Toshiyuki Takayanagi

List of Publications by Year
in descending order

87	1,110	394286 19	477173 29
papers	citations	h-index	g-index

90	90	90	788
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reduced dimensionality calculations of quantum reactive scattering for the H+CH4â†'H2+CH3 reaction. Journal of Chemical Physics, 1996, 104, 2237-2242.	1.2	97
2	Three-dimensional quantum reactive scattering calculations for the nonadiabatic (D+H2)+ reaction system. Journal of Chemical Physics, 2000, 112, 2615-2622.	1.2	60
3	van der Waals resonances in cumulative reaction probabilities for the F+H2, D2, and HD reactions. Journal of Chemical Physics, 1998, 109, 8929-8934.	1.2	51
4	Quantum scattering calculations for the electronically nonadiabatic Br(2P1/2)+H2â†'HBr+H reaction. Journal of Chemical Physics, 2000, 113, 7158-7164.	1.2	40
5	Nonadiabatic quantum reactive scattering calculations for the O(1D)+H2, D2, and HD reactions on the lowest three potential energy surfaces. Journal of Chemical Physics, 2002, 116, 2439-2446.	1.2	35
6	Photodissociation of Cl2 in helium clusters: an application of hybrid method of quantum wavepacket dynamics and path integral centroid molecular dynamics. Chemical Physics Letters, 2003, 372, 90-96.	1.2	34
7	Dynamics of dipole- and valence bound anions in iodide-adenine binary complexes: A time-resolved photoelectron imaging and quantum mechanical investigation. Journal of Chemical Physics, 2015, 143, 104308.	1.2	32
8	Theoretical study on photoexcitation dynamics of the K atom attached to helium clusters and the solvation structures of K*Hen exciplexes. Physical Chemistry Chemical Physics, 2004, 6, 3241.	1.3	31
9	Kinetic measurements for the reactions of ozone with crotonaldehyde and its methyl derivatives and calculations of transition-state theoryElectronic supplementary information (ESI) available: The stationary-point geometries optimized at B3LYP/6-31G(d,p) for the reactions of ozone with nine unsaturated carbonyls. See http://www.rsc.org/suppdata/cp/b4/b402496f/. Physical Chemistry Chemical Physics, 2004, 6, 3969.	1.3	31
10	Translational energy distributions of the products of the 193 and 157 nm photodissociation of chloroethylenes. Journal of Chemical Physics, 1997, 106, 10123-10133.	1.2	30
11	Accurate ab initio electronic structure calculations of the stable helium complex: HeBeO. Chemical Physics Letters, 2008, 454, 1-6.	1.2	28
12	Theoretical Study on the Mechanism of Low-Energy Dissociative Electron Attachment for Uracil. Journal of Physical Chemistry A, 2009, 113, 4795-4801.	1.1	27
13	Globalab initiopotential energy surfaces for the lowest three doublet states (1â€Š2Aâ€², 2â€Š2Aâ€², and 1â€Š2Aâ€³) of the BrH2 system. Journal of Chemical Physics, 2003, 119, 7838-7856.	1.2	26
14	Theoretical simulations on photoexcitation dynamics of the silver atom embedded in helium clusters. Journal of Chemical Physics, 2003, 119, 5478-5486.	1.2	24
15	Electron accommodation dynamics in the DNA base thymine. Journal of Chemical Physics, 2015, 143, 024312.	1.2	24
16	Theoretical study of an isotope effect on rate constants for the CH3+H2â†'CH4+H and CD3+H2â†'CD3H+H reactions using variational transition state theory and the multidimensional semiclassical tunneling method. Journal of Chemical Physics, 1999, 110, 10830-10842.	1.2	20
17	Quantum Dynamics Study on the Product Branching for the C(3P) + C2H2Reaction:Âcyclic-C3H versuslinear-C3Hâ€. Journal of Physical Chemistry A, 2006, 110, 361-366.	1.1	20
18	Theoretical study of the H+Br2 and Mu+Br2 reactions: A new ab initio potential energy surface and quantum dynamics calculations. Chemical Physics, 2007, 334, 109-116.	0.9	20

