Peter Saalfrank

List of Publications by Year
in descending order

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231 papers	7,793 citations	50170 46 h-index	76769 74 g-index
239 all docs	239 docs citations	239 times ranked	6329 citing authors

#	Article	IF	Citations
1	Aggregation in a High-Mobility n-Type Low-Bandgap Copolymer with Implications on Semicrystalline Morphology. Journal of the American Chemical Society, 2012, 134, 18303-18317.	6.6	395
2	orthoâ€Fluoroazobenzenes: Visible Light Switches with Very Longâ€Lived Z Isomers. Chemistry - A European Journal, 2014, 20, 16492-16501.	1.7	311
3	Quantum Chemical Investigation of Thermal Cis-to-Trans Isomerization of Azobenzene Derivatives: Substituent Effects, Solvent Effects, and Comparison to Experimental Data. Journal of Physical Chemistry A, 2009, 113, 6763-6773.	1.1	217
4	The multiconfiguration time-dependent Hartreeâ€“Fock method for quantum chemical calculations. Journal of Chemical Physics, 2005, 122, 124102.	1.2	196
5	Protonated Imineâ€Linked Covalent Organic Frameworks for Photocatalytic Hydrogen Evolution. Angewandte Chemie - International Edition, 2021, 60, 19797-19803.	7.2	171
6	Theory of photoinduced surface reactions of admolecules. Progress in Surface Science, 1999, 62, 239-303.	3.8	168
7	Time-dependent configuration-interaction calculations of laser-pulse-driven many-electron dynamics: Controlled dipole switching in lithium cyanide. Journal of Chemical Physics, 2005, 123, 074105.	1.2	163
8	Adsorption and photocatalytic splitting of water on graphitic carbon nitride: a combined first principles and semiempirical study. Physical Chemistry Chemical Physics, 2014, 16, 15917-15926.	1.3	151
9	Quantum Dynamical Approach to Ultrafast Molecular Desorption from Surfaces. Chemical Reviews, 2006, 106, 4116-4159.	23.0	145
10	Quantum Chemical Calculation of Excited States of Flavin-Related Molecules. Journal of Physical Chemistry A, 2003, 107, 140-147.	1.1	140
11	Quantum dynamics of bond breaking in a dissipative environment: Indirect and direct photodesorption of neutrals from metals. Journal of Chemical Physics, 1996, 105, 2441-2455.	1.2	118
12	Electrocatalytic Z â† E Isomerization of Azobenzenes. Journal of the American Chemical Society, 2017, 139, 335-341.	6.6	108
13	Molecular response properties from explicitly time-dependent configuration interaction methods. Journal of Chemical Physics, 2007, 127, 034107.	1.2	98
14	Femtosecond Stimulated Raman Spectroscopy of Flavin after Optical Excitation. Journal of Physical Chemistry B, 2011, 115, 3656-3680.	1.2	95
15	Density matrix description of laser-induced hot electron mediated photodesorption of NO from Pt(111). Chemical Physics Letters, 1994, 230, 463-472.	1.2	89
16	Surface oscillator models for dissociative sticking of molecular hydrogen at non-rigid surfaces. Surface Science, 1997, 373, 95-108.	0.8	82
17	Luminescence Detection of Open-Shell Transition-Metal Ions by Photoinduced Electron Transfer Controlled by Internal Charge Transfer of a Receptor. Angewandte Chemie - International Edition, 2007, 46, 1671-1674.	7.2	82
18	(TD-)DFT Calculation of Vibrational and Vibronic Spectra of Riboflavin in Solution. Journal of Physical Chemistry B, 2010, 114, 10826-10834.	1.2	82

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19	Microscopic Model of the Optical Absorption of Carbon Nanotubes Functionalized with Molecular Spiropyran Photoswitches. Physical Review Letters, 2011, 106, 097401.	2.9	81
20	On the Electronic Structure of Neutral and Ionic Azobenzenes and Their Possible Role as Surface Mounted Molecular Switches. Journal of Physical Chemistry B, 2006, 110, 16337-16345.	1.2	80
21	Stochastic wave packet vs. direct density matrix solution of Liouville-von Neumann equations for photodesorption problems. Chemical Physics, 1996, 211, 265-276.	0.9	77
22	Electronic Decoupling Approach to Quantitative Photoswitching in Linear Multiazobenzene Architectures. Journal of Physical Chemistry B, 2011, 115, 9930-9940.	1.2	77
