

Index

Symbols

β_2 , 91, 92
 C_{60} , 16, 25, 37, 93, 120, 156
 κ -Köhler theory, 143

A

ab initio, 55
abundance spectrum, 37, 77
abundances, 133
adiabatic separation, 49
aerosol, 137–139
aerosol growth, 140
aerosol science, 137
Ag clusters, 152
Ag nanoparticles, 122
aggregation, *see* gas aggregation
Aitken mode, 138
aliphatic chains, 135
alkaline, 7, 9–11, 14, 16, 35, 58, 65
amorphous carbon structures, 133
anisotropy, 92, 93
aromatic rings, 135
atmospheric particles, 137
atomic core, 116
atomic shells, 37, 79
atomic transitions, 42
atoms, 7

B

binding energy, 70
biocompatible polymers, 146
biological clearance, 156
biosensors, 149
blood-pool agents, 147
BO, *see* Born–Oppenheimer
BO molecular dynamics, 50
BO surface, 50, 51
BO-MD, *see* BO molecular dynamics

Born–Oppenheimer, 48
bulk equilibrium, 130

C

cancer therapies, 153
carbon nanotube functionalization, 149
carbon nanotubes, 149, 156
Car–Parrinello molecular dynamics, 50
catalysis, 121
catalysis and geometry, 122
catalytic efficiency, 122
CCN, *see* cloud condensation nuclei
charge resonance-enhanced ionization, 96
chemical binding, 9
chemotherapy, 151
chirp, 94, 100
chromophore, 147, 150, 152, 153
CI, *see* configuration interaction
cisplatin, 151, 155
classical, 161
Clemenger–Nilsson model, 58, 80
cloud condensation nuclei, 138, 140
cloud formation, 137
cluster deformation, 40
cluster shape, 80, 81, 85
cluster source, 25
cluster tailoring, 145
cluster temperature, 29
cluster-substrate coupling, 117
coating molecules, 105
coherent line broadening, 87
cohesive energy, 14
collective splitting, 85
collision, 32, 162
conduction gap, 120
conductivity, 11, 34
conductor, 11
configuration interaction, 56
contrast agents, 146

cooling, 51
 core electron, 5, 6, 8, 35, 42, 65, 95
 Coulomb explosion, 97
 Coulomb Hartree energy, 60
 Coulomb interaction, 83, 116
 Coulomb pressure, 98
 coupled oscillators, 109
 covalent binding, 15
 CP-MD, *see* Car–Parrinello molecular dynamics
 CREI, *see* charge resonance-enhanced ionization
 critical saturation ratio, 142, 143
 cytotoxicity, 156

D

damage, 153
 deformation, 68, 70, 86
 degrees of freedom, 115
 density functional theory, 8, 59
 density of states, 89, 124
 deposited clusters, 2, 19, 26
 designer material, 125
 DFT, *see* density functional theory
 dimer molecule, 9
 dipole antenna, 124
 dipole moment, 70
 dipole polarizability, 71
 dipole strength, 73
 dipole–dipole interaction, 109
 direct emission, 74
 disintegration, 105
 dissociation energies, 78
 distance-dependent tight binding, 53
 distorted-wave Born approximation, 32
 DNA, 146
 DNA double strand breaks, 155
 DNA sensors, 149
 drug delivery, 150, 152
 DWBA, *see* distorted-wave Born approximation

E

effective potential, 53
 electrical conductivity, 71
 electron gas, 129
 electron transmission, 119
 electronic shells, 37, 80
 electron–electron correlations, 87
 embedded clusters, 1, 2, 18, 19, 25, 26
 environment, 26
 exchange-correlation energy, 60
 exponential decrease, 90

F

FEL, *see* free-electron lasers
 Fermi momentum, 34, 62, 128
 ferromagnetic clusters, 154
 field-dominated regime, 90, 95
 finite fermion systems, 129
 fluorescence, 124
 fluorescence enhancement, 124
 force fields, 113
 fragmented resonance, 83
 free-electron lasers, 94
 frequency-dominated regime, 95
 fullerenes, 25, 37, 156

G

galaxy, 134
 gas aggregation, 25
 generalized-gradient approximation, 63
 GGA, *see* generalized-gradient approximation
 glass matrix, 104
 global shape parameters, 70
 global warming, 137
 glucose sensor, 149
 GNP, *see* gold nanoparticles
 gold cluster functionalization, 145
 gold clusters, 153, 155, 156
 gold nanoparticles, 147, 150
 gold nanoshell, 153, 157
 gold-silica nanoparticles, 154
 ground-state configuration, 51

