

Index

A

Ab initio, 2
Ab initio calculations, 9
Acceptor, 159
Activation barrier, 30
Adsorption, 125, 199
Adsorption energy, 57, 80, 126, 129, 134, 139
Al₂O₃(0001) surface, 204, 208
Al₂O₃ surface, 4, 199, 201, 205, 208
Al adatom, 60
Al adlayers, 61
Al composition, 47
AlGaN, 45
Al–H bonds, 75
All-electron, 20
Alloy semiconductors, 45
AlN, 1
Al–N bonds, 201, 207, 213
AlN/GaN superlattice, 4, 171, 177
AlN layer, 200, 207
AlN surface, 60, 75, 78
AlN(0001) surface, 60, 75, 78
AlN(1 $\bar{1}$ 00) surface, 75, 78
AlN(1 $\bar{1}$ 01) surface, 63, 77, 78, 133
AlN(1 $\bar{1}$ 02) surface, 133
AlN(11 $\bar{2}$ 0), 136
AlN(11 $\bar{2}$ 0) surface, 61, 77, 78
AlN(11 $\bar{2}$ 2), 63
AlN(11 $\bar{2}$ 2) surface, 77, 80, 129
Al–O bonds, 207
Approximation, 16
Atomic arrangement, 109, 116, 141
Atomic pseudo wave function, 20

B

Bachelet–Hamann–Schlüter, 22
Band alignment, 162, 165
Band bending, 165
Band gap, 38, 166
Band-gap energy, 155
Band offset, 152
Band structure, 38
Bazant, 25
Beam Equivalent Pressure (BEP), 55, 138
Bloch's theorem, 16, 18
Blue Light-Emitting Diodes (LEDs), 1
Bohr radius of the exciton, 118
Bond energy, 141
Bonding–antibonding gaps, 167
Bond network topology, 152
Bond order potential, 25
Bound electron, 159

C

Carbon doping, 195
Carbon incorporated surfaces, 195
C-atom doping, 160
Charged dislocations, 160
Charge Neutrality Level (CNL), 162, 166
Charge transfer, 166
Chemical and structural change, 206
Chemical potential, 31, 56
Cluster geometry, 155
Cohesive energy, 25, 36, 113
Compositional fluctuation, 116
Composition pulling effect, 122
Conduction Band Minimum (CBM), 38
4 core, 43

5/7 core, 43
 8 core, 43
 Correlation functional, 13
 Correlation potential, 15
 Coulomb repulsion, 189
 Covalent bond charge, 28
 Critical ionicity, 28
 Crystal field splitting, 39
 Crystal-field-split-off Hole (CH), 177
 Crystal slabs, 18
 Crystal-structure heredity, 149
 Crystal structures, 36, 139
 CsCl, 28

D

Dangling bond, 61, 72, 82, 140, 141, 156, 167
 Dangling bond counting model, 173
 Deep-level, 154
 Density-Functional Theory (DFT), 10
 Density of States (DOS), 188, 190
 Desorption of oxygen, 201, 203
 Diffusion coefficient, 32
 Diffusion length, 32, 128, 132, 135
 Dislocation, 2, 153
 Dislocation core, 156
 Dislocation core energy, 44
 Disorder-Induced Gap States (DIGS), 167
 Dissociation, 214
 Donor, 157
 Double 6-atom ring core, 46
 Driving force, 102

E

ECMC method, The, 140
 Edge and screw dislocations, 43
 Effective enthalpy of mixing, 119
 Elastic constants, 28
 Elastic energy loss, 155
 Electron and hole effective masses, 39
 Electron Counting (EC) rule, 59, 136, 140, 187, 194, 197
 Electron mobility, 160
 Electron transfer, 165
 Electrostatic interaction, 29
 Empirical interatomic potentials, 41
 Energy barrier, 127, 130, 131, 134, 137, 208, 214
 Equilibrium vapor pressure, 95
 Excess energy, 41
 Exchange-correlation energy, 11
 Exchange-correlation potential, 12

Exchange functional, 13
 Exchange potential, 14

F

{111} facet, 104
 Fcc-bulk structure, 149
 Fermi energy, 155, 164
 Formation energy, 56, 147, 172
 Formation rate, 214
 Fourier transformed, 17
 Free carriers, 160
 Free energies, 149