23	Inducing the Rotation of a Single Phenyl Ring with Tunneling Electrons. Journal of Physical Chemistry C, 2007, 111, 14843-14848.	1.5	72
24	Laser-induced electron dynamics including photoionization: A heuristic model within time-dependent configuration interaction theory. Journal of Chemical Physics, 2009, 131, 114304.	1.2	72
25	C K-edge NEXAFS spectra of graphene with physical and chemical defects: a study based on density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14083-14095.	1.3	70
26	Time-dependent approach to electronically excited states of molecules with the multiconfiguration time-dependent Hartree-Fock method. Journal of Chemical Physics, 2007, 126, 214106.	1.2	67
27	Role of electronic friction during the scattering of vibrationally excited nitric oxide molecules from Au(111). Physical Review B, 2010, 82, .	1.1	67
28	Faber and Newton polynomial integrators for open-system density matrix propagation. Journal of Chemical Physics, 1999, 110, 5538-5547.	1.2	64
29	Dissipative dynamics within the electronic friction approach: the femtosecond laser desorption of H2/D2 from Ru(0001). Physical Chemistry Chemical Physics, 2011, 13, 8659.	1.3	63
30	Open-system density-matrix approach to image-potential dynamics of electrons at Cu(100):â€ƒEnergy- and time-resolved two-photon photoemission spectra. Physical Review B, 2001, 64, .	1.1	61
31	Ab Initio Quantum Chemical Investigation of the First Steps of the Photocycle of Phototropin: A Model StudyÂ¶. Photochemistry and Photobiology, 2003, 77, 101.	1.3	60
32	Water adsorption at metal surfaces: A first-principles study of thep(3Ã—3)R30Â°H2Obilayer on Ru(0001). Physical Review B, 2005, 71, .	1.1	60
33	Photodesorption of neutrals from metal surfaces: a wave packet study. Chemical Physics, 1995, 193, 119-139.	0.9	59
34	Atomic-scale chemistry: Desorption of ammonia from Cu(111) induced by tunneling electrons. Chemical Physics Letters, 1999, 313, 544-552.	1.2	57
35	Theoretical study of vibration-phonon coupling of H adsorbed on a Si(100) surface. Journal of Chemical Physics, 2006, 124, 034710.	1.2	57
36	Hole Catalysis as a General Mechanism for Efficient and Wavelength-Independent Z â†' E Azobenzene Isomerization. CheM, 2018, 4, 1740-1755.	5.8	57

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37	Theory of laserâ€induced desorption of ammonia from Cu(111): Stateâ€resolved dynamics, isotope effects, and selective surface photochemistry. Journal of Chemical Physics, 1995, 103, 6720-6734.	1.2	56
38	Time-dependent configuration-interaction calculations of laser-driven dynamics in presence of dissipation. Journal of Chemical Physics, 2008, 129, 084302.	1.2	54
39	A local coherent-state approximation to system-bath quantum dynamics. Journal of Chemical Physics, 2006, 125, 194102.	1.2	52
40	Switching with orthogonal stimuli: electrochemical ring-closure and photochemical ring-opening of bis(thiazolyl)maleimides. Chemical Science, 2013, 4, 1028-1040.	3.7	52
41	Thermal Cis-to-Trans Isomerization of Azobenzene-Containing Molecules Enhanced by Gold Nanoparticles: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2015, 119, 17369-17377.	1.5	52
42	Optically probing Alâ€"O and Oâ€"H vibrations to characterize water adsorption and surface reconstruction on Î±-alumina: An experimental and theoretical study. Journal of Chemical Physics, 2015, 142, 054704.	1.2	52
43	Electronic structure of the molecular switch tetra-tert-butyl-azobenzene adsorbed on Ag(111). Applied Physics A: Materials Science and Processing, 2007, 88, 465-472.	1.1	50
44	cisâ€“trans Isomerisation of Substituted Aromatic Imines: A Comparative Experimental and Theoretical Study. ChemPhysChem, 2011, 12, 2311-2321.	1.0	50
45	Vibrationally excited products after the photodesorption of NO from Pt(111): a two-mode open-system density matrix approach. Chemical Physics Letters, 1997, 268, 291-299.	1.2	48
46	Computation of high-harmonic generation spectra of the hydrogen molecule using time-dependent configuration-interaction. Molecular Physics, 2016, 114, 947-956.	0.8	47