H

Hagena parameter, 24
 halogen, 7, 9, 11, 16
 harmonic oscillator, 58
 Hartree–Fock, 56
 He droplets, 107
 HF, *see* Hartree–Fock
 highest occupied molecular orbitals, 8
 highly oriented pyrolytic graphite, 2
 HOMO, *see* highest occupied molecular orbitals
 homogeneous electron gas, 63
 homogeneous matter, 129
 HOMO–LUMO gap, 81
 HOPG, *see* highly oriented pyrolytic graphite
 Hubbard model, 53
 Hückel, 52
 hydrodynamical flow, 98, 99
 hygroscopicity, 143
 hyperthermia, 154

I

independent particle picture, 60

infrared measurements, 135
 inner ionization, 96
 insulator, 11
 interaction potentials, 116
 interface, 113
 interstellar objects, 135
 ionic binding, 9–11, 15
 ionic core, 7, 8, 47
 ionic shells, 37
 ionization, 43, 88, 108
 ionization potential, 13, 70, 95
 ionization threshold, 92
 IP, *see* ionization potential
 isomer, 12
 isotropy, 93

J

Jahn–Teller effect, 80
 jellium, 62, 68, 86

K

Keldysh parameter, 95
 Kelvin effect, 141
 Kelvin equation, 141
 Köhler curve, 142
 Köhler theory, 141
 Kohn–Sham equations, 60
 Kohn–Sham potential, 68, 78
 Kohn–Sham scheme, 59
 KS, *see* Kohn–Sham equations

L

Landau fragmentation, 83, 86
 laser, 32
 laser field, 32
 laser frequency, 94
 laser intensity, 33, 94
 laser profile, 33
 LCAO, *see* linear combination of atomic orbitals
 LDA, *see* local density approximation
 Lennard-Jones, 53
 line broadening, 86
 linear combination of atomic orbitals, 52
 liquid ^3He , 129
 local density approximation, 60, 62
 local spin-density approximation, 62
 lowest unoccupied molecular orbital, 8
 LSDA, *see* local spin-density approximation
 luminescence, 109
 LUMO, *see* lowest unoccupied molecular orbital

M

magic numbers, 78, 80, 81, 131
 magnetic moment, 38, 106
 magnetic resonance, 146
 magnetic resonance imaging, 146
 magnetism, 106
 many-body problem, 47
 marker, 146
 mass spectrometer, 21
 mass spectrometry, 27
 MC, *see* Monte Carlo
 MCHF, *see* multiconfigurational HF
 MD, *see* molecular dynamics
 metabolic clearance, 144
 metallic binding, 15
 MgO surface, 103
 Mie, 2
 Mie frequency, *see* Mie plasmon frequency
 Mie plasmon frequency, 34
 Mie plasmon resonance, 81, 82, 84, 132
 Mie surface plasmon, 40, 110, 117
 mode coupling, 109
 molecular dynamics, 53
 molecular vibrations, 95
 moments of inertia, 71
 monomer separation energy, 70
 Monte Carlo, 52
 MPI, *see* multiphoton ionization
 MRI, *see* magnetic resonance imaging
 multiconfigurational HF, 57
 multiphoton, 162
 multiphoton ionization, 43, 88, 90, 95, 96
 multipole moments, 70

N

nanomaterial, 125
 nanomechanics, 120
 nanometer droplets, 143
 nanoplasma, 98
 nanoplasma model, 99
 nanotoxicity, 156
 near-field enhancement, 124
 nuclear giant resonances, 132
 nuclear matter, 129
 nucleation mechanism, 139
 nucleation mode, 138, 139

O

oblate, 40, 80, 85
 one-particle-one-hole, 56, 82
 one-photon process, 43, 89, 91
 ONIOM, 113
 optical absorption, 72, 82

