

Index

- ABL *see* alternating bond-length (ABL)
- acetylene rotation 33
- action spectrum 79, 80
- adsorbate density of states 49
- adsorbate Green's function 79
- adsorbate-induced resonance model 59
- adsorbate motions 26, 68
 - inelastic tunneling current 35
 - real-time monitoring of 83
 - vibrational excitation 50
- adsorbate self-energy energy shift 45
- Ag(111) 12–14
- Al–Al₂O₃–Pb tunneling junction 40
- alkali atom
 - chemisorptions 2
 - ionization of 5
 - valence electron of 2
- n*-alkanedithiol 131
- alkane thiolate junctions, IETS spectra for 41
- alternating bond-length (ABL) 111
- ambient temperature 129
- AND/NOT gates 30
- Arrhenius law, assumption of 55
- Arrhenius-like expression 51
- atomic force microscope (AFM) 130
 - metallic tip of 140
- atomic gold wire 49, 95, 105–107, 114
- atomic manipulation 27
- atomic orbital basis set 92
- atomic oxygen 29
- atomic reconstruction 128
- atomic-scale Joule heating 99
- atomic-scale systems, first-principles
 - transport calculations 97
- atomic switching device, atomic manipulation 27
- atomic wires
 - electron–phonon interaction 49
 - of single gold atoms 97
- Au(111)
 - NaCl ultrathin film grown on 167
 - STM-induced photon emission, from C₆₀ molecules adsorbed 168
- Au–S bonds 126
- Au wire 111, 112
 - left-originating eigenchannel scattering state 111
 - low transmission/reflection 111
- band-bending 171
- benzene/Si(100) HOMO resonance 212
- bias voltage 58
- biphenyl molecules
 - bistable movement of 173
 - chemisorbed adsorption configuration of 177
 - manipulation pulses 172
 - phenyl rings 178
 - on Si(100)-2 × 1 172, 174
 - during STM manipulation 176
 - STM topography of 174, 176
- Bloch state 111
- B3LYP hybrid exchange–correlation functional within Q-Chem 198
- BN nanotubes (BNNT) 15
 - conduction band 20
 - π conjugation 15
- Boltzmann distribution 51, 55
- Bose–Einstein distribution 111, 113, 114
- trans*-2-butene
 - negative ion geometry 214
 - reaction yield per electron 79
 - STM-controlled chemical reaction 78
- C2:C2 configuration
 - side view of 169
- CCD rotation, STM images of 81
- CdSe nanocrystals 178, 181
- CdSe nanorods, adsorption of 181
- C–F bonds 8, 11
- C₆F₆/Cu(111) surface
 - electron potential for 10
 - LT-STM image of 8
 - LUMO resonance of 9
 - NFE behavior 9
- chemical bond, thermal sensitivity of 130
- chemical potential 36, 42, 43
- chemisorption height 6

