Shinkoh Nanbu

List of Publications by Year
in descending order

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102	1,536	304743	377865
papers	citations	22 h-index	34 g-index

105	105	105	1349
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nonadiabatic bending dissociation in 16 valence electron system OCS. Journal of Chemical Physics, 1998, 109, 5778-5794.	3.0	114
2	Ab initio nonadiabatic quantum dynamics of cyclohexadiene/hexatriene ultrafast photoisomerization. Journal of Chemical Physics, 2006, 124, 084313.	3.0	78
3	Analysis of the Ultraviolet Absorption Cross Sections of Six Isotopically Substituted Nitrous Oxide Species Using 3D Wave Packet Propagationâ€. Journal of Physical Chemistry A, 2004, 108, 8905-8913.	2.5	56
4	A theoretical study of cyclohexadiene/hexatriene photochemical interconversion: multireference configuration interaction potential energy surfaces and transition probabilities for the radiationless decays. Chemical Physics Letters, 2005, 401, 487-491.	2.6	52
5	Nonadiabatic ab Initio Dynamics of Two Models of Schiff Base Retinal. Journal of Physical Chemistry A, 2009, 113, 4356-4366.	2.5	51
6	Theoretical study of the photodissociation cross sections and the photodissociation dynamics of hypochlorous acid. The Journal of Physical Chemistry, 1992, 96, 2103-2111.	2.9	47
7	Future perspectives of nonadiabatic chemical dynamics. Chemical Science, 2010, 1, 663.	7.4	47
8	Bisindolylmaleimides with Large Stokes Shift and Long-Lasting Chemiluminescence Properties. Organic Letters, 2007, 9, 3583-3586.	4.6	45
9	QM/MM Trajectory Surface Hopping Approach to Photoisomerization of Rhodopsin and Isorhodopsin: The Origin of Faster and More Efficient Isomerization for Rhodopsin. Journal of Physical Chemistry B, 2012, 116, 8009-8023.	2.6	43
10	Laser control of reactions of photoswitching functional molecules. Journal of Chemical Physics, 2006, 125, 034307.	3.0	32
11	Theoretical studies of absorption cross sections for the CÌƒâ€‰B12-XÌƒâ€‰A11 system of sulfur dioxide and isotope effects. Journal of Chemical Physics, 2010, 132, 024301.	3.0	32
12	A comparative study of the quantum dynamics and rate constants of the O(3P)+HCl reaction described by two potential surfaces. Journal of Chemical Physics, 2000, 113, 227-236.	3.0	31
13	Nuclear motion driven by the Rennerâ€“Teller effect as observed in the resonant Auger decay to the XÌƒ2Î electronic ground state of N2O+. Journal of Chemical Physics, 2001, 115, 864-869.	3.0	31
14	Nonadiabatic ab Initio Dynamics of a Model Protonated Schiff Base of 9-cis Retinal. Journal of Physical Chemistry A, 2010, 114, 8190-8201.	2.5	30
15	Millimeter-wave spectroscopy of the internal-rotation band of the Heâ€“HCN complex and the intermolecular potential energy surface. Journal of Chemical Physics, 2002, 117, 7041-7050.	3.0	29
16	Ab initio study of sulfur isotope fractionation in the reaction of OCS with OH. Chemical Physics Letters, 2008, 450, 214-220.	2.6	27
17	Photoabsorption crossâ€section measurements of³²S, ³³S, ³⁴S, and ³⁶S sulfur dioxide for the B¹Bˉ₁â€X¹A₁ absorption band. Journal of Geophysical Research, 2012, 117, .	3.3	27
18	Strongly Chemiluminescent Acridinium Esters under Neutral Conditions: Synthesis, Properties, Determination, and Theoretical Study. Journal of Organic Chemistry, 2017, 82, 2450-2461.	3.2	26

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19	OCS photolytic isotope effects from first principles: sulfur and carbon isotopes, temperature dependence and implications for the stratosphere. Atmospheric Chemistry and Physics, 2013, 13, 1511-1520.	4.9	25