G

Ga adatoms, 66
 Ga adlayer, 67
 GaAs(001), 58
 Ga-C bond, 197
 Ga-Ga dimers, 192
 Ga monolayer, 66, 192
 GaN, 1
 GaN(0001), 64
 GaN(0001) surface, 80, 83
 GaN(000 $\bar{1}$) surface, 66, 80, 83
 GaN(1 $\bar{1}$ 00) and (1120) surfaces, 67, 82, 83
 GaN(1101) surface, 82, 85, 191, 195
 GaN(11 $\bar{2}$) surface, 82, 85
 Ga vacancy, 66
 Generalized Gradient Approximation (GGA), 15
 Gibbs energy, 100
 Growth kinetics, 125
 Growth processes, 125, 142
 Growth rate, 128, 213

H

2H-AlN, 139
 4H-AlN, 139, 142
 Hartree-Fock approximation, 16
 Heat of formation, 56
 Heavy-Hole (HH), 40, 177
 Hexagonal, 36
 High H₂ pressures, 193
 Hohenberg and Kohn, 10
 Homogeneous electron gas, 13
 4H-SiC, 136
 4H-SiC(11 $\bar{2}$ 0), 136
 H-terminated surface, 193
 Hybrid exchange-correlation functionals, 16
 Hydride Vapor Phase Epitaxy (HVPE), 199
 Hydrogen, 191

Hydrogen adsorption, 74
Hydrogen chemical potential, 196

I

Iconicity, 28
Ideal surface, The, 61
III/V ratio, 142
 $\text{In}_x\text{Ga}_{1-x}\text{N}$, 109
 $\text{In}_x\text{Ga}_{1-x}\text{N}$ on $\text{In}_y\text{Ga}_{1-y}\text{N}$, 4
In adatom, 71, 189
In adlayer, 74, 189
InAs, 172
In bilayer, 71, 73, 188
In composition, 48
Incorporation, 191
Indium incorporation, 109, 118
 InGaN , 40, 45, 171
 InGaN quantum well, 4, 109
In–In dimer, 156
In monolayer, 71, 74
 InN , 1, 70
 InN semipolar surfaces, 72
 $\text{InN}(0001)$ surface, 70
 $\text{InN}(000\bar{1})$, 71
 $\text{InN}(000\bar{1})$ surface, 70, 187
 $\text{InN}(0001)$ and $(000\bar{1})$ surface, 85
 $\text{InN}(\bar{1}\bar{1}00)$ and $(\bar{1}\bar{1}01)$ surfaces, 87
 $\text{InN}(\bar{1}\bar{1}00)$ and $(11\bar{2}0)$ surfaces, 72, 188
 $\text{InN}(\bar{1}\bar{1}01)$ surface, 73
 $\text{InN}(11\bar{2}2)$ surface, 74
 $\text{InN}(11\bar{2}0)$ and $(11\bar{2}2)$ surfaces, 87
In-plane alignment, 201, 203
Interface physics, 166
Inversion symmetry, 152
Inward diffusion, 208
Ionic charge, 28

K

Keating model, 24
Khor-Das Sarma, 25, 27
Kinetic Monte Carlo (KMC), 30
Kleinman and Bylander, 23
KMC simulations, 210
Kohn-Sham equations, 11

L

Laser Diodes (LDs), 1
Lattice constraint, 111
Lifetime, 32, 128, 132, 135
Light- and crystal-holes, 40
Light-Hole (LH), 177

Local Density Approximation (LDA), 13
Localization length, 159
Localized excitons, 111
Low H_2 pressures, 192

M

MC simulations, 112
Metallic In–In bonds, 174, 187
Metallic reconstruction, 68
Metal-Induced Gap States (MIGS), 167
Metal/InN interfaces, 161
Metal Organic Vapor Phase Epitaxy (MOVPE), 4, 55, 74, 95, 118, 125, 126, 193, 199
Metal-polarity surface, 146
Metropolis Monte Carlo (MMC), 30
{1010}m facet, 104
Mg-acceptor doping, 160
Mg adsorption, 191
Mg doping, 186, 191
Mg-incorporated surfaces, 186
Migration, 125, 127, 130, 131
Miscibility, 40
Miscibility gap, 111
Molecular Beam Epitaxy (MBE), 4, 55, 118, 125, 193
Momentum matrix element, 181
Monte Carlo (MC), 2
Monte Carlo simulations, 30

