

Index

a

adsorbed CO flexibility 26–28
 (SP³-C) alkane polymerization 143–145
 alkoxy isophthalic acids (ISA) 55
 alkoxy substituted
 dehydrobenzo[12]annulenes
 (DBA) 54
 (SP¹-C) alkyne-Glaser coupling 151–152
 anthracene derivatives on HOPG surface
 75
 Arrhenius equation 117, 118, 125
 (SP²-C) aryl & alkene polymerization
 145–151
 aryl–aryl dehydrogenation coupling
 145–148
 as-fabricated SL-WSe₂ FET device on
 SiO₂/Si substrate 187, 188
 assembly-assisted on-surface reactions
 118, 129
 asymmetric linkers 82–86
 ATAT adenine 214
 AT-modified Pd/Al₂O₃ catalyst 126
 atomic force microscopy (AFM) 3, 9, 10,
 210
 Au(111) surface 32, 38, 47, 61, 64, 206
 Au-thiolate self-assembled monolayer
 (SAM) synthesis 207
 azide–alkyne cycloaddition 159–160

b

BDFPTP on Au(111) 120, 121
 1,4-benzenediboronic acid (BDBA) 212

5-(benzyloxy) isophthalic acid derivative
 (BIC) 55
 Bergman reaction 161–162
 bias pulse technique 36, 37
 bicomponent systems 46, 52
 bisDBA-C12 72, 73
 1,2-bis(2-ethynyl phenyl)ethyne/Ag (100)
 35
 boronic acid condensation 156–157
 bulk quasicrystalline materials 114
 butyllithium (BuLi) treatment 179, 180

c

calix[8]arene on Au(111) surface 47
 calixarenes 47
 carbon containing species 37
 carboxylic acid groups 50, 107, 164, 200,
 205
 carboxylic acid homodimer 200
 carboxylic acid hydrogen-bonded
 homo-dimer 201
 carboxylic acid moieties 201
 carboxylic acid supramolecular synthons
 200–205
 carboxylic acid synthon 201, 213
 C₈₂ entrapment 206
 C₆₀F₄₈ adsorption on SL-WSe₂/graphite
 185
 C₆₀F₄₈/graphene, molecular density in
 187
 C₆₀F₄₈/WSe₂/graphite heterostructure,
 photoemission spectra of 187,
 188