20	Assignment of surface IR absorption spectra observed in the oxidation reactions: 2H+H2O/Si(100) and H2O+H/Si(100). Surface Science, 2005, 575, 330-342.	1.9	24
21	Carbonyl sulfide isotopologues: Ultraviolet absorption cross sections and stratospheric photolysis. Journal of Chemical Physics, 2009, 131, 024307.	3.0	24
22	Characterization of the E Isomer of Tetrasubstituted [5]Cumulene and Trapping of the Z Isomer as a Zirconocene Complex. Organometallics, 2011, 30, 3544-3548.	2.3	24
23	Clarification of nonadiabatic chemical dynamics by the Zhu-Nakamura theory of nonadiabatic transition: from tri-atomic systems to reactions in solutions. International Reviews in Physical Chemistry, 2017, 36, 229-285.	2.3	24
24	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM I.. Journal of Theoretical and Computational Chemistry, 2002, 01, 263-273.	1.8	23
25	Molecular switching in one-dimensional finite periodic nonadiabatic tunneling potential systems. Journal of Chemical Physics, 1997, 107, 5445-5459.	3.0	22
26	Collision Energy Dependence of the O(1D) + HCl â† ' OH + Cl(2P) Reaction Studied by Crossed Beam Scattering and Quasiclassical Trajectory Calculations on Ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2008, 112, 818-825.	2.5	22
27	Theoretical Study of Photophysical Properties of Bisindolylmaleimide Derivatives. Journal of Physical Chemistry A, 2009, 113, 8213-8220.	2.5	22
28	Quantum dynamical study of the O(D1)+HCl reaction employing three electronic state potential energy surfaces. Journal of Chemical Physics, 2008, 128, 014308.	3.0	21
29	Nonadiabatic calculations of ultraviolet absorption cross section of sulfur monoxide: Isotopic effects on the photodissociation reaction. Journal of Chemical Physics, 2014, 140, 044319.	3.0	20
30	Theoretical study of the potential energy surfaces and dynamics of CaNC/CaCN. Journal of Chemical Physics, 1997, 106, 8073-8083.	3.0	19
31	Development of semiclassical molecular dynamics simulation method. Physical Chemistry Chemical Physics, 2016, 18, 11972-11985.	2.8	18
32	Nonadiabatic ab initio molecular dynamics of photoisomerization reaction between 1,3-cyclohexadiene and 1,3,5-cis-hexatriene. Chemical Physics, 2015, 459, 45-53.	1.9	16
33	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM II.. Journal of Theoretical and Computational Chemistry, 2002, 01, 275-284.	1.8	15
34	Quantum Mechanical Calculation of Energy Dependence of OCl/OH Product Branching Ratio and Product Quantum State Distributions for the O(¹D) + HCl Reaction on All Three Contributing Electronic State Potential Energy Surfaces. Journal of Physical Chemistry A, 2008, 112, 7947-7960.	2.5	14
35	Dinuclear Ruthenium(III)â€"Ruthenium(IV) Complexes, Having a Doubly Oxido-Bridged and Acetato- or Nitrato-Capped Framework. Inorganic Chemistry, 2016, 55, 6830-6832.	4.0	14
36	A theoretical study on vibrational spectra of C84 fullerenes: results for C2, D2, and D2d isomers. Computational and Theoretical Chemistry, 1999, 461-462, 453-461.	1.5	13

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37	Theoretical studies of vacuum ultraviolet emission spectra of NeLi+ and ArLi+. Journal of Chemical Physics, 1991, 94, 3707-3714.	3.0	12
38	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM III.. Journal of Theoretical and Computational Chemistry, 2002, 01, 285-293.	1.8	12
39	Theoretical study of water-induced oxidation reaction on a bare Si surface: H2O+Si(100)â€“(2Ã—1). Chemical Physics Letters, 2006, 424, 133-138.	2.6	12