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19	The photodissociation dynamics of dichloroethenes at 214 and 220 nm. Journal of Chemical Physics, 1993, 99, 1703-1709.	1.2	19
20	Theoretical study of kinetic isotope effects on rate constants for the H2+C2Hâ†'H+C2H2 reaction and its isotopic variants. Journal of Chemical Physics, 2000, 113, 4060-4072.	1.2	19
21	An ab initio molecular orbital study of even-membered hydrogen cluster cations: H6+,â€‰H8+,â€‰H10+,â€‰H12+, and H14+. Journal of Chemical Physics, 1998, 109, 4327-4334.	1.2	18
22	Automated reaction path searches for spinâ€forbidden reactions. Journal of Computational Chemistry, 2018, 39, 1319-1326.	1.5	18
23	Ab initio study of small acetonitrile cluster anions. Journal of Chemical Physics, 2005, 122, 244307.	1.2	17
24	Photodissociation Dynamics of 1-Bromo-1-chloro-2,2,2-trifluoroethane at 157 nm. Journal of Physical Chemistry A, 1997, 101, 6647-6652.	1.1	15
25	Dynamical Calculations of Charge-Transfer-to-Solvent Excited States of Small I-(CH3CN)nClusters. Journal of Physical Chemistry A, 2006, 110, 7011-7018.	1.1	15
26	Dynamical calculations for the H+para, orthoâ€H2 reactions at low temperatures: Effect of rotational energy of reagent H2 molecule. Journal of Chemical Physics, 1991, 95, 4154-4159.	1.2	14
27	Preferential Câ€“Cl bond rupture from 1â€bromoâ€2â€chloroâ€1,1,2â€trifluoroethane following photoabsorption via n(Cl)â†'Ïƒ*(Câ€“Cl) transition. Journal of Chemical Physics, 1995, 103, 1710-1713.	1.2	12
28	Theoretical study of the non-Arrhenius temperature dependence of thermal rate constants for the H+H2Sâ†'H2+SH reaction. Journal of Chemical Physics, 1999, 111, 10529-10536.	1.2	12
29	Path-integral molecular dynamics simulations of BeO embedded in helium clusters: Formation of the stable HeBeO complex. Chemical Physics, 2008, 354, 38-43.	0.9	12
30	Positron binding to hydrocarbon molecules: calculation using the positronâ€“electron correlation polarization potential. European Physical Journal D, 2019, 73, 1.	0.6	12
31	Automated reaction path search calculations of spin-inversion mechanisms in the 6,4,2Nbâ€¯+â€¯C2H4 reaction. Computational and Theoretical Chemistry, 2019, 1155, 31-37.	1.1	12
32	Positronâ€“electron correlationâ€polarization potential model for positron binding in polyatomic molecules. Journal of Computational Chemistry, 2020, 41, 1576-1585.	1.5	12
33	Spinâ€inversion mechanisms in O 2 binding to a model heme complex revisited by density function theory calculations. Journal of Computational Chemistry, 2020, 41, 1130-1138.	1.5	12
34	COMPUTATIONAL METHODS FOR POLYATOMIC BIMOLECULAR REACTIONS. , 1998, , 1-33.		11
35	Theoretical calculations of the prereaction process of the H-Â·Â·Â·HD van der Waals molecule. Physical Chemistry Chemical Physics, 2000, 2, 665-670.	1.3	11
36	Theoretical analysis of the transition-state spectrum of the cyclooctatetraene unimolecular reaction: Three degree-of-freedom model calculations. Chemical Physics Letters, 2015, 634, 134-139.	1.2	11