- chlorobenzene 197, 202, 206
 C–H mode, with IETS 81
 Chulkov potentials 2, 5, 10
 C8 junctions
 stretching distance of 132
 thermodynamic breakdown 132
 CM mode 77
 C₆₀ molecular crystal
 3D band structure of 19
 C₆₀ molecule 117
 hexagon–pentagon bond 115
 C₆₀ molecule quantum wire
 σ and π symmetry bands 18
 C_n stretching distance 134, 135
 C₆₀ nanocrystals, STM image of 167
 CO–Ag stretch mode, vibrational
 excitations 29
 Co atom 58
 coherent ladder climbing
 displaced ion-excited state, potential
 energy curve for 60
 electron scattering 60
 tunneling current 59, 61
 vs. incoherent process 61–63
 CO hopping
 hopping probability 65
 parameters 71
 single-electron process of 64
 CO molecules, STM image of 32
 conductance curves
 external damping 113
 vs. voltages 116
 conductance quantum 133
 conduction band 5, 11, 15, 19, 20
 contact resistance 139–140
 copper surfaces
 C₆₀ molecules 15
 NFE band formation 17
 C–O–Si bonds 169
 C–O stretch mode 69, 73
 anharmonic coupling 71
 energy transfer from 29
 intermode coupling rates of 73
 STM-IETS spectrum of 64
 Co tunneling 58
 Coulomb blockade 105
 Coulomb interaction 2, 4
 Coulomb tail 15
 CO vibrations 66, 160
 C₆₀ quantum wires, NFE states of 3
 C–Si bonds, butterfly configuration 170, 173
 current-carrying electrons 126
 current-induced local heating
 instability 123
 in molecular junctions
 chemical bond breakdown,
 thermodynamic theory of 129–130
 single-molecule junctions, repeated
 creation of 130–131
 thermal effect 128
 molecular junctions *vs.* metallic point
 contacts 127–128
 single-alkanedithiol junctions
 bias and molecular length dependence
 of 134–135
 conductance, bias dependence
 of 133–134
 electron tunneling 131
 thermodynamic dissociation 132–133
 in single-molecule junctions 124
 theory of 125–127
 current-induced vibrational excitation 57
 current–voltage (*I–V*) characteristics 103, 108
 Cu(100) surface
 acetylene, schematic drawing of 64
 NH₃ translation motion of 74
 single acetylene molecule on
 dependencies of 28
 Cu(111) surface
 Co adatom hopping rate 57
 IP-state wave function of 11
 partial C₆₀ molecule monolayer
 topographic image of 17
 1, 4-cyclohexadiene 214–215
 cyclohexene 214, 216
 cyclopentene/Si(100) 3, 90, 91, 174, 176, 198
 desorption of 216
 electron-stimulated desorption of 82
 ionic equilibrium displacements of 209
 STM images of 202–203
 dangling bond 199
 DCM *see* dielectric continuum model (DCM)
 density functional theory (DFT)
 B3LYP method 101
 calculations 73, 74
 Hamiltonian 200
 mean-field potential 96
 NEGF methods 90, 92–96, 100
 scattering states 100
 density of states (DOS) 5, 103, 149
 desorption induced by an electric
 field (DIEF) 204
 desorption induced by electronic transition
 (DIET) 59, 174
 desorption induced by multiple electronic
 transitions (DIMET) 59
 desorption yield *vs.* voltage data 204
 deuterium molecule, single-level model 114
 DFT *see* density functional theory (DFT)
 DFT-NEGF transport method 91
 inelastic transport
 Born approximation 100
 eigenchannel scattering 100
 electron–phonon interactions 101–105
 hydrocarbon molecules 101
 nonequilibrium electron system 99
 DIEF *see* dynamics induced by electric
 field (DIEF)
 dielectric continuum model (DCM) 9, 10