- chemical bonding 25, 183, 191
 - chemical synthetic processes 117
 - chiral supramolecular catalysts 122
 - C₅₇H₃₃N₃ Pt (111) surface 145, 146
 - click reaction 159–161
 - close-packed arrangement 201
 - clover-leave Fe(TMA)₄ complexes with Fe
 - on Cu(100) 88
 - C₆₀ molecules 48, 203
 - co-crystallisation 45, 46, 60, 103
 - complexity 81
 - corannulene 61
 - coronene 53
 - covalent-organic frameworks 211
 - crown ethers 47
 - 15-crown-5-ether-substituted cobalt(II)
 - phthalocyanine 47
 - cryogenic SPM systems 11
 - CuAAC reaction 160
 - Cu adatom lattice 94
 - cyanuric acid-melamine (CAM) system
 - 210
 - cyclic hydrogen-bonded FcCOOH
 - pentamers 107, 109
 - cyclisation processes 34
 - cyclocondensation, of TAPB/Ag (111)
 - 159
 - cyclotrimerization, of acetyls 159
- d**
- DBA/COR/ISA system on Au(111) surface
 - 66, 67
 - DBA/COR/ISA system on HOPG surface
 - 65, 66
 - decanethiol molecules 206
 - defect engineering, of 2D TMDs 177–179
 - dehalogenation, Heck reaction 141–143
 - dehalogenative homocoupling, of
 - tribromonethyl-substituted precursors 139
 - dehydrogenation
 - (SP³-C) alkane polymerization 143–145
 - (SP²-C) arylalkene polymerization 145–148
 - dehydrogenation coupling, between
 - benzylic groups 143
 - dehydrogenation of
 - 4,4''-diamino-*p*-terphenyl (DATP) 152, 153
 - density functional theory (DFT)
 - calculations 107
 - diacetylene polymerisation 164–165
 - dialkyl(iso)phthalates 60, 61
 - dibenzo-18-crown-6 (DB18C6)
 - monolayers 47
 - dibenzothiophene (DBT) adsorption on
 - MoS₂ nanoclusters 175, 176
 - diboronic acid self-condensation 158
 - 10,10'-dibromo-9,9'-bianthryl precursor
 - monomer (DBPM) polymerization 146, 147
 - Diels–Alder reaction 160
 - diene moieties on Cu (110) surface,
 - stereoselective synthesis of 151
 - differential charge density (DCD) 185
 - dimerization 159
 - discrete pinwheel phase 105
 - ditopic bi-carboxylic linker 86
 - ditopic bi-pyridyl linkers 86
- e**
- edge passivation approach 150
 - electronic screening at organic/2D TMD
 - interface 190–192
 - electronic screening effect 182, 183
 - electrostatic catalysis, of Diels–Alder
 - reaction 161
 - energy level alignment (ELA)
 - at heterointerfaces 182
 - at interface 181–184
 - energy level lineup (ELL) 181
 - ethylene oxide, cyclic oligomers of 47
 - Eu/para-quaterphenyl-dicarbonitrile
 - (qdc) metal-organic coordination 112, 113
- f**
- Fe phthalocyanine (FePc) molecules on
 - Ag(110) 128, 129

Feringa's MonoPhos ligands 122
 Fermi levels 183
 ferrocenecarboxylic acid (FcCOOH)
 107, 108, 204
 flexible nanodevices, organics-2D TMD
 192
 flower structure 200
 5-fold metal-organic coordination center
 91
 four-component systems 71
 host-guest architectures 72–75
 non-host-guest architectures
 75–76
 fractal Sierpinski triangles 82
 fractal structures 82
 furfural hydrogenation on Pd catalysts
 127

g

giant cyclic porphyrin nanorings with C₆₀
 via host-guest interactions on
 Au(111) 49
 Glaser coupling 120
 of 1,4-diethynyl-2,5-dihexylbenzene on
 metal surfaces 120
 reactions 152
 granular alloy phase 105, 107
 graphene nanoribbons (GNRs)
 bottom-up fabrication of 148–150
 synthesis and characterisation
 32–34
 graphite surface 54, 104, 105
 guanine 52
 guest-induced phase transitions, in
 self-assembled monolayers 56

h

Heck reaction 141–143
 heteromolecular supramolecular
 synthons 213
 hexagonal boron nitride (hBN) substrate
 210
 hexaido-substituted macrocyclocyclo-
 hexam-m-phenylene (CHP)
 molecule 138, 139

2H-4FTPP/Au(111) 38
 hierarchical dehydrogenation, of aromatic
 amine 152
 highly-oriented pyrolytic graphite
 (HOPG) substrate 201, 204
 homo-coupling, of terminal alkene
 150–151
 Hoogsteen-style hydrogen-bonding 213
 host-guest architectures
 four-component systems 72–75
 surface-confined 2D-COFs 58
 two-component systems 46–59
 host-guest chemistry 47, 48
 host networks
 formed by aromatic tricarboxylic acids
 52
 from intrinsically porous building
 blocks 46–49
 from self-assembly of building blocks
 49–59
 sustained by van der Waals interactions
 between alkyl chains 53–57
 hydrogen-bond acceptor (C=O) 200
 hydrogen-bond donor (OH) 200
 hydrogen-bonded frameworks 199
 hydrogen-bonded host networks 50
 hydrogen-bonding interactions 199
 hydrogen-bonds 104, 199