47	Photoisomerization Ability of Molecular Switches Adsorbed on Au(111): Comparison between Azobenzene and Stilbene Derivatives. Journal of Physical Chemistry C, 2010, 114, 1231-1239.	1.5	46
48	Electronic structure of a subnanometer wide bottom-up fabricated graphene nanoribbon: End states, band gap, and dispersion. Physical Review B, 2012, 86, .	1.1	46
49	Nonlinear optical response of photochromic azobenzene-functionalized self-assembled monolayers. Physical Chemistry Chemical Physics, 2015, 17, 18079-18086.	1.3	44
50	Quantum size effects in metal films:â€ƒEnergies and charge densities of Pb(111) grown on Cu(111). Physical Review B, 2001, 63, .	1.1	43
51	Optimal control in a dissipative system: Vibrational excitation of COâˆ•Cu(100) by IR pulses. Journal of Chemical Physics, 2006, 124, 234706.	1.2	43
52	Exciting flavins: Absorption spectra and spinâ€“orbit coupling in lightâ€“oxygenâ€“voltage (LOV) domains. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 290-300.	2.0	43
53	Reversible Photoswitching of the Interfacial Nonlinear Optical Response. Journal of Physical Chemistry Letters, 2015, 6, 505-509.	2.1	42
54	Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects. Journal of Physical Chemistry Letters, 2016, 7, 3591-3596.	2.1	42

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55	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). Physical Review B, 2016, 93, .	1.1	42
56	Vibrational lifetimes of hydrogen on lead films: An ab initio molecular dynamics with electronic friction (AIMDEF) study. Journal of Chemical Physics, 2014, 141, 234702.	1.2	40
57	Hydrogen transfer in vibrationally relaxing benzoic acid dimers: Timeâ€dependent density matrix dynamics and infrared spectra. Journal of Chemical Physics, 1996, 104, 2869-2882.	1.2	37
58	STM-Induced Desorption of Hydrogen from a Silicon Surface:Â An Open-System Density Matrix Study. Journal of Physical Chemistry B, 1998, 102, 8029-8035.	1.2	37
59	Electronic damping of anharmonic adsorbate vibrations at metallic surfaces. Physical Review B, 2010, 81, .	1.1	37
60	On the electronic and geometrical structure of the trans- and cis-isomer of tetra-tert-butyl-azobenzene on Au(111). Physical Chemistry Chemical Physics, 2010, 12, 4488.	1.3	37
61	Quantum dynamical aspects of rotationally and vibrationally mediated photochemistry in matrices and at surfaces HCl/DCl in Ar and NH3/ND3 at Cu(111). Journal of the Chemical Society, Faraday Transactions, 1997, 93, 957-967.	1.7	36
62	Experimental Characterization of Unimolecular Water Dissociative Adsorption on Î±-Alumina. Journal of Physical Chemistry C, 2014, 118, 13623-13630.	1.5	34
63	Resonance Raman and vibronic absorption spectra with Duschinsky rotation from a time-dependent perspective: Application to Î²-carotene. Journal of Chemical Physics, 2012, 137, 22A534.	1.2	33
64	On the Role of Electronic Friction for Dissociative Adsorption and Scattering of Hydrogen Molecules at a Ru(0001) Surface. Journal of Physical Chemistry A, 2013, 117, 8761-8769.	1.1	33
65	Cis-to-Trans Isomerization of Azobenzene Derivatives Studied with Transition Path Sampling and Quantum Mechanical/Molecular Mechanical Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 2042-2051.	2.3	33
66	Timeâ€independent quantum dynamics for diatomâ€“surface scattering. Journal of Chemical Physics, 1993, 98, 9040-9052.	1.2	32
67	The Photoinduced E â†' Z Isomerization of Bisazobenzenes: A Surface Hopping Molecular Dynamics Study. Journal of Physical Chemistry A, 2015, 119, 5026-5037.	1.1	31
68	Ground state properties and infrared spectra of anharmonic vibrational polaritons of small molecules in cavities. Journal of Chemical Physics, 2021, 154, 104311.	1.2	31
69	Controlled surface photochemistry: Bond- and isotope-selective photodesorption of neutrals by adsorbate vibrational preparation with infrared laser pulses. Journal of Chemical Physics, 1997, 107, 10723-10735.	1.2	30
70	Femtosecond-Laser Desorption of H₂ (D₂) from Ru(0001): Quantum and Classical Approaches. Journal of Physical Chemistry C, 2009, 113, 7790-7801.	1.5	30
