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	Reaction barriers on non-conducting surfaces beyond periodic local MP2: Diffusion of hydrogen on Î±-Al2O3(0001) as a test case. Journal of Chemical Physics, 2022, 156, 074109.	1.2	5
2	The electronic structure of the metalâ€“organic interface of isolated ligand coated gold nanoparticles. Nanoscale Advances, 2022, 4, 1599-1607.	2.2	7
3	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
4	Towards low-energy-light-driven bistable photoswitches: ortho-fluoroaminoazobenzenes. Photochemical and Photobiological Sciences, 2022, 21, 159-173.	1.6	15
5	Cavity-altered thermal isomerization rates and dynamical resonant localization in vibro-polaritonic chemistry. Journal of Chemical Physics, 2022, 156, 154305.	1.2	19
6	Water on porous, nitrogen-containing layered carbon materials: the performance of computational model chemistries. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
7	Cavity-induced non-adiabatic dynamics and spectroscopy of molecular rovibrational polaritons studied by multi-mode quantum models. Journal of Chemical Physics, 2022, 157, .	1.2	8
8	â€œInvertedâ€•CO molecules on NaCl(100): a quantum mechanical study. Physical Chemistry Chemical Physics, 2021, 23, 7860-7874.	1.3	5
9	Vibrational energy relaxation of interfacial OH on a water-covered Î±-Al₂O₃(0001) surface: a non-equilibrium ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 7714-7723.	1.3	10
10	Many-electron dynamics in laser-driven molecules: wavefunction theory vs. density functional theory. Physical Chemistry Chemical Physics, 2021, 23, 13544-13560.	1.3	19
11	Raman Enhancement of Nanoparticle Dimers Self-Assembled Using DNA Origami Nanotriangles. Molecules, 2021, 26, 1684.	1.7	8
12	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
13	Seemingly asymmetric atom-localized electronic densities following laser-dissociation of homonuclear diatomics. Journal of Chemical Physics, 2021, 154, 234305.	1.2	3
14	Quantum Chemistry Treatment of Silicon-Hydrogen Bond Rupture by Nonequilibrium Carriers in Semiconductor Devices. Physical Review Applied, 2021, 16, .	1.5	5
15	Protonated Imineâ€Linked Covalent Organic Frameworks for Photocatalytic Hydrogen Evolution. Angewandte Chemie - International Edition, 2021, 60, 19797-19803.	7.2	171
16	Photoisomerization of an Azobenzeneâ€Containing Surfactant Within a Micelle. ChemPhotoChem, 2021, 5, 926-932.	1.5	12
17	A thermofield-based multilayer multiconfigurational time-dependent Hartree approach to non-adiabatic quantum dynamics at finite temperature. Journal of Chemical Physics, 2021, 155, 134109.	1.2	5
18	The Role of Structural Flexibility in Plasmonâ€Driven Coupling Reactions: Kinetic Limitations in the Dimerization of Nitroâ€Benzenes. Advanced Materials Interfaces, 2021, 8, 2101344.	1.9	8

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19	Gaussian-Type Orbital Calculations for High Harmonic Generation in Vibrating Molecules: Benchmarks for H₂⁺. Journal of Chemical Theory and Computation, 2021, 17, 7353-7365.	2.3	6
20	Surface Hopping Dynamics for Azobenzene Photoisomerization: Effects of Packing Density on Surfaces, Fluorination, and Excitation Wavelength. Journal of Physical Chemistry C, 2020, 124, 26287-26295.	1.5	7
21	A hierarchical effective mode approach to phonon-driven multilevel vibrational relaxation dynamics at surfaces. Journal of Chemical Physics, 2020, 153, 064704.	1.2	5
22	On the Borate-Catalyzed Electrochemical Reduction of Phosphine Oxide: A Computational Study. Journal of Physical Chemistry A, 2020, 124, 10239-10245.	1.1	4
23	Molecular attochemistry: Correlated electron dynamics driven by light. Advances in Quantum Chemistry, 2020, 81, 15-50.	0.4	15
24	A quantum-mechanical tier model for phonon-driven vibrational relaxation dynamics of adsorbates at surfaces. Journal of Chemical Physics, 2019, 150, 244105.	1.2	7
25	Vibrationally Broadened Optical Spectra of Selected Radicals and Cations Derived from Adamantane: A Time-Dependent Correlation Function Approach. Journal of Physical Chemistry A, 2019, 123, 8871-8880.	1.1	12