i

imide groups 205, 210
 imide hydrogen-bonds 205
 imidization condensation reaction 156
 indole-2-carboxylic acid 112
 interdigitation, of alkyl chains 54
 ion binding chemistry 47
 isophthalic acid (ISA) 65, 201

k

knitted pinwheel phase 105, 106

l

Langmuir–Blodgett technique 165
 Lennard Jones Potentials 26, 28

light-induced metal-free homocoupling,
 of 4-ethynylbenzoic PEBA on
 highly oriented pyrolytic graphite
 (HOPG) 120, 122

linear alkane polymerization, on Au (100)
 surface 144

liquid-solid phase transformation 184,
 185

local dispersion interactions 24

local electrostatic interactions 25

low-energy electron diffraction (LEED)
 104

m

(3-mercaptopropyl) trimethoxysilane
 (MPS) molecules 177

metal-ligand coordination 81

molecular self-assembly 43, 118, 131

molecular synthesis 199

“molecular zipper” method 137

monolayer TMDs, atomic structure of
 173

multi-component self-assembly 45, 86

multi component supramolecular systems
 43

multiple binding modes 90

multiple-level (hierarchical) interaction
 88

n

nanographenes 4, 55

nanoscience 148

2,6-naphthalenedicarboxylic acid (NDCA),
 metal-catalyzed polymerization
 157

naphthalene-1,4:5,8-tetracarboxylic
 diimide (NTCDI) 205

ncAFM imaging 21

amplitude calibration 22

apparent dissipation and mechanical
 coupling, of qPlus sensor 22

degree of crosstalk 23

drift and creep 21–22

force inversion 20, 23

on-surface reactions characterisation
 29

evolution 34–38

graphene based nanostructures
 32–34

practical considerations 31

sub-molecular contrast at single bond
 level 23

probe particle response 25–26, 28

tip-sample junction forces 24–25,
 27

N-heterocyclic carbenes (NHC)-Cu (111)
 162–163

noncontact AFM (ncAFM) 12, 15

noncontact atomic force microscopy
 (ncAFM) technique 3, 5

non-covalent bonding interactions 104

non-covalent interactions 1, 44, 104, 118

non-host-guest type three-component
 systems 69–71

non-host-guest type two-component
 networks 60

non-site specific interactions 24

o

octadecafluoro derivative, of
 hexakis-(phenylethynyl)benzene
 55

1D intrinsic/p-doped interface, electronic
 properties of 187, 189

on-surface chemical reactions

Bergman reaction 161–162

click reaction 159–161

dehalogenation

Heck reaction 141, 143

Sonogashira cross-coupling 141

Ullmann coupling 136–141

dehydration reaction

boronic acid condensation 156–157

cyclotrimerization, of acetyls 159

decarboxylative polymerization
 157–159

imidization condensation reaction
 156

Schiff-base reaction 153–155

- dehydrogenation
 - (SP³-C) alkane polymerization 143–145
 - (SP₂-C) arylalkene polymerization 145–148
 - diacetylene polymerization 164
 - N-heterocyclic carbene formation and dimerization 162–163
 - σ-bond metathesis 163–164
 - on-surface host-guest chemistry 46
 - on-surface reaction 130
 - pathways 124–125
 - selectivity 119–123
 - sites 125–130
 - on-surface reactions
 - characterisation, ncAFM imaging
 - graphene based nanostructures synthesis and 32–34
 - practical considerations 31
 - SPM under UHV conditions 12–15
 - on-surface synthesis 135
 - organic-2D TMD hybrid structures 172
 - organic-2D TMD interfaces 180
 - atomic structure 174–177
 - electronic screening effect 190–192
 - energy level alignment (ELA) 181–184
 - interfacial charge transfer 184–190
 - p-n heterojunctions 192–193
 - organic light-emitting diodes (OLEDs) 172
 - organics 172, 192
 - organic semiconducting materials 171
- p**
- palladium catalysts 127
 - parallel two-dimensional structures 202
 - Pauli repulsion 25