N

N adatom, 196, 199, 202
Narrow bandgap, 176
Near-band-edge emission, 181
Nearest neighbor, 174
 NH_3 , 199
 NH_3 molecule, 204
N–H bond, 82
Nitridation, 198
III-nitride compounds, 1
Nitrogen adsorption, 211
Nitrogen incorporated $\text{Al}_2\text{O}_3(0001)$ surface, 199
Nitrogen incorporated Al_2O_3 surfaces, 205
Nitrogen substitution, 200, 203
Nitrogen vacancy, 171
N/III ratio, 95, 101
N–N bonds, 80
N–N dimer, 157
NO molecules, 199
Nonlocal pseudopotential, 19

- Nonpolar orientations, 61, 186
 Non-radiative recombination centers, 118
 Norm-conserving, 20
 N-polarity surface, 146
 Nudged Elastic Band (NEB) method, 208
 N vacancy, 159
- O**
- O-atom doping, 160
 (1102) orientation, 199
 Outward diffusion, 208
- P**
- Partial pressure, 101
 Partition functions, 57
 Perdew, Burke, and Ernzerhof (GGA-PBE96), 15
 Perdew and Wang (GGA-PW91), 15
 Phase diagram, 122
 Phase separation, 42
 Photoluminescence (PL), 109
 Plane-wave basis set, 16
 Point defects, 153
 Polarity inversion, 146
 Potential Energy Surface (PES), 126, 129, 136, 139
 2p orbitals, 177
 Pressure, 57
 Pseudopotential, 18
 Pseudopotential methods, 2
 Pseudo-(1 × 1) surface, 65
 P-type conductivity, 191
 P-type doping, 195
 P-type InN, 160
- Q**
- Quantum confinement effects, 180
 Quantum-Confinement Stark Effect (QCSE), 180, 191
- R**
- Rate-limiting, 210
 Reaction energy, 208
 Regular-solution model, 120
 Repeated-slab geometry, 147, 162
 Repeated unit-cell, 155
- S**
- Sapphire (Al₂O₃), 198
 Scanning Tunneling Microscopy (STM), 64
 Schottky barrier, 4, 161
 Schottky Barrier Height (SBH), 163
 Schrödinger equation, 9
 Secondary-Ion-Mass Spectroscopy (SIMS), 187, 191
 Seebeck coefficient, 160
 Semipolar GaN(1101) surface, 68
 Semipolar GaN(1122) surface, 68
 Semipolar orientations, 62, 191
 Separable pseudopotential, 23
 Sp³ orbitals, 166
 Spherical Bessel functions, 23
 Spherical harmonics, 19
 Spin-orbit coupling, 177
 Stacking fault, 152
 Stillinger-Weber (SW), 25, 44
 Stoichiometry, 199, 202, 206
 Strain effect, 151
 Strain energy, 43
 Substitutional Mg atoms, 186, 192
 Superlattices (SLs), 109
 (0001) surface, 199
 Surface energy, 97, 99, 105
 Surface formation energies, 59
 Surface phase diagrams, 4, 55, 104, 127, 138, 194, 197, 204, 205
 Surface polarity, 146
 Surface-polarity inversion, 4
 Surface reconstruction, 55
 (2 × 2) surface, The, 60, 66
- T**
- Temperature, 57
 Tetrahedral clusters, 111
 Thermodynamic analysis, 97, 114
 Thermodynamic equilibrium, 149
 Thermodynamic stability, 41
 Threading dislocations, 42
 Tight-binding calculations, 175
 β-tin, 28
 Tomas-Fermi screening length, 159
 Transcription effect, 150
 Transfer integral, 175
 Transition state, 208
 Troullier and Martins, 21
 Two-dimensional metals, 152
 Two-monolayer model, 146
- U**
- Ultrasoft pseudopotentials, 24
 Unintentional electron carriers, 153

V

V/III ratio, 136

Valence Band Maximum (VBM), 38

Valence electrons, 18

Valence-Force-Field (VFF), 41

W

Wurtzite, 25, 36

Wurtzite structure, 146

XX-ray Photoemission Spectroscopy (XPS),
186, 213**Z**

Zinc Blende (ZB), 25, 36

Zincblende structure, 146