26	Discriminating organic isomers by high harmonic generation: A time-dependent configuration interaction singles study. Journal of Chemical Physics, 2019, 150, 234114.	1.2	21
27	Vibrational spectra of dissociatively adsorbed D2O on Al-terminated Î±-Al2O3(0001) surfaces from ab initio molecular dynamics. Journal of Chemical Physics, 2019, 150, 244701.	1.2	9
28	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
29	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
30	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
31	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
32	Control of Oxidation and Spin State in a Single-Molecule Junction. ACS Nano, 2018, 12, 3172-3177.	7.3	18
33	Vibrationally resolved photoelectron spectra of lower diamondoids: A time-dependent approach. Journal of Chemical Physics, 2018, 148, 044310.	1.2	9
34	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
35	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
36	Muonic molecular ions<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>p</mml:mi><mml:mi>p</mml:mi><mml:mi>Î¼</mml:mi></mml:mrow></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>p</mml:mi><mml:mi>d</mml:mi><mml:mi>Î¼</mml:mi></mml:mrow></mml:math> by superintense VUV laser pulses: Postexcitation muonic and nuclear oscillations and high-order harmonic generation. Physical Review A, 2018, 97, .	1.0	2

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37	Water Molecular Beam Scattering at Î±-Al₂O₃(0001): An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 15494-15504.	1.5	4
38	Hole Catalysis as a General Mechanism for Efficient and Wavelength-Independent Z â†' E Azobenzene Isomerization. CheM, 2018, 4, 1740-1755.	5.8	57
39	Vibrationally resolved absorption and fluorescence spectra of perylene and N-substituted derivatives from autocorrelation function approaches. Chemical Physics, 2018, 515, 728-736.	0.9	9
40	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
41	A novel system-bath Hamiltonian for vibration-phonon coupling: Formulation, and application to the relaxation of Siâ€"H and Siâ€"D bending modes of H/D:Si(100)-(2 Ã— 1). Chemical Physics, 2017, 482, 69-80.	0.9	6
42	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
43	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
44	Electrocatalytic Z â†' E Isomerization of Azobenzenes. Journal of the American Chemical Society, 2017, 139, 335-341.	6.6	108
45	Strong Anisotropic Interaction Controls Unusual Sticking and Scattering of CO at Ru(0001). Physical Review Letters, 2017, 119, 146101.	2.9	17
46	Isotopic effects in vibrational relaxation dynamics of H on a Si(100) surface. Journal of Chemical Physics, 2017, 147, 144703.	1.2	5
47	Thermal isomerization of azobenzenes: on the performance of Eyring transition state theory. Journal of Physics Condensed Matter, 2017, 29, 314002.	0.7	19
48	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
49	CO Molecules on a NaCl(100) Surface: Structures, Energetics, and Vibrational Davydov Splittings at Various Coverages. Journal of Physical Chemistry C, 2016, 120, 12637-12653.	1.5	12
50	Characterization of water dissociation on Î±-Al₂O₃(11Ì„02): theory and experiment. Physical Chemistry Chemical Physics, 2016, 18, 14822-14832.	1.3	13
51	Fluorination of the Hydroxylated Î±-Al₂O₃ (0001) and Its Implications for Water Adsorption: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 9713-9718.	1.5	9
52	Dynamics of Azobenzene Dimer Photoisomerization: Electronic and Steric Effects. Journal of Physical Chemistry Letters, 2016, 7, 3591-3596.	2.1	42
53	Femtosecond-laser-driven molecular dynamics on surfaces: Photodesorption of molecular oxygen from Ag(110). Physical Review B, 2016, 93, .	1.1	42
54	Excited States of Xanthene Analogues: Photofragmentation and Calculations by CC2 and Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2016, 17, 3129-3138.	1.0	15

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55	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