 - Penrose tiling 111, 204
 - pentacene/MoS₂ photovoltaic device 192, 193
 - perchlorinated
 - hexa-*peri*-hexabenzocoronene (PCHBC) 61
 - periodic self-assembled structures 104
 - perylene-3,4:9,10-tetracarboxylic dianhydride (PTCDA) 211
 - perylene-3,4:9,10-tetracarboxylicdiimide (PTCDI) 205
 - phase engineering, of 2D TMDs 179–180
 - phase separation 44
 - phenylacetylene and iodobenzene
 - heterocoupling on Au (100) 141
 - 1,4-phenylenediboronic acid (PDBA)
 - molecular conversion 156, 157
 - photoemission spectroscopy (PES) 187
 - pick-mix-and-link strategy 148
 - p-n heterojunctions, organic-2D TMD
 - interfaces 192–193
 - polymeric diacetylene (PDA) 164
 - polyphenyl-dicarbonitrile linkers on Au(111) 96
 - potential hydrogen-bonding
 - supramolecular synthons 205
 - pristine 2D transition metal
 - dichalcogenides 172
 - PTCDI-melamine bimolecular host
 - networks 62
 - PTCDI/melamine/(3BPEB-OH)/C₆₀ 73
 - PTCDI-melamine/C₇₀ host-guest system 63
 - PTCDI-melamine framework 208
 - PTCDI-melamine host network 62–64, 73
 - PTCDI-melamine host system on Au(111) 72
 - PTCDI-melamine network 205
 - PtSe₂ monolayer 174–175
- q**
- quasicrystalline self-assembled
 - monolayers 114
 - quasicrystals
 - characterization 104
 - defined 103
 - quasiperiodicity analysis 104
 - p*-quaterphenyl-3,3''',5,5'''-tetracarboxylic acid (QPTC) 51, 202

p-quinquephenyl-3,3'',5,5''-
tetracarboxylic acid (QQPTC)
204

r

random mixing 44, 60, 62
random tiling 105, 111
rhombus tiling 4, 105, 200–204

s

scanning probe microscopy (SPM) 9
 defining characteristic 10
 feature 10
 techniques 3, 5
 ultra-high vacuum (UHV) conditions
 11
 benefits 11
 challenges 11
 molecule-substrate systems,
 characterisation of 12–15
 ncAFM 15–16
 on-surface reactions 11–12
 sample preparation 11
scanning tunnelling microscopy (STM)
 3, 9, 43, 47, 84, 104, 119, 135, 189,
 201
Schiff-base reaction 153–155
self-assembly 46, 86
 of building blocks, host networks from
 49–59
 of ethynyl-iodophenanthrene on
 Ag(111) 88
 of 1,3,5-tris[4-(pyridin-4-yl)phenyl]
 benzene on Cu(111) 93
self-assembly process 5
Sierpinski triangles 82, 84, 85, 213
 σ -bond metathesis, of silylated alkynes
 164
site selective guest adsorption 68–70
solution-based chemistry 135
Sonogashira cross-coupling 141
stimuli-responsive host-guest systems
 49, 57
stimulus responsive two-component
 host-guest systems 53

sub-molecular contrast at single bond
 level, ncAFM imaging 23
probe particle response 25
 adsorbed CO flexibility 26–28
 chemical sensitivity 29
 electrostatics 28–29
tip-sample junction forces 24–25
 chemical bonding 25
 local dispersion interactions 24
 local electrostatic interactions 25
 non-site specific interactions 24
 Pauli repulsion 24–25
substrate-induced confinement effect
 119
supramolecular architectures 96
supramolecular chemistry 1, 9, 122
supramolecular coordination
 self-assembly 81
supramolecular synthon approach 199
supramolecular synthons 49, 199, 201,
 205, 213
surface-based frameworks 200, 215
surface-based supramolecular chemistry
 4
surface-confined 2D-COFs 57–59
surface confinement effect 118
surface diffraction techniques 104
surface functionalization, of 2D TMDs
 177
 defect engineering 177–179
 phase engineering 179–180
surface molecular self-assembly 119
surface oxygen reduction reaction 128
surface reactions 118
switchable bicomponent system 52

t

p-terphenyl-3,5,3',5'-tetracarboxylic acid
 (TPTC) 201
 at graphite/nonanoic acid interface,
 STM image of 106
 molecule structure 105
 monolayer 52
 self-assembly 104