- optical field ionization, 95
 optical response, 40, 72, 86, 104
 orientation averaging, 92
 outer ionization, 96
- P**
 PAD, *see* photoelectron angular distribution
 PAH, *see* polycyclic aromatic hydrocarbon
 Pauli repulsion, 116
 PCR, *see* polymerase chain reaction
 PES, *see* photoelectron spectroscopy
 PES/PAD, 44, 92
 photoabsorption, 40
 photocatalysis, 122
 photoelectron angular distribution, 44, 91, 119
 photoelectron spectroscopy, 13, 43, 89
 photon-induced ionization, 96
 photosensitizers, 147
 photothermal therapy, 150, 153
 planetary nebulae, 135
 plasmonic resonance energy transfer, 147
 polarization interaction, 116
 polarization potentials, 67
 polycyclic aromatic hydrocarbon, 124, 134
 polymer hydrogels, 151
 polymerase chain reaction, 149
 ponderomotive potential, 94
 potential energy surface, 50
 power spectrum, 73
 PRET, *see* plasmonic resonance energy transfer
 prodrug, 151
 projectile, 32
 prolate, 40, 80, 85
 pseudo wave functions, 67
 pseudojellium, 69
 pseudomass, 50
 pseudopotentials, 65
 PsP, *see* pseudopotentials
 pulse delay, 107
 pulse length, 100
 pump and probe, 107
- Q**
 QM/MM, *see* quantum mechanical/molecular mechanical
 quadrupole moment, 70, 80
 quantum dots, 132
 quantum mechanical/molecular mechanical, 112
- R**
 radiative forcing, 137
 radiosensitizer, 150
 radiotherapy, 155
 random-phase approximation, 63, 72
 Raoult's law, 141
 rare gas clusters, 100
 rare gas matrix, 103, 117
 recoil energies, 98
 reflectron, 38
 relative humidity, 140
 relaxation, 5, 6, 52, 74
 residual interaction, 83
 resonance conditions, 100
 resonance mechanism, 100
 resonance width, 82, 83
 Rh nanostructures, 106
 RNA, 146
 root-mean-square radius, 70
 RPA, *see* random-phase approximation
- S**
 saturating fermion systems, 127
 saturation density, 128
 saturation ratio, 140
 saturation vapor pressure, 141
 self-interaction correction, 63, 70
 semiclassical approaches, 64, 79
 sensor, 147
 shell closures, 77, 131
 shell oscillations, 131
 shell structure, 7
 short-range potential, 117
 short-range repulsion, 116
 SIC, *see* self-interaction correction
 single-electron energy, 36, 43, 67, 70, 80
 Slater approximation, 63
 Slater determinant, 56
 Slater exchange energy functional, 63
 soft jellium, 68
 solute molecule, 141
 spectral analysis, 73
 spectral fragmentation, 73
 SPION, *see* superparamagnetic ion oxide nanoparticles
 splitting, 85
 superatoms, 125
 supernova, 133
 supernova ejecta model, 133
 superparamagnetic ion oxide nanoparticles, 146
 supersaturation, 141
 supershells, 79
 supersonic jet, 21, 23
 surface plasmon, *see* Mie surface plasmon
 surface plasmon resonance, 147

surface source, 25
surface states, 122

T

TDDFT-MD, 51
TDHF, *see* time-dependent HF
TDLDA, *see* time-dependent local density approximation
TDLDA-MD, 87
therapeutic window, 151
thermal broadening, 83, 87
thermal emission, 74, 89
thermal shape fluctuations, 86
Thomas–Fermi approximation, 64
tight binding, 52
time of flight, 21, 37
time scales, 6
time-dependent HF, 56
time-dependent KS equations, 60
time-dependent local density approximation, 63
time-resolved analysis, 107
TOF, *see* time of flight
toxicity, 156
trajectory surface hopping, 51
transferability, 66
triaxial, 81, 85, 86

U

ultrafine aerosol network, 138
ultrafine aerosols, 138
unidentified infrared bands, 134, 135

V

valence electron, 5, 8, 40, 42, 43, 47, 65, 97, 116
van der Waals binding, 10, 11, 15
van der Waals cluster, 15, 53
vapor phase, 141
vascular targeting, 145
velocity map imaging, 44, 92
visible light, 95
Vlasov equation, 64
Vlasov–Uehling–Uhlenbeck, 64
VMI, *see* velocity map imaging
VUU, *see* Vlasov–Uehling–Uhlenbeck

W

water activation, 138, 140, 143
water activity, 141
water liquid droplet, 141
water molecules, 105
Weisskopf formula, 74
Wigner–Seitz, 128
Wigner–Seitz radius, 35, 62
Woods–Saxon shell model, 58

X

XMCD, *see* X-ray magnetic circular dichroism
X-ray magnetic circular dichroism, 107
X-ray regime, 95
X-ray spectrum, 42

Z

ZEKE, *see* zero electron kinetic energy
zero electron kinetic energy, 43