 63–66
 heterocyclic of non-planar nanographenes 71–74
 planar nanographenes 56–63
 seven-membered rings 169
 surface-assisted (cyclo)dehydration 74–76
 twisting of nanographenes 67
 selenium annulation 227
 seven-membered ring
 early stage 165–168
 last stage 168–174
 shaped nanographenes (SNGs) 67, 68, 180, 290, 293, 371
 sila[7]helicene derivative 115
 silahelicenes 113, 115
 silylated pentacenophane 200
 single crystal X-ray structure 226
 single organic molecules (SOMs) 428
 single-wall carbon nanotubes (SWCNTs) 243, 244, 255, 258
 six-membered ring-based PAHs
 anthracene and phenanthrene 247–248
 larger PAHs 249–251

- six-membered ring-based PAHs (*contd.*)
 naphthalene 244–247
 pyrene and perylene 248–249
 solution-phase and on-surface chemistry
 366–373
 of nanographenes 371–373
 surface-assisted cyclodehydrogenation
 reaction 367–369
 solution-phase synthesis 277, 280, 284,
 488
 solvent-separated-ion products (SSIPs)
 452, 453, 468
 Sonogashira coupling 233, 259, 261, 280,
 281, 436, 468
 Sonogashira/Diels–Alder/Scholl sequence
 437
 spin chains 501–504
 spin $\frac{1}{2}$ non-Kekulé nanographenes
 489–492
 S-shaped C_{26} PAH dibenzo[*c,l*]chrysene
 203
 stable open-shell Kekulé NGs 485–486,
 504
 π – π stacking interactions 280
 stepwise organic synthesis 224
 substituted [6]helicenes 119
 superconducting quantum interference
 device (SQUID) 270, 271, 273,
 494
 supercritical fluid chromatography (SFC)
 434
 super[7]helicene 133, 134
 (super)helicenes 95, 326
 supertwistacene 87, 135
 surface-assisted (cyclo)dehydration
 74–76
 surface-assisted cyclodehydrogenation
 reaction 367–369
 surface-assisted Ullmann type reactions
 369–371
 Suzuki–Miyaura coupling 70, 157, 166,
 167, 170, 172, 179, 181, 214, 271,
 278, 280, 382
 Suzuki–Miyaura cross-coupling 205,
 246, 307, 309, 330, 331, 392, 433
- t**
 teranthene 269–271, 415, 417
 teropyrenophanes (C_{36}) 205, 207–211
p-terphenyl-containing macrocycles 205
 tetratracene, synthetic route 272
 terylene 195
 tetrabenz[*a,c,h,j*]anthracenes (C_{30})
 205–207
 tetrabenz[*a,c,h,j*]anthracenophanes 206
peri-tetracene 269, 271, 273–275, 279
 tetrahydrofuran (THF) 72, 108, 113, 114,
 116, 117, 123, 124, 126, 128, 130,
 199, 202, 204, 207, 210, 213, 214,
 216–218, 259, 261, 270, 272–274,
 283, 284, 305, 307, 308, 327, 332,
 387, 392, 450, 453–455, 458–460,
 462, 464–469
 tetramethylethylenediamine (TMEDA)
 452, 454
 1,1,8,8-tetramethyl[8](2,11)teropyreno-
 phane 207, 209
 tetraphenylene 59, 175, 176
 tetrathia[4.4](3,11)dibenzo[*c,l*]chryseno-
 phane 203
 tetrathia[7]helicene 72, 109, 110
 thermally activated delayed fluorescence
 (TADF) 315, 316
 [15]thiahelicene 129
 thia[6]helicene derivative 121
 thiahelicenes 109, 114, 115
 thieno-based monkey saddle PAH 331
 thiophene based monkey saddle PAH
 334, 335
 third-order saddle 328
 Thomas–Fermi kinetic energy density
 11
 three-dimensional conjugated chiral
 nanographene 133
 tip-induced patterned function 35–37
 top-down approach 152–153
 topological phase transition 349, 350,
 352, 353
 topological quantum phase
 transition, acene polymer family
 350

- TPA-based upconverted-CPL (TP-UCPL) 435
- transition dipole moment 427, 429, 436, 440
- transition metal-catalyzed [2 + 2 + 2] alkyne cycloisomerisation 112
- transition metal-catalyzed [2 + 2 + 2] cycloisomerization of π -electron systems 111–117
- transition metal-catalyzed hydroarylation of alkynes 119–120
- transition state theory 346, 355
- triangular nanographenes 268, 275–278
- triangular zigzag edged NGs 275
- [3]triangulene 277, 368, 371, 419, 489, 492–495, 501
- [*n*]triangulene 275, 277, 492, 496, 497, 504
- tribenzo[*ff*, *ij*, *rst*]pentaphene (TBP) 249, 251
- tribromo truxene 331
- trimeric cyclophane 200
- trimeric pentacenophanes 200
- trimethylenemethane 398, 399
- triphenylene 59, 181, 249, 452, 453, 455
- triply-bridged cyclophane 209
- triply-bridged [8.2.2]pyrenophane 207–208
- triply fused corannulene 134
- triply fused [7]helicene 134
- triply [5]helicene-bridged (1,3,5)cyclophane 196
- trismide nanographene 227–229
- tritylated dibenzo[5]helicene 136, 137
- truxene precursor 328, 330
- truxene tris(aldehyde) 330
- Tschitschibabin diradical 398, 399
- Tschitschibabin molecule 403
- twistacene 87, 123, 135, 381–393
- two-dimensional (2D) honeycomb lattice 31
- 2D isochemical shielding surface (2D-ICSS) 271
- two-photon absorption (TPA) 434, 435, 437
- u**
- Ullmann couplings 75, 345, 369, 370, 371, 373, 374
- ultra-high vacuum (UHV) 75, 275, 360, 363, 364, 366, 367, 369, 484, 504
- ultralong azagraphene nanoribbons 135
- unbridged heteroarene 212
- undecabenz[7]superhelicene 131, 132
- unsubstituted [8]circulene 175, 324
- v**
- vacuum thermolysis 204, 389
- van der Waals molecular nanographenes 225–230
- variable temperature EPR (VT-EPR) spectroscopy 283, 490
- vibrational CD (VCD) 427
- virtually enantiopure S-shaped double diaza[10]helicene derivative 119
- visible light 231, 248, 382, 390
- Vögtle belt 153
- w**
- Wang's synthesis 184
- warped nanographene (WNG) 325, 461–463
- wavefunction character 9, 10, 15, 398, 400–402
- wet chemical reactions 35, 39
- Wittig reaction 86, 153, 156, 157, 184
- Wu and Isobe's synthesis 197
- x**
- X-ray crystallography 67, 181, 186, 246, 490
- X-ray diffraction (XRD) 66, 225, 226, 231, 234, 279, 314, 384, 434, 450–453, 456, 459, 462, 463, 466, 468, 470
- y**
- Yamamoto coupling 133, 153, 154, 156, 172, 185, 186, 368
- ynedinitriles 115
- Young's modules 31

Z

- zero mode states 401
- zethrene 404–407, 411
- zigzag carbon nanotube 151, 246, 323, 324
- zigzag-edged nanographenes (Z-NGs) 267
 - circumarenes 279–283
 - peri*-acenes 268–275
 - peri*-acenoacenes 278–279
 - triangular nanographenes 275–278
- zig-zag (ZG NR) 409, 410
- zirconocene-based bridge-forming reaction 200
- zirconocene coupling 154
- zirconocene-mediated methodology 200