- 5,10,15,20-tetra(4-pyridyl) porphyrin
four-fold symmetric linker 86
- thermal-induced Ullmann reactions, of
TPP derivatives 137
- thio-adamantyl functionalised PTCDI,
(SAdam)₂-PTCDI 209
- thio-adamantyl groups 209
- thio-adamantyl side chains 209
- thiopropyl groups 209
- three-component systems 62
non-host-guest systems 69–71
one-component host network and two
different guests 65–69
two-component host network and guest
62–64
- thymine hydrogen-bonds 213
- tip-induced on-surface Ullmann reaction
136
- “tip manipulation” approach 136
- TOAT molecule 28, 30
- 1,4-triazole products 160
- trimesic acid (TMA) 50, 105, 201
- 5,10,15-tri(4-pyridyl)-20-phenylporphyrin
84
- 1,3,5-tris(4-carboxyphenyl)benzene (BTB)
50, 52, 201
- 1,3,5-tris(4-iodophenyl)benzene (TIPB)
208
- 1,3,5-tris(*E*)-2-(3,5-didecyloxyphenyl)-
ethenyl]benzene (TSB35) 54
- 1,3,5-tris-(4-ethynylphenyl)benzene
(Ext-TEB) molecules 151
- 1,3,5-trispyridylbenzene three-fold
symmetric linker 86
- two-component self-assembly
systems 45
using fluorophilic interactions 58
- two-component systems
based on surface-confined 2D-COFs)
57–59
host-guest architectures 46–59
non-host-guest architectures 59–62
- two-dimensional (2D) atomically layered
materials 171
- two-dimensional (2D) crystal engineering
44
- 2D co-crystals 46
- 2D covalent networks 137, 138
- 2D graphene structure synthesis 33
- 2D surface covalent organic frameworks
(2D-sCOFs) 46
- 2D transition metal dichalcogenides 5
exotic properties 171
Heck reaction 141–143
Sonogashira cross-coupling 141
surface functionalization by organics
177–180
Ullmann coupling 136–141
- two-dimensional hydrogen-bonded
structure 201
- two-dimensional (2D) molecular
assembly 118
- two-dimensional self-assembled
frameworks 199
- two-dimensional supramolecular
chemistry on surfaces 3
- ## U
- Ullman-like pathway 208
- Ullmann coupling, of BBP on Ag(111)
129, 130
- Ullmann reactions of BBP on Ag(111)
124
- ultra-high resolution imaging, of organic
molecules 16
- qPlus sensor construction 18
- sample preparation 16
CO deposition 17–18
decoupling layers 18
organic molecule deposition at low
temperature 17
- tip functionalisation 19–21
- tip preparation 19–21
- ultra-high vacuum (UHV) 201
- underpotential deposition (UPD) methods
207
- Ureido-4[1*H*]-ureidopyrimidone (UP)
ligands 122

V

- vacancies, surface engineering 178
- vacancy densities 179
- van der Waals interactions 4, 5, 50–57
- van der Waals-stabilized networks 57

W

- Wanzlick-type dimerization 163
- Watson-Crick base-pairing 214

X

- X-ray photoelectron spectroscopy (XPS)
3, 9

Z

- zigzag-edge structures (ZGNR)
148
- ZnPc/ZnOEP/C₆₀ at electrolyte/Au(111)
interface 69, 71