- Diels Alder process 201–202
- DIET *see* desorption induced by electronic transition (DIET)
- dimer stretch coordinate, expectation value 215
- DIMET *see* desorption induced by multiple electronic transitions (DIMET)
- Dirac point 15
- dynamic reaction coordinate (DRC) calculations 200
- dynamics induced by electric field (DIEF) 170
- dynamics induced by electronic transition (DIET) 170
- EHP *see* electron–hole pair (EHP)
- EHP excitations *see* electron–hole pairs (EHP) excitations
- Eigenchannel transmissions 97
- Eigler switch 27, 50
- elastic conductance 47
- elastic scattering process 39
- elastic transport channels
eigenchannels 96–99
- elastic tunneling process 39, 48
- electric transport properties 200
- electromagnetic field 186
laser–STM 185–188
polarization of 178
- electromigration 123–124
- electron affinity 9
- electron attachment 158, 160
CO motion 34
electronic excitation processes 158
STM image of 159
- electron binding energy 7
- electron conduction 108
- electron detachment 160
- electron–electron interaction 125
- electron–electron scattering processes 124
- electron–hole damping constant 112
- electron–hole pair (EHP)
damping rate 73
excitations 31, 38, 43, 45, 62, 66, 68, 71, 72, 112, 207
formation of 157
light adsorption 139
- electronic excitations 112, 157, 172
of adsorbed molecules 169
of atoms and molecules 157
molecular dynamics 157
schematics of 158
with STM 157
- electronic Hamiltonian 101
- electronic molecular states, heat generation 140
- electronic resonant excitation 204
- electronic switches, multistable function 172
- electronic transition 158
- electronic transition mechanism 163, 166
- electronic tunneling matrix elements 37
- electron impact, importance of 158
- electron-induced excitation 140
- electron liquid, hydrodynamic theory of 126
- electron–phonon coupling 127
- electron–phonon interactions 39, 46, 125, 134
Born approximation 101–103
ionic heating 127
lowest-order expansion 103–105
- electron–phonon scattering 79
- electron repulsion 7
- electron scattering 60
- electron transport mechanisms
modeling of 91
molecular wires 98
- electron–vibrational coupling constants 55
- electron–vibration coupling 60, 82
- electron–vibration interaction 78
- electron viscosity 127
- energy barrier 128, 129
- energy conservation 70
- e–ph interaction 102
- escape-rate matrix 94
- ethylene 215
- exchange–correlation 198–199
- excitation–deexcitation cycles 34
- Fano-type asymmetry 59
- Fe(CO) product
formation of 29
single bond formation 29
- Fermi distributions 42, 43
- Fermi energy 49, 94, 97, 111, 151, 186
- Fermi functions 102, 111
- Fermi level (E_F) 4, 47, 53, 55, 70, 94, 149, 168
- Fermi’s golden rule (FGR) 110
scattering rate, LOE rate, comparison 110
- Fermi surface 15
- fluorescence 167, 189
- four-atom gold wire
differential conductance 107, 113
geometry of 106
- free alkali atoms, ionization potential of 7
- free molecules, electronic properties of 2
- frustrated rotation (FR) mode, excitation of 31
- FT mode 58
- Gaussian basis sets 198
- Ge(111)-c(2 × 8) surface
H atoms, desorption of 163
- Ge–H
antibonding orbitals of 162
STM tip 166
- generic system, semi-infinite electrode 92
- geometrically asymmetric systems 104
- Ge surface 161

- hydrogen, desorption of 166
- gold electrode 95, 97, 100, 107, 210
- golden rule 100
- Green's function 43, 48, 93, 102, 109
- GW method 3

- Hamiltonian matrix 93
- Hamiltonian submatrix 210
- Hartree diagram 103
- heat capacity 124
- heat-carrying molecular wire 128
- heat conduction 41, 50
- heat dissipation 140, 147
- HF mode, deexcitation of 76
- highest occupied molecular orbital (HOMO) 3, 168, 211, 213
 - DFT-optimized geometry 210
 - electron affinity level 2
 - energy 8
- high-frequency (HF) mode 68, 69, 76
 - deexcitation of 76
 - intramolecular mode 35, 50
 - tunneling electron 35
 - stretch mode
 - excitation of 65
 - single tunneling electron 33
- Hilbert space 92
- Hilbert transform 104
- hole injection 168
- HOMO *see* highest occupied molecular orbital (HOMO)
- H–Si system 50
- hydrodynamic damping 133
- hydrogenated silicon (Si(100):H) 180, 183, 186
- hydrogen atoms 183
 - desorption of 160, 173
 - STM manipulation of 162
 - with STM tip 164
- hydrogen-bond exchange reaction 58
- hydrogen desorption 165
- hydrogen extraction process 163
- hydrogen phthalocyanine (H₂Pc) molecules 183