71	Current versus Temperature-Induced Switching in a Single-Molecule Tunnel Junction: 1,5 Cyclooctadiene on Si(001). Nano Letters, 2009, 9, 2996-3000.	4.5	30
72	Systematic Investigation of Photoinduced Electron Transfer Controlled by Internal Charge Transfer and Its Consequences for Selective PdCl₂ Coordination. Chemistry - A European Journal, 2010, 16, 1819-1825.	1.7	30

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73	Dissipative many-electron dynamics of ionizing systems. Journal of Chemical Physics, 2011, 134, 044311.	1.2	30
74	Diarylethene Molecules on a Ag(111) Surface: Stability and Electron-Induced Switching. Journal of Physical Chemistry C, 2015, 119, 4874-4883.	1.5	30
75	Nonadiabatic Effects in the Photodissociation and Electronic Spectroscopy of HMn(CO)3(dab):Â Quantum Wave Packet Dynamics Based onab InitioPotentials. The Journal of Physical Chemistry, 1996, 100, 3368-3376.	2.9	29
76	Photon-assisted tunneling versus tunneling of excited electrons in metal?insulator?metal junctions. Applied Physics A: Materials Science and Processing, 2004, 78, 189-199.	1.1	29
77	Monotonically convergent algorithms for solving quantum optimal control problems described by an integrodifferential equation of motion. Physical Review A, 2007, 75, .	1.0	29
78	A new analytical potential energy surface for the adsorption system CO/Cu(100). Journal of Chemical Physics, 2010, 132, 074108.	1.2	29
79	Combination of a CT modulated PET and an intramolecular excimer formation to quantify PdCl2 by large fluorescence enhancement. Chemical Communications, 2010, 46, 2034.	2.2	29
80	Optical absorption and excitonic coupling in azobenzenes forming self-assembled monolayers: a study based on density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 21608.	1.3	29
81	Photodesorption of NO from a metal surface: quantum dynamical implications of a two-mode model. Chemical Physics, 2000, 251, 51-69.	0.9	28
82	Selective excitation of coupled CO vibrations on a dissipative Cu(100) surface by shaped infrared laser pulses. Journal of Chemical Physics, 2008, 128, 194709.	1.2	28
83	Femtosecond-laser induced dynamics of CO on Ru(0001): Deep insights from a hot-electron friction model including surface motion. Physical Review B, 2016, 94, .	1.1	28
84	Two-Dimensional Nonlinear Optical Switching Materials: Molecular Engineering toward High Nonlinear Optical Contrasts. Journal of Physical Chemistry C, 2018, 122, 25555-25564.	1.5	28
85	Quantum size effects in thin lead films. Surface Science, 1992, 274, 449-456.	0.8	27
86	Open-system quantum dynamics for laser-induced DIET and DIMET. Surface Science, 1997, 390, 1-10.	0.8	27
87	Selective subsurface absorption of hydrogen in palladium using laser distillation. Journal of Chemical Physics, 2009, 131, 084716.	1.2	26
88	Stochastic approach to laser-induced ultrafast dynamics: the desorption of H2/D2 from Ru(0001). Physical Chemistry Chemical Physics, 2010, 12, 14082.	1.3	26
89	The Chemistry of Water on Î±-Alumina: Kinetics and Nuclear Quantum Effects from First Principles. Journal of Physical Chemistry C, 2012, 116, 26829-26840.	1.5	26
90	Vibrationally resolved absorption, emission and resonance Raman spectra of diamondoids: a study based on time-dependent correlation functions. Physical Chemistry Chemical Physics, 2014, 16, 144-158.	1.3	26

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91	Femtosecond laser induced desorption of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>,</mml:mo><mml:msub><mml:mi mathvariant="normal">D</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> , and HD from Ru(0001): Dynamical promotion and suppression studied with ab initio molecular dynamics with electronic friction. Physical Review B, 2017, 95, .	1.1	26
92	Isotope and Quantum Effects in Vibrational State Distributions of Photodesorbed Ammonia. Physical Review Letters, 1997, 78, 1174-1177.	2.9	25