56	Excited States of Xanthene Analogues: Photofragmentation and Calculations by CC2 and Time-Dependent Density Functional Theory. ChemPhysChem, 2016, 17, 2951-2951.	1.0	0
57	Controlling the high frequency response of H2 by ultra-short tailored laser pulses: A time-dependent configuration interaction study. Journal of Chemical Physics, 2016, 144, 044301.	1.2	11
58	A detailed assignment of NEXAFS resonances of imidazolium based ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 8654-8661.	1.3	15
59	Femtosecond laser pulse induced desorption: A molecular dynamics simulation. Nuclear Instruments & Methods in Physics Research B, 2016, 382, 114-118.	0.6	18
60	Computation of high-harmonic generation spectra of the hydrogen molecule using time-dependent configuration-interaction. Molecular Physics, 2016, 114, 947-956.	0.8	47
61	Reversible Photoswitching of the Interfacial Nonlinear Optical Response. Journal of Physical Chemistry Letters, 2015, 6, 505-509.	2.1	42
62	Diarylethene Molecules on a Ag(111) Surface: Stability and Electron-Induced Switching. Journal of Physical Chemistry C, 2015, 119, 4874-4883.	1.5	30
63	A combined quantum chemical/molecular dynamics study of X-ray photoelectron spectra of polyvinyl alcohol using oligomer models. Journal of Electron Spectroscopy and Related Phenomena, 2015, 199, 38-45.	0.8	5
64	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
65	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
66	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
67	Nonlinear optical response of photochromic azobenzene-functionalized self-assembled monolayers. Physical Chemistry Chemical Physics, 2015, 17, 18079-18086.	1.3	44
68	A multi-reference study of the byproduct formation for a ring-closed dithienylethene photoswitch. Physical Chemistry Chemical Physics, 2015, 17, 14088-14095.	1.3	11
69	Measures for the non-Markovianity of a harmonic oscillator coupled to a discrete bath derived from numerically exact references. European Physical Journal D, 2015, 69, 1.	0.6	6
70	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
71	Semiclassical modelling of finite-pulse effects on non-adiabatic photodynamics via initial condition filtering: The predissociation of NaI as a test case. Journal of Chemical Physics, 2015, 142, 194107.	1.2	8
72	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

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73	Comparing thermal wave function methods for multi-configuration time-dependent Hartree simulations. Journal of Chemical Physics, 2014, 140, 044106.	1.2	17
74	A six-dimensional potential energy surface for Ru(0001)(2Ã—2):CO. Journal of Chemical Physics, 2014, 141, 094704.	1.2	12
75	Electronic structure changes during the surface-assisted formation of a graphene nanoribbon. Journal of Chemical Physics, 2014, 140, 024701.	1.2	19
76	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
77	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
78	orthoâ€Fluoroazobenzenes: Visible Light Switches with Very Longâ€Lived Z Isomers. Chemistry - A European Journal, 2014, 20, 16492-16501.	1.7	311
79	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
80	Experimental Characterization of Unimolecular Water Dissociative Adsorption on Î±-Alumina. Journal of Physical Chemistry C, 2014, 118, 13623-13630.	1.5	34
81	Frontispiece:ortho-Fluoroazobenzenes: Visible Light Switches with Very Long-LivedZIsomers. Chemistry - A European Journal, 2014, 20, n/a-n/a.	1.7	0
82	Switching with orthogonal stimuli: electrochemical ring-closure and photochemical ring-opening of bis(thiazolyl)maleimides. Chemical Science, 2013, 4, 1028-1040.	3.7	52
83	Electron correlation dynamics in atoms and molecules. Journal of Chemical Physics, 2013, 138, 164108.	1.2	6
84	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
85	Quantum Dynamical Simulations of the Femtosecondâ€Laserâ€Induced Ultrafast Desorption of H₂ and D₂ from Ru(0001). ChemPhysChem, 2013, 14, 1471-1478.	1.0	5
86	Theory of Non-adiabatic Molecular Dynamics at Surfaces. Springer Series in Surface Sciences, 2013, , 323-348.	0.3	3
87	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