- IETS *see* inelastic electron tunneling spectroscopy (IETS)
- image charge 4–8
- image potential (IP) 4
 - atomic units 2, 4
 - wave functions 11
- incoherent process 62
- inelastic current 45, 46
- inelastic electron transfers, schematic representation of 53
- inelastic electron tunneling (IET) spectra 28, 41
 - via* adsorbate-induced resonance 37
- inelastic electron tunneling spectroscopy (IETS) 28, 48, 79, 81, 124
 - on alkanedithiol self-assembled monolayers (SAM) 100
 - bond-breaking 31
 - propensity rules 108–111
 - signal 72, 107
 - of single adsorbed atoms 26
 - vibrational spectroscopy 28
- inelastic fraction 46
- inelastic phonon-assisted scattering 41
- inelastic scattering
 - peaks 108
 - processes 38
- inelastic transport
 - in atomic-scale device 42
 - with DFT-NEGF 99–101
 - NEGF-SCBA scheme for 102
- inelastic tunneling 36, 57, 67
 - conductance 38
 - fraction 45
 - process 53, 99
- inelastic tunneling current-driven motions
 - of single adsorbates 35
 - action spectroscopy 78–83
 - anharmonic mode coupling 63
 - coherent ladder climbing 59–63
 - real-space observation 83
 - STM-IETS, theory of 35
 - vibrational excitation, with STM 50–59
- inelastic tunneling rate
 - absolute value of 54
 - vibrational excitation 38
- intrinsic quantum tunneling 58
- ion-excited state, potential energy curve 60
- ionization potential 2

- Joule heating 123

- Keldysh NEGF method 41
 - electron tunneling, nonequilibrium process of 42
 - for IETS 42
- Knudsen cell 124
- Kohn–Sham eigenfunctions 3
- Kondo effect, single-atom visualization of 156

- ladder-climbing process 57
 - harmonic potential 51
- Landauer–Büttiker form 96–97, 104
- laser-induced thermal desorption (LITD) 186
- laser irradiation 188
- laser–STM experiment 185
- LDOS *see* local density of states (LDOS)
- LEED *see* low-energy electron diffraction (LEED)
- lesser Green's function 94, 102
- LITD *see* laser-induced thermal desorption (LITD)
- local density of states (LDOS) 12, 160

- Lorentzian function 40
- Löwdin population analysis (LPA) 200
- low-energy electron diffraction (LEED) 6
- lowest-order expansion (LOE) 103
 - approximation 105, 108
 - on molecular junctions 107
 - expression 104
- lowest unoccupied molecular orbital (LUMO)
 - 2, 168, 211
 - IP-state hybridization 11
 - resonances 8, 11, 153
- low-temperature scanning tunneling microscopy (LT-STM) 3
- LPA *see* Löwdin population analysis (LPA)
- LT-STM *see* low-temperature scanning tunneling microscopy (LT-STM)
- LUMO *see* lowest unoccupied molecular orbital (LUMO)

- mean-field approximation 101
- mean free path 124
- mesoscopic quantum transport 97
- metal–molecule interfaces, electronic structure of 4
- metal–organic interface
 - hybrid NFE band formation
 - C_{60} quantum well state 8–11
 - PTCDA 12–14
 - NFE behavior 14
- metal surfaces
 - image charge interaction 4–8
 - vibrational mode 33
- microscopic mechanism 32
- molecular-overlayer-covered metal surface
 - electronic structure of 9
- molecular-scale electronic devices 123
- molecular temperature, applied
 - bias 152–153
- molecular vibration decay, mechanisms of 149
- Mott–Schottky theory
 - for band alignment
 - semiconductor interfaces 1
- multiple-electron process 31

- NaCl layer
 - STM-induced photon emission, from C_{60} molecules adsorbed 168
- nanoscale conductor, inelastic processes 97
- nanoscale transport systems 91
- nano-surface chemistry 30
- natural population analysis (NPA) 200
- near edge X-ray absorption fine structure (NEXAFS) 12, 169
- nearly-free-electron (NFE) bands 3
 - binding energy 10
 - dispersions of 8
 - effective mass 14
 - metal-like band formation 19
 - 2PP intensity 13
 - probability density 10
- NEB method *see* nudge elastic band (NEB) method
- NEGF *see* nonequilibrium Green’s function (NEGF)
- NEXAFS *see* near edge X-ray absorption fine structure (NEXAFS)
- NH_3 molecules, STM images of 74, 75
- N–H stretch mode 73, 74, 77
- Ni(111) 156
- noble metals 6, 14
- nonequilibrium Green’s function (NEGF)
 - 41, 90, 91, 92, 101, 152, 200
 - DFT approach 211
 - DFT transport calculations 210
 - SCBA expression 103
 - transport calculations 201
- NPA *see* natural population analysis (NPA)
- nuclear wave packet
 - snapshots of 214
- nudge elastic band (NEB) method 175