40	Raman spectroscopic study on isomers of photochromic 1,2-bis(2,5-dimethyl-3-thienyl)perfluorocyclopentene in crystal and stability of the closed-ring forms in the open-ring forms. Chemical Physics Letters, 2008, 454, 42-48.	2.6	12
41	Control of Chemical Dynamics by Lasers: Theoretical Considerations. Journal of Physical Chemistry A, 2010, 114, 6171-6187.	2.5	12
42	Fluorescence and chemiluminescence properties of indolylmaleimides: experimental and theoretical studies. Physical Chemistry Chemical Physics, 2010, 12, 9783.	2.8	11
43	Photochemical dynamics of indolylmaleimide derivatives. Physical Chemistry Chemical Physics, 2012, 14, 11546.	2.8	11
44	Haptotropic Shift of [5]Cumulenes in Zirconocene Complexes and Effects of Steric Factors. Organometallics, 2014, 33, 5220-5230.	2.3	11
45	Effects of Cyclodextrins on Intramolecular Photoinduced Electron Transfer in a Boronic Acid Fluorophore. Analytical Sciences, 2014, 30, 643-648.	1.6	11
46	Atomic hydrogen transmission through five-membered carbon ring by the mechanism of non-adiabatic tunneling. Chemical Physics, 2006, 324, 721-732.	1.9	10
47	Intramolecular energy transfer in 3-amino-N-(7â€²-methoxy-4â€²-methylcoumaryl)phthalimide. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 208, 21-26.	3.9	10
48	Isotopomer Fractionation in the UV Photolysis of N2O: 3. 3D Ab Initio Surfaces and Anharmonic Effectsâ€. Journal of Physical Chemistry A, 2010, 114, 9700-9708.	2.5	10
49	Theoretical study of the potential energy surfaces and bound states of HCP. Journal of Chemical Physics, 2000, 112, 5866-5876.	3.0	9
50	Three-pairs of doublet bands assigned toSiH2scissoring modes observed inH2O-induced oxidation of Si(100) surfaces. Physical Review B, 2004, 69, .	3.2	9
51	Remarkable suppression of the excited-state double-proton transfer in the 7-azaindole dimer due to substitution of the dimethylamino group studied by electronic spectroscopy in the gas phase. Chemical Physics Letters, 2007, 443, 194-198.	2.6	9
52	Electronic Spectra of Two Long-Lived Photoproducts: Double-Proton Transfer in 7-Hydroxyquinoline Dimer in a 2-Methyltetrahydrofuran Glass Matrix. Journal of Physical Chemistry A, 2010, 114, 5041-5048.	2.5	9
53	First principle study of proton transfer in the green fluorescent protein (GFP): Ab initio PES in a cluster model. Computational and Theoretical Chemistry, 2012, 990, 185-193.	2.5	9
54	Theoretical analysis of the oxygen insertion process in the oxidation reactions of H2O+H/Si(100) and 2H+H2O/Si(100): a molecular orbital calculation and an analysis of tunneling reaction. Chemical Physics Letters, 2004, 383, 523-527.	2.6	8

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55	Ab initio calculated structures of conformers for 1,3-dimethoxy-p-tert-butylcalix[4]crown-5-ether complexed with potassium cation. Computational and Theoretical Chemistry, 2005, 722, 117-123.	1.5	8
56	Vibrational energies for the XÌƒA11, AÌƒB11, and BÌƒA11 states of SiH2â^•SiD2 and related transition probabilities based on global potential energy surfaces. Journal of Chemical Physics, 2005, 122, 144307.	3.0	8
57	Electronically nonadiabatic wave packet propagation using frozen Gaussian scattering. Journal of Chemical Physics, 2015, 143, 114103.	3.0	8
58	Synthesis, chemiluminescence, and application of 2,4-disubstituted phenyl 10-methyl-10Î»4-acridine-9-carboxylates. Dyes and Pigments, 2019, 170, 107628.	3.7	8
59	Total Absorption Cross Section for UV Excitation of Sulfur Monoxide. Journal of Physical Chemistry A, 2019, 123, 3697-3702.	2.5	8
60	Synthesis and Structureâ€Photophysics Evaluation of 2â€Nâ€Aminoâ€quinazolines: Small Molecule Fluorophores for Solution and Solid State. Chemistry - an Asian Journal, 2021, 16, 2087-2099.	3.3	8