88	Excitation, relaxation, and quantum diffusion of CO on copper. Physical Review B, 2012, 86, .	1.1	23
89	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
90	Current versus temperature-induced switching of a single molecule: Open-system density matrix theory for 1,5-cyclooctadiene on Si(100). Journal of Chemical Physics, 2012, 136, 094705.	1.2	6

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91	STM-switching of organic molecules on semiconductor surfaces: an above threshold density matrix model for 1,5 cyclooctadiene on Si(100). Journal of Physics Condensed Matter, 2012, 24, 394009.	0.7	3
92	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
93	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
94	Tribute to JÃ¶rn Manz. Journal of Physical Chemistry A, 2012, 116, 11041-11042.	1.1	0
95	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
96	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
97	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
98	Non-adiabatic excited state dynamics of riboflavin after photoexcitation. Physical Chemistry Chemical Physics, 2012, 14, 8693.	1.3	21
99	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
100	Selective Excitation of Moleculeâ€Surface Vibrations in H₂ and D₂ Dissociatively Adsorbed on Ru(0001). Israel Journal of Chemistry, 2012, 52, 438-451.	1.0	10
101	Quantum chemical modeling of the kinetic isotope effect of the carboxylation step in RuBisCO. Journal of Molecular Modeling, 2012, 18, 1877-1883.	0.8	4
102	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
103	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
104	The Effects of Electronâ€“Hole Pair Coupling on the Infrared Laser-Controlled Vibrational Excitation of NO on Au(111). Journal of Physical Chemistry A, 2011, 115, 10698-10707.	1.1	11
105	Femtosecond Stimulated Raman Spectroscopy of Flavin after Optical Excitation. Journal of Physical Chemistry B, 2011, 115, 3656-3680.	1.2	95
106	Electronic Decoupling Approach to Quantitative Photoswitching in Linear Multiazobenzene Architectures. Journal of Physical Chemistry B, 2011, 115, 9930-9940.	1.2	77
107	Dissipative many-electron dynamics of ionizing systems. Journal of Chemical Physics, 2011, 134, 044311.	1.2	30
108	Laser-controlled switching of molecular arrays in an dissipative environment. Physical Review B, 2011, 83, .	1.1	7

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109	Microscopic Model of the Optical Absorption of Carbon Nanotubes Functionalized with Molecular Spiropyran Photoswitches. Physical Review Letters, 2011, 106, 097401.	2.9	81
110	Adsorption and (photo-) electrochemical splitting of water on rutile ruthenium dioxide. Europhysics Letters, 2011, 93, 68001.	0.7	11
111	cisâ€“trans Isomerisation of Substituted Aromatic Imines: A Comparative Experimental and Theoretical Study. ChemPhysChem, 2011, 12, 2311-2321.	1.0	50
112	Ab initio calculations for XPS chemical shifts of poly(vinyl-trifluoroacetate) using trimer models. Surface Science, 2011, 605, 1516-1524.	0.8	8
113	(TD-)DFT Calculation of Vibrational and Vibronic Spectra of Riboflavin in Solution. Journal of Physical Chemistry B, 2010, 114, 10826-10834.	1.2	82
114	Time-dependent response of dissipative electron systems. Physical Review A, 2010, 81, .	1.0	21
115	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
116	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
117	Electronic damping of anharmonic adsorbate vibrations at metallic surfaces. Physical Review B, 2010, 81, .	1.1	37
118	Role of electronic friction during the scattering of vibrationally excited nitric oxide molecules from Au(111). Physical Review B, 2010, 82, .	1.1	67
119	Ab initio Electron Dynamics with the Multi-Configuration Time-Dependent Hartree-Fock Method. Zeitschrift Fur Physikalische Chemie, 2010, 224, 569-581.	1.4	7
120	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
121	A new analytical potential energy surface for the adsorption system CO/Cu(100). Journal of Chemical Physics, 2010, 132, 074108.	1.2	29
122	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