- O_2 bond-breaking, mechanism of
 - by tunneling electrons 31
- octanedithiol 140
- O/Cu(110) surface
 - nine C_{60} molecule chain
 - topographic image of 17
 - single C_{60} molecule
 - dI/dV images of 16
- oligo-phenylene ethynylene (OPE) molecule
 - 97, 98, 110
 - eigenchannel scattering states for 100
 - IETS spectra 109
- oligo-phenylene vinylene (OPV) molecule
 - 98
 - IETS spectra 109
 - left eigenchannel scattering state 99
- O_2 molecules
 - dissociation rate of 30
 - fcc sites, STM image of 30
- O–O stretch mode 61
 - lineshape analysis of 31
 - single excitation of 32
- OPV molecule *see* oligo-phenylene vinylene (OPV) molecule

- Pauli exclusion 6
- Pauli master equation 51
- Pb(111) 142–143, 149, 151
- Pd(110)
 - CO, C–O stretch mode of 63
 - CO hopping 32, 71, 74
- PDOS *see* projected density of states (PDOS)
- perturbation theory 70
- 3,4,9,10-perylene-tetracarboxylic-dianhydride (PCDTA) 3
- PES *see* potential energy surface (PES)
- phonon
 - distribution function 44, 45, 47

- elastic scattering of 125
- energy transfer 84
 - LOE equation for 110
- excitations 51, 66
 - frequency 63
 - power dissipation 111
- phonon bands, in Pt electrodes 114
- phonon emission 38, 39, 102
 - phase diagram 50
- phosphonate capped CdSe nanorod STM
 - topography of 182
- photoelectron emission 188
- photon
 - adsorption 186
 - emission 168
- photovoltage 188
- pico-SPM 130
- piezoelectric transducer 130–131
- Planck's constant 133
- polyacenes 11, 12, 14
- polyatomic processes 207
- potential energy surface (PES) 60
 - for neutral and positively charged 213
 - vibrational system 206
- power law
 - atom transfer rate 27
 - dependence of 50
 - simulation of 57
- power spectrum 146, 152
- 2PP measurements *see* two-photon
 - photoemission (2PP) measurements
- π - π^* transition
 - electronic excitation of 169
- projected density of states (PDOS) 211
 - ab initio* calculation of 82
- propene
 - negative ion equilibrium geometries
 - of 216
 - positive ion 214
- PTCDA/Ag(111) interface 13
 - covalent bonding 12
 - NFE behavior 13
 - NFE character of 14
 - 2PP spectra 13
 - topographic STM image of 13
- PTCDA films, π - π stacking of 12
- pulsed valve technique 181

- quantum defect 4
- quantum dynamics 200
- quantum wells 3
- quantum wire 3, 15, 18
- quasi-Boltzmann distribution 61
- quasiparticle 3
- quasi-stationary distribution, Boltzmann
 - distribution 51

- reaction coordinate (RC) mode 26, 50, 66,
 - 68, 73, 76
 - direct excitation of 62
 - O–O stretch mode 34
 - for rotational motion 73
 - tunneling electrons 34
- resonance lifetime 200, 206, 211–212
- right-hand color STM topography 180
- Rydberg-like IP states 4
- Rydberg series 15