61	He*(2â€Š3S) Penning ionization of H2S. I. Theoretical Franckâ€“Condon factors for the H2S(XÌƒâ€Š1A1,vâ€²=0)â†'H2S+(XÌƒâ€Š2B1,Ãƒâ€Š2A1) ionization and H2S+(Ãƒâ€“XÌƒ) transition. Journal of Chemical Physics, 2003, 119, 5874-5881.	3.0	7
62	Chemiluminescence Change of Polyphenol Dendrimers with Different Core Molecules. Organic Letters, 2008, 10, 5171-5174.	4.6	7
63	Application of particle-mesh Ewald summation to ONIOM theory. Chemical Physics, 2015, 461, 47-57.	1.9	7
64	The excimer emission spectra and the interaction potential energy of the ground and excited states of He and alkali-metal ion systems. Chemical Physics Letters, 1992, 192, 443-450.	2.6	6
65	Theoretical study of vibrational spectra of p-tert-butylcalix[4]crown-6-ether complexed with ethyl ammonium cation. Chemical Physics Letters, 2003, 374, 572-576.	2.6	6
66	HOCl Ro-Vibrational Bound-State Calculations for Nonzero Total Angular Momentumâ€. Journal of Physical Chemistry A, 2006, 110, 5468-5474.	2.5	6
67	Quantum Calculation of Ro-vibrational States:â€‰ Methodology and DOCl Application Results. Journal of Physical Chemistry A, 2008, 112, 4141-4147.	2.5	6
68	Fluorescence properties of 2-aryl substituted indoles. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 905-908.	3.9	6
69	Acridinium Ester Chemiluminescence: Methyl Substitution on the Acridine Moiety. Journal of Oleo Science, 2021, 70, 1677-1684.	1.4	6
70	Theoretical transition probabilities for the AÌƒÎ1-XÌƒÎ£+1 system of AlNC and AlCN isomers based on global potential energy surfaces. Journal of Chemical Physics, 2006, 124, 224301.	3.0	5
71	Isotope effects in the dissociation of the BÌƒA11 state of SiH2, SiHD, and SiD2 using three-dimensional wave packet propagation. Journal of Chemical Physics, 2006, 124, 114308.	3.0	5
72	The vibrational structure of the XÌƒA11â^'AÌƒB11 and AÌƒB11â^'BÌƒA11 band systems of GeH2â^•GeD2 based on global potential energy surfaces. Journal of Chemical Physics, 2007, 126, 044313.	3.0	5

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73	Theoretical study of photo-physical properties of indolylmaleimide derivatives. Physical Chemistry Chemical Physics, 2012, 14, 3017.	2.8	5
74	Theoretical study of electronic properties and isotope effects in the UV absorption spectrum of disulfur. Chemical Physics, 2019, 516, 108-115.	1.9	5
75	Framework Conversion of Oxido-Bridged Dinuclear Ruthenium Complexes. Inorganic Chemistry, 2020, 59, 612-622.	4.0	5
76	Theoretical emission spectra of NeAl+ and ArAl+ in the vacuum ultraviolet region. Chemical Physics Letters, 1988, 146, 275-279.	2.6	4
77	He*(2â€Š3S) penning ionization of H2S. II. Formation of the SH+(Aâ€Š3Î) and H2S+(Ãƒâ€Š2A1) ions. Journal of Chemical Physics, 2003, 119, 5882-5888.	3.0	4
78	First-Principle Study of Atomic Hydrogen Interaction with a Fluorinated Corannulene Radical. Australian Journal of Chemistry, 2010, 63, 371.	0.9	4
79	A theoretical study of SiCN and SiNC in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mover accent="true"><mml:mrow><mml:mi>X</mml:mi></mml:mrow><mml:mrow><mml:mo>Ëœ</mml:mo></mml:mrow></mml:mover> electronic state based on global potential energy surfaces. Chemical Physics Letters, 2011, 514, 239-243.	2.6	4
80	Unsymmetric indolylmaleimides: Synthesis, photophysical properties and amyloid detection. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 289, 39-46.	3.9	4
81	Development of efficient time-evolution method based on three-term recurrence relation. Journal of Chemical Physics, 2015, 142, 204104.	3.0	4