93	Electron transport through molecules treated by LCAO-MO Greenâ€™s functions with absorbing boundaries. Chemical Physics Letters, 2004, 386, 17-24.	1.2	25
94	Guided locally optimal control of quantum dynamics in dissipative environments. Physical Review A, 2008, 78, .	1.0	25
95	Long-range intermolecular charge transfer induced by laser pulses: an explicitly time-dependent configuration interaction approach. Physical Chemistry Chemical Physics, 2009, 11, 3875.	1.3	25
96	Energetics and gap engineering in alternating layer and intralayer substituted boron-nitrogen-carbon compounds. Synthetic Metals, 1992, 52, 1-19.	2.1	24
97	The dissociation of diatomic molecules on vibrating surfaces: A semiclassical generalized Langevin approach. Journal of Chemical Physics, 1998, 108, 4226-4236.	1.2	24
98	The coupled channel density matrix method for open quantum systems: Formulation and application to the vibrational relaxation of molecules scattering from nonrigid surfaces. Journal of Chemical Physics, 1998, 108, 3045-3056.	1.2	24
99	Open-system density matrix description of femtosecond laser desorption of electronically and vibrationally relaxing adsorbates: Single- and two-pulse scenarios. Journal of Chemical Physics, 2002, 116, 7189-7199.	1.2	24
100	Density matrix model for hydrogen transfer in the benzoic acid dimer. Chemical Physics Letters, 1995, 245, 201-208.	1.2	23
101	Dissipation in anharmonic molecular systems: beyond the linear coupling limit. Chemical Physics, 2001, 268, 65-78.	0.9	23
102	Serine in BLUF domains displays spectral importance in computational models. Journal of Photochemistry and Photobiology B: Biology, 2009, 94, 87-95.	1.7	23
103	Excitation, relaxation, and quantum diffusion of CO on copper. Physical Review B, 2012, 86, .	1.1	23
104	Vibrational spectroscopy of hydroxylated Î±-Al2O3(0001) surfaces with and without water: An ab initio molecular dynamics study. Journal of Chemical Physics, 2018, 149, 014707.	1.2	23
105	Classical and quantum-mechanical modeling of the stimulated desorption of ammonia from Cu(111). Surface Science, 1996, 363, 179-184.	0.8	22
106	A new pump & dump strategy to control chemical reactivity at surfaces: application to photoisomerization of adsorbates. Chemical Physics Letters, 1999, 301, 509-516.	1.2	22
107	Open-system quantum dynamics for gas-surface scattering: Nonlinear dissipation and mapped Fourier grid methods. Journal of Chemical Physics, 2000, 113, 8753-8761.	1.2	22
108	Manipulation of adsorbates with electric fields. Journal of Chemical Physics, 2000, 113, 3780-3791.	1.2	21

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109	STM and laser-driven atom switch: â€,An open-system density-matrix study of H/Si(100). Physical Review B, 2003, 67, .	1.1	21
110	Time-dependent response of dissipative electron systems. Physical Review A, 2010, 81, .	1.0	21
111	Non-adiabatic excited state dynamics of riboflavin after photoexcitation. Physical Chemistry Chemical Physics, 2012, 14, 8693.	1.3	21
112	Vibrationally resolved optical spectra of modified diamondoids obtained from time-dependent correlation function methods. Physical Chemistry Chemical Physics, 2015, 17, 19656-19669.	1.3	21
113	An efficient first principles method for molecular pump-probe NEXAFS spectra: Application to thymine and azobenzene. Journal of Chemical Physics, 2018, 149, 144112.	1.2	21
114	Discriminating organic isomers by high harmonic generation: A time-dependent configuration interaction singles study. Journal of Chemical Physics, 2019, 150, 234114.	1.2	21
115	From laser control of vibrationally mediated photodissociation to photodesorption: Model simulations of breaking metal-ligand bonds in organometallic molecules, clusters, and adsorbates at surfaces. International Journal of Quantum Chemistry, 1996, 57, 595-609.	1.0	20
116	A tight-binding Green's function approach to adsorbate electronic ground and excited states and their lifetimes. Surface Science, 1998, 410, 21-38.	0.8	20
117	Vibrational relaxation rates for H on a Si(100):(2Ã—1) surface: a two-dimensional model. Chemical Physics Letters, 2001, 350, 191-197.	1.2	20