- SAMOs *see* superatom molecular orbitals (SAMOs)
- scanning tunneling
 - microscopy/spectroscopy (STM/STS) 8,
 - 26, 92, 130, 156, 196
 - break-junction approach 133
 - break-junction measurement
 - schematic illustration of 131
 - current–distance characteristics 140
 - driven surface desorption reaction 199
 - IETS, theory of
 - adsorbate-induced resonance model
 - of 35–41
 - elastic/inelastic current 45–50
 - Keldysh NEGF theories of 78
 - nonequilibrium Green's function (NEGF)
 - method 41–45
 - IETS spectra 63
 - imaging 63
 - induced desorption process 206
 - single-molecule manipulation 30
 - tip junction
 - electromagnetic field 186
 - topographic imaging 28, 29
 - topography, molecular models 180
 - tunneling process, energy diagram of 36
 - tunnel junction 201
 - ultrahigh vacuum (UHV) 198
- Schrödinger equation 15
- second-harmonic generation (SHG) 186
- self-assembled monolayers (SAM) 100
- self-consistent Born approximation (SCBA)
 - 101–103
- semiconductor electronics technology 91
- semiconductor surfaces
 - hydrogen passivates 178
 - single adsorbates on 57
- seven-atom Au atomic chain
 - eigenchannel scattering state 98
- SHG *see* second-harmonic generation (SHG)
- shockley surface (SS) state 12
- Si–C bonds
 - cleavage process 82
 - electronic states of 170, 212
- SiC(0001) 3 × 3 reconstruction
 - local modification of 185
- Si–H bonds 163, 165, 186
 - antibonding orbitals of 162
 - σ - σ^* electronic transition of 166
- Si₆H₁₂ cluster
 - cyclohexene, equilibrium geometries
 - of 216

- Si(100):H surface
 alkene molecules 201
 cyclopentene molecule 202
 hydrogen atoms
 STM desorption of 182
 isolated cyclopentene molecule, schematic of 199
 pentacene molecule, STM topographies of 181
 STM topographic image of 198
 submonolayer coverage of 198
 silicon dangling bonds 161, 164
 silicon dimer, central role of 208
 silicon–organic hybrid systems 197
 silicon surfaces
 hydrogen atoms, desorption of 186
 molecular dynamics on 179
 STM images 169
 simple two-dimensional potential wells, schematics of 34
 single C_{60} molecular junctions 139, 141
 on Au(111) 142, 143
 Cu(100), degradation spectrum 148
 current-driven thermal process 145
 current *vs.* tip approach plots 145
 degradation spectrum 148, 150, 152
 differential conductance spectra of 143
 heat dissipation
 mechanism of 149–152
 molecular vibration decay, mechanisms of 149
 STM tip 148
 heat generation 152–153
 large-scale STM images 142
 logarithmic current–distance 144
 LUMO-derived resonance
 dI/dV spectra 151
 STM image of 147
 STS spectrum 146
 submonolayer amount 141
 submonolayer coverage of 142
 single-electron process 31
 by coherent multiple-step jumps 62
 desorption mechanism 197
 schematic illustration of 67
 via anharmonic mode coupling
 CO, hopping probability 65
 CO, IETS spectrum 66
 CO hopping 71, 74
 C–O stretch mode 72, 73
 Cu(100) surface, NH_3 molecule 64
 EHP excitations 68, 70
 HF mode, Hamiltonian of 69
 NH_3 hopping 72
 STM–IETS spectra 63
 two-electron processes 74–77
 single-electron resonance process
 cyclopentene, desorption of 205
 single-molecule imaging 28
 single-molecule junction
 current-carrying electrons 125
 heat capacity of 124
 repeated creation of 130–131
 single-molecule motions 83
 single-molecule nanomachines, electronic control of
 electronic excitation
 electron attachment 157–166
 electron–hole pair attachment 166–168
 electronic transition 166
 molecules manipulation 168–172
 biphenyl, on Si(100) 172–176
 laser–STM 185–188
 passivated/insulating surfaces 179–184
 on wide-band-gap semiconductors 183–184
 single-molecule-wide C_{60} quantum wires
 NFE bands for 15
 and quantum wells 3
 Si(100) surface 169
 benzene, butterfly configuration of 208
 benzene desorption 207
 biphenyl molecule
 chemisorbed adsorption configuration of 172, 177
 cyclopentene desorption, current-driven dynamics of 196
 Si(100) surface, cyclopentene desorption process 196–212
 Si(100)-(2 × 1) surface 169
 biphenyl molecules adsorbed on 171
 cyclopentene desorption yield 83
 STM topography 180
 Trima molecule on 169
 Si(100)(2 × 1):H surface
 hydrogen, laser desorption of 187
 STM topography of 164
 Si(111)-7 × 7 surface
 STM image of 159
 source–drain bias 146
 step-by-step ladder-climbing process 31
 STM/STS *see* scanning tunneling microscopy/spectroscopy (STM/STS)
 superatom molecular orbitals (SAMOs) 16
 derived bands, NFE properties of 18
 energy 20
 hybridization 17, 18
 quantum structures, LDOS images of 18
 superatom states
 metal-like hybridization of
 BN nanotubes 15
 C60, superatom states of 16–17
 Dirac point 15
 intermolecular charge transport properties 14
 NFE band formation 17–20
 surface chemical reactions
 adsorbate motions 83
 microscopic mechanisms of 27, 83
 surface Diels–Alder process 201