123	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
124	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
125	Ab initio Electron Dynamics with the Multi-Configuration Time-Dependent Hartree-Fock Method. , 2010, , 279-291.		0
126	Selective subsurface absorption of hydrogen in palladium using laser distillation. Journal of Chemical Physics, 2009, 131, 084716.	1.2	26

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127	Serine in BLUF domains displays spectral importance in computational models. Journal of Photochemistry and Photobiology B: Biology, 2009, 94, 87-95.	1.7	23
128	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
129	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
130	Time-evolution operator method for non-Markovian density matrix propagation in time and space representation: Application to laser association of OH in an environment. Physical Review A, 2009, 79, .	1.0	10
131	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
132	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
133	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
134	Open-system density matrix description of an STM-driven atomic switch: H on Si(100). Applied Physics A: Materials Science and Processing, 2008, 93, 319-333.	1.1	9
135	Theoretical and experimental investigation of novel iron(II)-based spin crossover compounds. Chemical Physics, 2008, 347, 514-522.	0.9	11
136	Controlling the photodesorption of adspecies from surfaces. Surface Science, 2008, 602, 3153-3161.	0.8	1
137	Time-dependent configuration-interaction calculations of laser-driven dynamics in presence of dissipation. Journal of Chemical Physics, 2008, 129, 084302.	1.2	54
138	Guided locally optimal control of quantum dynamics in dissipative environments. Physical Review A, 2008, 78, .	1.0	25
139	A hybrid local/global optimal control algorithm for dissipative systems with time-dependent targets: Formulation and application to relaxing adsorbates. Journal of Chemical Physics, 2008, 128, 074104.	1.2	9
140	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
141	Monotonically convergent algorithms for solving quantum optimal control problems described by an integrodifferential equation of motion. Physical Review A, 2007, 75, .	1.0	29
142	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
143	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
144	Inducing the Rotation of a Single Phenyl Ring with Tunneling Electrons. Journal of Physical Chemistry C, 2007, 111, 14843-14848.	1.5	72

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145	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
146	Molecular response properties from explicitly time-dependent configuration interaction methods. Journal of Chemical Physics, 2007, 127, 034107.	1.2	98
147	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
148	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
149	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
150	Laser-induced charge transfer and photodesorption of Cs at Cu(111): quantum dynamical model simulations. Applied Physics A: Materials Science and Processing, 2007, 88, 535-546.	1.1	7
151	Vibrationally enhanced associative photodesorption of molecular hydrogen from Ru(0001). Chemical Physics, 2007, 338, 299-311.	0.9	19
152	Ultrafast dynamics of photoinduced processes at surfaces and interfaces. , 2007, , 387-484.		2
153	A local coherent-state approximation to system-bath quantum dynamics. Journal of Chemical Physics, 2006, 125, 194102.	1.2	52
154	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
155	Quantum Dynamical Approach to Ultrafast Molecular Desorption from Surfaces. Chemical Reviews, 2006, 106, 4116-4159.	23.0	145
156	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
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	Theoretical study of vibration-phonon coupling of H adsorbed on a Si(100) surface. Journal of Chemical Physics, 2006, 124, 034710.	1.2	57
159	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
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