

SUBJECT INDEX

4th Power, 3

A

Ag (Silver), 57
AIREBO, 4
Alkali Halides of NaCl Type, 13
Alkali Metals, 51
Aluminophosphate, 9
AMBER, 131
Ar (Argon), 58
Aspherical Molecules, 50
Axelrod-Teller, 109

B

Berne-Pechukas, 8
Beest-Kramer-Santen (BKS), 9
Biochemical AMBER, 131
Biochemical CHARMM, 133
Biochemical GROMACS, 136
Biswas-Hamann, 11
Born Repulsive, 12
Born-Huggins-Mayer, 13
Born-Mayer, 14
Born-Pauling, 19
Breakable Bond Interaction-Quartic, 82
Brenner, 21, 31
Brenner II (REBO), 25
Buckingham, 33

C

C (Carbon), 94, 100, 102
C₆₀ Clusters Formation, 37
Charged Atoms, 39
Chelikowsky, 37
CFF, 132
CHARMM, 133
CO, 84
Cu, 57
COMPASS, 134
Cosine Angular, 110
Cosine Dihedral, 119
Coulombic (Any Charged Atom), 39
Cubic Metals, 77

D

D₂, 85
Diep-Johnson, 41
Dipole, 43
Dissipative particle dynamics (DPD), 44
DREIDING, 134

E

Ellipsoid Gaussians, 8
Embedded-Atom Method (EAM), 45
ESFF Dihedral, 120
Exponential 3-Body, 112
Exponential Dihedral, 122

F

Finite Extensible Nonlinear Elastic
(FENE), 46
Fermi-Dirac, 47
Feuston-Garofalini, 48

G

Gay-Berne, 50
Ge (Germanium), 90
GROMAX, 136
Guo-Thirumalai Dihedral, 122

H

HO₂, 67
H₂F, 65
H₂O, 48, 105
Harmonic, 53
Harmonic Angle, 113
Harmonic-Cosine Dihedral, 123
Harmonic Dihedral, 124
Hybrid Extended Rydberg, 51
Hydrocarbons, 4, 21, 25
Hydrogen, 41, 59, 79, 84, 85

I

Inert Gas-Hydrogen Halide, 61
Inert Monatomic Molecules, 60
Ionic Compounds, 19

Ionic Crystal, 12
Inorganic Molecules, 134, 135, 137, 138
Inverted Gaussian, 54

K

Kaxiras-Pandey, Murrell-Mottarm, 55

L

Lennard-Jones, 57, 58, 59, 60, 61,
LiFH, 12

M

Metals, 45, 132
Murrell-Carter-Farantos-Huxley-Varandas
(MCFHV), 63, 65, 67, 69
Mittal-Chaplot, 71
Modified Stillinger-Weber, 73
Morse, 77
Murrell-Mottram Angle, 114

N

Neutral Ground-State Atoms with $Z=2$ to 105,
14

O

OPLS Dihedral, 125
Organic Molecules, 131, 132, 134, 135, 137
Oxygen, 73

P

Particles with Charge and/or Point Dipole
Moment-Dipole, 43
Particles that Exchange Massive Scalable Field-
Yukawa, 104
Polymers, 46, 132, 134, 135, 136, 137, 138
Polynomial, 81
Polynomial Dihedral, 126
Pt (Platinum), 105

Q

Quartic, 82

R

ReaxFF, 137
Rector-Swol, 83
Rydberg (Extended), 84

S

Semiconductors, 45
Si (Silicon), 11, 31, 55, 73, 79, 89, 92, 94,
95, 97, 99, 100
Silica, 9
Silvera-Goldman, 85
Silvera-Goldman/Deep-Johnson, 86
Squared Cosine Angle, 111
Squared Harmonic, 88
Stillinger-Weber, 89, 90, 92

T

Tang-Toennies-van der Walls Potential
Model, 93
Tersoff, 94, 95, 97, 99
Tersoff-Brenner, 100
Triple Cosine Dihedral, 127

U

UFF, 138
Urey-Bradley Angle, 115

Y

Yamaguchi-Maruyama, 102
Yukawa, 104

Z

Zhu-Philpott, 105