- surface potential
 - adsorption-induced change 4
 - modification of 181
- synchrotron radiation 158
- tadpole diagram *see* Hartree diagram
- p*-terphenyl-4,4'-diacetyl ketone, adsorption
 - and manipulation of 168
- thermal conductivity 127
- thermal cooling 127
- thermal energy 128
- thermal fluctuations 129
- thermodynamic dissociation, stretching
 - distance 133
- thermodynamic theory 133
- time-of-flight (TOF) measurements 186
- time-resolved twophoton photoemission (TR-2PP) 8
- trima molecule
 - adsorption of 184
 - STM study of 169
- TR-2PP *see* time-resolved twophoton photoemission (TR-2PP)
- tunnel current
 - negative bias pulse 176
 - during negative bias pulse 175
- tunneling barrier 98
- tunneling conductance 39, 40
- tunneling current 60, 61, 73
 - atom transfer rate
 - power-law dependence of 27
 - desorption rate 205
 - desorption yield 164
 - induced motions, physical mechanisms
 - of 33
 - inelastic component of 80
- tunneling electrons 27, 32, 70
 - decays 71
- two-level fluctuation (TLF) 115, 128
- two-photon photoemission (2PP)
 - measurements 2
- UHV *see* ultra high vacuum (UHV)
- ultra high vacuum (UHV) 141
- umbrella mode
 - multiple excitation of 65
- vacuum ultraviolet (VUV)
 - irradiation 188
 - light 188
- van der Waals distance 18
- van der Waals interaction 181
- vibrational distribution function 47, 48
- vibrational energy 147
- vibrational energy absorption 149
- vibrational energy shift 43
- vibrational energy transfer 72
- vibrational excitation, with STM
 - adsorbate motions
 - Γ_{ist} , physical meaning of 52–55
 - inelastic tunneling current, numerical calculations of 55–59
 - vibrational ladder climbing—vibrational heating 50–52
- vibrational generating rate, temperature dependence of 56
- vibrational heating
 - inelastic tunneling electrons 50
 - Si–H bond 163
- vibrational ladder
 - adatom–substrate bond excitations 28
 - quasi-Boltzmann distribution 51
 - tunneling current 31
- vibrational linewidths 55
- vibrationally assisted tunneling model 57
- vibrations
 - current, heating of 111–117
 - types of 107
- vibronic coupling 206–207, 212
- voltage dependence
 - I*–*V* 103
 - thermal effect 55, 56
- voltage drop 95
- VUV irradiation *see* vacuum ultraviolet (VUV) irradiation
- wave packet propagation (WPP) method 6, 8
- WPP method *see* wave packet propagation (WPP) method
- Xe atom bound 27
- xenon atoms
 - on nickel surface 27