118	Infrared-laser driven vibrational excitation of relaxing adsorbates: Quantum dynamical aspects. Journal of Chemical Physics, 1999, 110, 6500-6510.	1.2	19
119	Vibrationally enhanced associative photodesorption of molecular hydrogen from Ru(0001). Chemical Physics, 2007, 338, 299-311.	0.9	19
120	Electronic structure changes during the surface-assisted formation of a graphene nanoribbon. Journal of Chemical Physics, 2014, 140, 024701.	1.2	19
121	Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. Journal of Physics Condensed Matter, 2017, 29, 314002.	0.7	19
122	Many-electron dynamics in laser-driven molecules: wavefunction theory vs. density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 13544-13560.	1.3	19
123	A Dual pHâ€•and Lightâ€Responsive Spiropyranâ€Based Surfactant: Investigations on Its Switching Behavior and Remote Control over Emulsion Stability. Angewandte Chemie - International Edition, 2022, 61, .	7.2	19
124	Cavity-altered thermal isomerization rates and dynamical resonant localization in vibro-polaritonic chemistry. Journal of Chemical Physics, 2022, 156, 154305.	1.2	19
125	Dissociative sticking of diatomic molecules on cold, non-rigid surfaces: comparison of quantal and semiclassical surface oscillator models. Surface Science, 1998, 409, 37-45.	0.8	18
126	Direct and indirect DIET and DIMET from semiconductor and metal surfaces: What can we learn from â€˜toy modelsâ€™?. Faraday Discussions, 2000, 117, 65-83.	1.6	18

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127	Free vibrational relaxation of H adsorbed on a Si(1 0 0) surface investigated with the multi-configurational time-dependent Hartree method. Chemical Physics Letters, 2006, 433, 91-96.	1.2	18
128	Surface hopping dynamics of direct trans â†' cis photoswitching of an azobenzene derivative in constrained adsorbate geometries. Journal of Chemical Physics, 2012, 137, 234701.	1.2	18
129	Reduced and Exact Quantum Dynamics of the Vibrational Relaxation of a Molecular System Interacting with a Finite-Dimensional Bath. Journal of Physical Chemistry A, 2012, 116, 11118-11127.	1.1	18
130	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 114-118.	0.6	18
131	Control of Oxidation and Spin State in a Single-Molecule Junction. ACS Nano, 2018, 12, 3172-3177.	7.3	18
132	Variational wave packet method for dissipative photodesorption problems. Chemical Physics Letters, 1998, 288, 383-390.	1.2	17
133	Absorption and Fluorescence Excitation Spectra of 9-(N-carbazolyl)-anthracene:Â Effects of Intramolecular Vibrational Redistribution and Diabatic Transitions Involving Electron Transferâ€. Journal of Physical Chemistry A, 2001, 105, 2911-2924.	1.1	17
134	Mode-selective excitation of hydrogen atoms on a Si surface: Non-Markovian and Markovian treatment of infrared laser driven dissipative quantum dynamics. Physical Review B, 2007, 75, .	1.1	17
135	Comparing thermal wave function methods for multi-configuration time-dependent Hartree simulations. Journal of Chemical Physics, 2014, 140, 044106.	1.2	17
136	Strong Anisotropic Interaction Controls Unusual Sticking and Scattering of CO at Ru(0001). Physical Review Letters, 2017, 119, 146101.	2.9	17
137	Water Dissociative Adsorption on Î±-Al₂O₃(112Ì…0) Is Controlled by Surface Site Undercoordination, Density, and Topology. Journal of Physical Chemistry C, 2018, 122, 6573-6584.	1.5	17
138	Quantum-mechanical rates for gas-surface processes. Surface Science, 1994, 303, 206-230.	0.8	16
139	Quantum Theory of Photodesorption of Neutrals from Metals: Ab Initio Calculations and Active Control. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 1347-1352.	0.9	16
140	â€œFreeâ€•nuclear density propagation in two dimensions the coupled-channel density matrix method and its application to inelastic molecule-surface scattering. Chemical Physics, 1997, 219, 43-55.	0.9	16
141	Enhancement of femtosecond-laser-induced molecular desorption by thin metal films. Physical Review B, 2004, 69, .	1.1	16