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37	From photoelectron detachment spectra of BrHBrâ¯, BrDBrâ¯ and IHIâ¯, IDIâ¯ to vibrational bonding of BrMuBr and IMuI. Journal of Chemical Physics, 2015, 142, 164308.	1.2	11
38	On the ionâ€pair dissociation mechanisms in the small NaClÂ·(H 2 O) 6 cluster: A perspective from reaction path search calculations. Journal of Computational Chemistry, 2018, 39, 1835-1842.	1.5	11
39	Path integral molecular dynamics combined with discrete-variable-representation approach: the effect of solvation structures on vibrational spectra of Cl2 in helium clusters. Chemical Physics Letters, 2002, 362, 504-510.	1.2	10
40	Spinâ€inversion mechanisms in the reactions of transition metal cations (Sc⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 632 T reaction path search calculations. International Journal of Quantum Chemistry, 2019, 119, e25908.	1.0	10
41	Ab initio calculations for the N(2D) + CH4 reaction: Does the N(2D) atom really insert into CH bonds of alkane molecules?. International Journal of Quantum Chemistry, 2000, 79, 190-197.	1.0	9
42	Synthesis and Some Properties of Bis(ruthenocenyl)thiophene Derivatives â€“ Possible Spin-Coupling in the Two-Electron Oxidized Species of Dinuclear Ruthenocenes Bridged by Thiophene Derivatives. European Journal of Inorganic Chemistry, 2006, 2006, 4577-4588.	1.0	9
43	Computational Analysis of Two-State Reactivity in Î²-Hydride Elimination Mechanisms of Fe(II)â€“ and Co(II)â€“Alkyl Complexes Supported by Î²-Diketiminate Ligand. Organometallics, 2019, 38, 3582-3589.	1.1	9
44	A quantum reactive scattering study of the spin-forbidden CH(Xâ€Š2Î)+N2(Xâ€Š1Î£g+)â†'HCN(Xâ€Š1Î£+)+N(4S) reaction. Journal of Chemical Physics, 2002, 116, 7065-7072.	1.2	8
45	DEVELOPMENT OF A THREE-DIMENSIONAL AB INITIO POTENTIAL ENERGY SURFACE FOR THE Heâ€“Cl2(X) SYSTEM AND ITS APPLICATION TO SOLVATION STRUCTURES IN THE HenCl2 CLUSTERS. Journal of Theoretical and Computational Chemistry, 2005, 04, 197-207.	1.8	8
46	Photoexcited Ag ejection from a low-temperature He cluster: a simulation study by nonadiabatic Ehrenfest ring-polymer molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 13798-13806.	1.3	8
47	Construction of global ab initio potential energy surfaces for the HNS system and quantum dynamics calculations for the S(3P)+NH(X3Î£)â†'NS(X2Î)+H(2S) and N(4S)+SH(X2Î)â†'NS(X2Î)+H(2S) reactions. Chemical Physics, 2014, 439, 63-70.	0.9	7
48	First-principles simulations of transition state spectra of the I + HI and I + DI reactions and vibrational bonding in IMuI. Chemical Physics, 2015, 457, 51-56.	0.9	7
49	Ab Initio Molecular Orbital Study of the N(2D) + HCN(1Î£) Reaction. Journal of Physical Chemistry A, 1999, 103, 9323-9329.	1.1	6
50	Photodissociation dynamics of CBrClF2 at 157.6 nm. I. Experimental study using photofragment translational spectroscopy. Journal of Chemical Physics, 2001, 114, 1617-1623.	1.2	6
51	Ring-Polymer Molecular Dynamics Calculations of Thermal Rate Coefficients and Branching Ratios for the Interstellar H₃⁺ + CO â†' H₂ + HCO⁺/HOC⁺ Reaction and Its Deuterated Analogue. Journal of Physical Chemistry A, 2021, 125, 10750-10756.	1.1	6
52	Spin-orbit branching in the collision-induced dissociation reaction of He(1S0)+HF(Xâ€Š1Î£0+)â†'He(1S0)+H(2S1/2)+F(2P3/2,1/2). Journal of Chemical Physics, 2001, 115, 6385-6393.	1.2	5
53	Semiclassical dynamics of electron attachment to guanineâ€“cytosine base pair. Chemical Physics Letters, 2015, 625, 174-178.	1.2	5
54	Reduction of OH vibrational frequencies in amino acids by positron attachment. Journal of Computational Chemistry, 2018, 39, 2060-2066.	1.5	5

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55	Quantum Simulation Verifies the Stability of an 18â€Coordinated Actiniumâ€“Helium Complex. Chemistry - A European Journal, 2018, 24, 12716-12721.	1.7	5
56	Hydration Effect on Positron Binding Ability of Proline: Positron Attachment Induces Proton-Transfer To Form Zwitterionic Structure. Journal of Physical Chemistry A, 2019, 123, 1217-1224.	1.1	5
57	Quantum dynamics calculation of the annihilation spectrum for positronâ€“proline scattering. Computational and Theoretical Chemistry, 2019, 1147, 1-7.	1.1	5
58	Positron binding in chloroethenes: Modeling positron-electron correlation-polarization potentials for molecular calculations. Physical Review A, 2020, 102, .	1.0	5
59	Reduced-Dimensionality Quantum Dynamics Study of the 3Fe(CO)4 + H2 â†' 1FeH2(CO)4 Spin-inversion Reaction. Molecules, 2020, 25, 882.	1.7	5
60	Nuclear Quantum Effects in H₂ Adsorption Dynamics on a Small Water Cluster Studied with Ring-Polymer Molecular Dynamics Simulations. ACS Earth and Space Chemistry, 2022, 6, 1390-1396.	1.2	5
61	Tunneling in the H2S+O(3P)â†'HS+OH reaction: A theoretical study. Journal of Chemical Physics, 1996, 104, 1953-1957.	1.2	4
62	Ab initio prediction of vibrational states of the HeCuF helium-containing complex. Chemical Physics Letters, 2012, 539-540, 15-18.	1.2	4
63	Franckâ€“Condon simulations of transition-state spectra for the OH + H₂O and OD + D₂O reactions. Physical Chemistry Chemical Physics, 2020, 22, 20685-20692.	1.3	4
64	Application of Reaction Path Search Calculations to Potential Energy Surface Fits. Journal of Physical Chemistry A, 2021, 125, 3994-4002.	1.1	4
65	Two-state reactivity in the acetylene cyclotrimerization reaction catalyzed by a single atomic transition-metal ion: The case for V+ and Fe+. Computational and Theoretical Chemistry, 2022, 1211, 113682.	1.1	4
66	Real wave packet and flux analysis studies of the H + F₂ â†' HF + F reaction. International Journal of Quantum Chemistry, 2012, 112, 2348-2354.	1.0	3
67	The effects of water microsolvation on the C 2 O 4 â^' â†" CO 2 Â·CO 2 â^' core switching reaction: Perspective from exploration of pathways on the potential energy surfaces of small [(CO 2) 2 (H 2 O) n] â^' (n = 1 and 2) clusters. Computational and Theoretical Chemistry, 2017, 1105, 61-68.	1.1	3
68	Quantum dynamics calculations for e+â€¯+â€¯LiHâ€¯â†'â€¯Li+â€¯+â€¯[Hâ^';â€¯e+] dissociative positron attachment using a pseudopotential model. Computational and Theoretical Chemistry, 2018, 1123, 135-141.	1.1	3
69	SN1 reaction mechanisms of tert-butyl chloride in aqueous solution: What can be learned from reaction path search calculations and trajectory calculations for small hydrated clusters?. Computational and Theoretical Chemistry, 2021, 1201, 113278.	1.1	3
70	Nonadiabatic relaxation dynamics of water anion cluster and its isotope effects by ring-polymer molecular dynamics simulation. International Journal of Quantum Chemistry, 2014, 114, 636-641.	1.0	2
71	Nonadiabatic quantum dynamics calculations of transition state spectroscopy of I + HI and I + DI reactions: the existence of long life vibrational bonding resonances. Physical Chemistry Chemical Physics, 2017, 19, 29125-29133.	1.3	2
72	Nuclear quantum effects in the direct ionization process of pure helium clusters: path-integral and ring-polymer molecular dynamics simulations on the diatomics-in-molecule potential energy surfaces. Physical Chemistry Chemical Physics, 2018, 20, 26489-26499.	1.3	2