82	Formation of HCl+(A2Î£+) and HBr+(A2Î£+) Resulting from He(23S) Penning Ionization of HCl and HBr. Journal of Physical Chemistry A, 2002, 106, 6068-6074.	2.5	3
83	INITIAL ROTATIONAL QUANTUM STATE EXCITATION AND ISOTOPIC EFFECTS FOR THE O(¹D)+HCl â†' OH+Cl (OCl+H) REACTION. Journal of Theoretical and Computational Chemistry, 2009, 08, 1003-1024.	1.8	3
84	Nonadiabatic ab initio molecular dynamics with PME-ONIOM scheme of photoisomerization reaction between 1,3-cyclohexadiene and 1,3,5-cis-hexatriene in solution phase. Chemical Physics, 2017, 485-486, 45-59.	1.9	3
85	Enhancement effect on the chemiluminescence of acridinium esters under neutral conditions. Luminescence, 2018, 33, 345-348.	2.9	3
86	Chemiluminescence of methoxycarbonylphenyl 10-methyl-10Î»4 -2,7-disubstituted acridine-9-carboxylate derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 403, 112851.	3.9	3
87	Non-Adiabatic Bending Dissociation of OCS Induced by Orbital Unlocking. ACS Symposium Series, 2002, , 300-313.	0.5	2
88	H atom-induced oxidation reaction on water-terminated Si surface, 2H + H2O/Si(1 0 0)â€"(2 Ã— 1): A theoretical study. Chemical Physics Letters, 2005, 412, 347-352.	2.6	2
89	Quantum mechanical study of atomic hydrogen interaction with a fluorinated boron-substituted coronene radical. Journal of Physics Condensed Matter, 2009, 21, 144209.	1.8	2
90	Theoretical study of ultraviolet induced photodissociation dynamics of sulfuric acid. Chemical Physics, 2015, 452, 17-24.	1.9	2

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91	Reactions of Azides Coordinated to Ruthenium(II) Centers with Haloalkanes To Afford Nitrogenâ€Containing Moieties. European Journal of Inorganic Chemistry, 2017, 2017, 2998-3007.	2.0	2
92	Potential energy surfaces of some low-lying states of fluoroformyl radical FCO. Chemical Physics, 1994, 184, 97-106.	1.9	1
93	THEORETICAL TRANSITION PROBABILITIES FOR THE $ilde{A}^{2}A_{1} -ilde{X}^{2}B_{1}$ SYSTEM OF H2O+ AND D2O+ AND RELATED FRANCKâ€“CONDON FACTORS BASED ON GLOBAL POTENTIAL ENERGY SURFACES. Journal of Theoretical and Computational Chemistry, 2005, 04, 225-245.	1.8	1
94	Isomerization reaction between linear AlNC and AlCN including the XÌƒ 1Î£+ and AÌƒ 1Î states studied by three-dimensional wave packet propagation. Journal of Chemical Physics, 2011, 135, 024305.	3.0	1
95	A Nonadiabatic Ab Initio Dynamics Study on Rhodopsin and Its Analog Isorhodopsin: Chemical Dynamics Reasons behind Selection of Rhodopsin by Life. Chemistry Letters, 2011, 40, 1395-1397.	1.3	1
96	Theoretical Molecular Dynamics Simulation of the DIF-1 Receptor Activation. Bulletin of the Chemical Society of Japan, 2019, 92, 1436-1443.	3.2	1
97	Theoretical analysis of the kinetic isotope effect on carboxylation in RubisCO. Journal of Computational Chemistry, 2020, 41, 1116-1123.	3.3	1
98	Chemiluminescence enhancement of 1,2â€di[3,4,5â€tri(3,4,5â€trihydroxybenzoyloxy)benzoyloxy] benzene in the presence of quaternary ammonium ions. Luminescence, 2010, 25, 360-363.	2.9	0
99	THEORETICAL STUDY OF PHOTO-PHYSICAL PROCESSES IN 2-ARYL SUBSTITUTED INDOLES. Journal of Theoretical and Computational Chemistry, 2012, 11, 1311-1322.	1.8	0
100	The Nonadiabatic Trajectory. , 2017, , .		0
101	Real-Time TDHF/TDDFT Calculation with Efficient Time-Evolution Based on Three-Term Recurrence Relation. Journal of Computer Chemistry Japan, 2014, 13, 184-186.	0.1	0
102	Nâ€“C bond formation between two anilines coordinated to a ruthenium center in cis-form affording a 3,5-cyclohexadiene-1,2-diimine moiety. RSC Advances, 2021, 11, 36644-36650.	3.6	0