142	Temperature effects for vibrational relaxation of hydrogen adsorbed on Si(100): a stochastic multiconfigurational time-dependent Hartree (MCTDH) study. Theoretical Chemistry Accounts, 2010, 127, 183-193.	0.5	16
143	Concept of a Single Temperature for Highly Nonequilibrium Laser-Induced Hydrogen Desorption from a Ruthenium Surface. Physical Review Letters, 2012, 109, 098303.	2.9	16
144	Exciton Splitting of Adsorbed and Free 4-Nitroazobenzene Dimers: A Quantum Chemical Study. Journal of Physical Chemistry A, 2016, 120, 3055-3070.	1.1	16

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145	Vibrational response and motion of carbon monoxide on Cu(100) driven by femtosecond laser pulses: Molecular dynamics with electronic friction. Physical Review B, 2019, 100, .	1.1	16
146	Electronic structure of undoped and dopedLa2CuO4: A Hartree-Fock cluster study. Physical Review B, 1990, 41, 8824-8832.	1.1	15
147	Effect of substrate vibrations on the sticking of atoms at surfaces: A critical comparison of different propagation methods for the H/Cu(100) system. Journal of Chemical Physics, 2000, 112, 10571-10581.	1.2	15
148	Quantum theoretical study of electron solvation dynamics in ice layers on a Cu(111) surface. Journal of Chemical Physics, 2005, 122, 234710.	1.2	15
149	Excited States of Xanthene Analogues: Photofragmentation and Calculations by CC2 and Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2016, 17, 3129-3138.	1.0	15
150	A detailed assignment of NEXAFS resonances of imidazolium based ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 8654-8661.	1.3	15
151	Photoswitching of azobenzene-containing self-assembled monolayers as a tool for control over silicon surface electronic properties. Journal of Chemical Physics, 2017, 146, 104703.	1.2	15
152	Theoretical Surface Science Beyond Gradient-Corrected Density Functional Theory: Water at Î±-Al₂O₃(0001) as a Case Study. Journal of Physical Chemistry C, 2019, 123, 6675-6684.	1.5	15
153	Molecular attochemistry: Correlated electron dynamics driven by light. Advances in Quantum Chemistry, 2020, 81, 15-50.	0.4	15
154	Towards low-energy-light-driven bistable photoswitches: ortho-fluoroaminoazobenzenes. Photochemical and Photobiological Sciences, 2022, 21, 159-173.	1.6	15
155	Molecular Dynamics Simulation of the LOV2 Domain fromAdiantum capillus-veneris. Journal of Chemical Information and Computer Sciences, 2004, 44, 1788-1793.	2.8	14
156	Laser-driven coupled electron-nuclear dynamics: Quantum mechanical simulation of molecular photodesorption from metal films. Physical Review B, 2005, 72, .	1.1	14
157	Quantum dynamics of laser-induced desorption from metal and semiconductor surfaces, and related phenomena. Journal of Physics Condensed Matter, 2006, 18, S1425-S1459.	0.7	14
158	Breaking Relaxing Bonds at a H:Si(100)-(2 Ã— 1) Surface with Infrared Laser Pulses. Journal of Physical Chemistry C, 2007, 111, 5432-5440.	1.5	13
159	Characterization of water dissociation on Î±-Al₂O₃(11Ì„02): theory and experiment. Physical Chemistry Chemical Physics, 2016, 18, 14822-14832.	1.3	13
160	Ab initio cluster and band structure calculations on systems modeling La2CuO4. Effects of charge transfer between the different planes, Madelung potentials, doping and correlations. Physica C: Superconductivity and Its Applications, 1992, 196, 340-356.	0.6	12
161	Theory of electron stimulated desorption and dissociation of CO at transition metals. Journal of Chemical Physics, 2002, 117, 4489-4498.	1.2	12
162	Laser-driven electron dynamics at interfaces. Israel Journal of Chemistry, 2005, 45, 205-215.	1.0	12

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163	BLUF Hydrogen network dynamics and UV/Vis spectra: A combined molecular dynamics and quantum chemical study. Journal of Computational Chemistry, 2012, 33, 2233-2242.	1.5	12
164	A six-dimensional potential energy surface for Ru(0001)(2Ã—2):CO. Journal of Chemical Physics, 2014, 141, 094704.	1.2	12
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