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73	Theoretical calculations of photoelectron spectrum of (Auâ€“CO2)â^' anion. Computational and Theoretical Chemistry, 2018, 1140, 56-62.	1.1	2
74	Theoretical calculation of positron annihilation spectrum using positronâ€electron correlationâ€polarization potential. International Journal of Quantum Chemistry, 2020, 120, e26376.	1.0	2
75	Spinâ€inversion mechanisms in O 2 binding to a model heme compound: A perspective from nonadiabatic wave packet calculations. Journal of Computational Chemistry, 2020, 41, 2527-2537.	1.5	2
76	Quantum calculations of the photoelectron spectra of the OHâ^'Â·NH3 anion: implications for OH + NH3 â†' H2O + NH2 reaction dynamics. Physical Chemistry Chemical Physics, 2021, 23, 6950-6958.	1.3	2
77	New Perspectives in Muonium Chemical Reactions. Journal of Computer Chemistry Japan, 2016, 15, 119-123.	0.0	2
78	Metastable dissociation of multiphoton-ionized xenon clusters. Rapid Communications in Mass Spectrometry, 1991, 5, 303-306.	0.7	1
79	Fundamental peak disappears upon binding of a noble gas: a case of the vibrational spectrum of PtCO in an argon matrix. Physical Chemistry Chemical Physics, 2018, 20, 3296-3302.	1.3	1
80	Theoretical Analysis of the Formylmethylene Anion Photoelectron Spectrum: Importance of Wolff Rearrangement Dynamics. Journal of Physical Chemistry A, 2020, 124, 9721-9728.	1.1	1
81	Quantum dynamics analysis of transition-state spectrum for the SH + H2S â†' H2S + SH reaction. Physical Chemistry Chemical Physics, 2020, 22, 19845-19854.	1.3	1
82	Theoretical study of the dissociative photodetachment dynamics of the hydrated superoxide anion cluster. Physical Chemistry Chemical Physics, 2021, 23, 16958-16965.	1.3	1
83	On-the-Fly Ring-Polymer Molecular Dynamics Calculations of the Dissociative Photodetachment Process of the Oxalate Anion. Molecules, 2021, 26, 7250.	1.7	1
84	Contribution of vibrational overtone excitations to positron annihilation rates for benzene and naphthalene. Physical Review A, 2021, 104, .	1.0	1
85	Ionization dynamics of Ne-doped helium clusters at low temperature: Ring-polymer molecular dynamics simulations including electronically nonadiabatic transitions. Computational and Theoretical Chemistry, 2019, 1163, 112537.	1.1	0
86	Theoretical Study on the Spectroscopic Observation of Intersystem Crossing between ³B₁ and ¹A₁ States of GeH₂ Using the GeH₂^{â€“} (²B₁) Anion. Journal of Physical Chemistry A, 2019, 123, 5734-5740.	1.1	0
87	An Invitation to Muon and Muonium Chemistry Research. Journal of Computer Chemistry Japan, 2020, 19, 51-56.	0.0	0