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	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
2	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
3	Theoretical study of the dissociative photodetachment dynamics of the hydrated superoxide anion cluster. Physical Chemistry Chemical Physics, 2021, 23, 16958-16965.	1.3	1
4	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
5	Application of Reaction Path Search Calculations to Potential Energy Surface Fits. Journal of Physical Chemistry A, 2021, 125, 3994-4002.	1.1	4
6	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
7	On-the-Fly Ring-Polymer Molecular Dynamics Calculations of the Dissociative Photodetachment Process of the Oxalate Anion. Molecules, 2021, 26, 7250.	1.7	1
8	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
9	Contribution of vibrational overtone excitations to positron annihilation rates for benzene and naphthalene. Physical Review A, 2021, 104, .	1.0	1
10	Theoretical calculation of positron annihilation spectrum using positronâ€electron correlationâ€polarization potential. International Journal of Quantum Chemistry, 2020, 120, e26376.	1.0	2
11	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
12	Positron binding in chloroethenes: Modeling positron-electron correlation-polarization potentials for molecular calculations. Physical Review A, 2020, 102, .	1.0	5
13	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
14	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
15	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
16	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
17	Positronâ€“electron correlationâ€polarization potential model for positron binding in polyatomic molecules. Journal of Computational Chemistry, 2020, 41, 1576-1585.	1.5	12
18	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

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19	An Invitation to Muon and Muonium Chemistry Research. Journal of Computer Chemistry Japan, 2020, 19, 51-56.	0.0	0
20	Positron binding to hydrocarbon molecules: calculation using the positronâ€“electron correlation polarization potential. European Physical Journal D, 2019, 73, 1.	0.6	12
21	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
22	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
23	Spinâ€inversion mechanisms in the reactions of transition metal cations (Sc⁺,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5 reaction path search calculations. International Journal of Quantum Chemistry, 2019, 119, e25908.	1.0	10
24	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
25	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
26	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
27	Quantum dynamics calculation of the annihilation spectrum for positronâ€“proline scattering. Computational and Theoretical Chemistry, 2019, 1147, 1-7.	1.1	5
28	Automated reaction path searches for spinâ€forbidden reactions. Journal of Computational Chemistry, 2018, 39, 1319-1326.	1.5	18
29	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
30	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
31	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
32	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
33	Reduction of OH vibrational frequencies in amino acids by positron attachment. Journal of Computational Chemistry, 2018, 39, 2060-2066.	1.5	5
34	Theoretical calculations of photoelectron spectrum of (Auâ€“CO2)â‹¯ anion. Computational and Theoretical Chemistry, 2018, 1140, 56-62.	1.1	2
35	Quantum Simulation Verifies the Stability of an 18â€Coordinated Actiniumâ€“Helium Complex. Chemistry - A European Journal, 2018, 24, 12716-12721.	1.7	5
36	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

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37	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
38	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
39	New Perspectives in Muonium Chemical Reactions. Journal of Computer Chemistry Japan, 2016, 15, 119-123.	0.0	2
40	Electron accommodation dynamics in the DNA base thymine. Journal of Chemical Physics, 2015, 143, 024312.	1.2	24
41	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
42	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
43	Semiclassical dynamics of electron attachment to guanineâ€"cytosine base pair. Chemical Physics Letters, 2015, 625, 174-178.	1.2	5
44	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
45	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
46	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
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	Ab initio prediction of vibrational states of the HeCuF helium-containing complex. Chemical Physics Letters, 2012, 539-540, 15-18.	1.2	4
49	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
50	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
51	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
52	Accurate ab initio electronic structure calculations of the stable helium complex: HeBeO. Chemical Physics Letters, 2008, 454, 1-6.	1.2	28
53	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
54	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

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55	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
56	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
57	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
58	Ab initio study of small acetonitrile cluster anions. Journal of Chemical Physics, 2005, 122, 244307.	1.2	17
59	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
60	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
61	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
62	Theoretical simulations on photoexcitation dynamics of the silver atom embedded in helium clusters. Journal of Chemical Physics, 2003, 119, 5478-5486.	1.2	24
63	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
64	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
65	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
66	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
67	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
68	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
69	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
70	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
71	Three-dimensional quantum reactive scattering calculations for the nonadiabatic (D+H2)+ reaction system. Journal of Chemical Physics, 2000, 112, 2615-2622.	1.2	60
72	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

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73	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
74	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
75	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
76	Ab Initio Molecular Orbital Study of the N(2D) + HCN(1Î£) Reaction. Journal of Physical Chemistry A, 1999, 103, 9323-9329.	1.1	6
77	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
78	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
79	COMPUTATIONAL METHODS FOR POLYATOMIC BIMOLECULAR REACTIONS. , 1998, , 1-33.		11
80	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
81	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
82	Tunneling in the H2S+O(3P)â†'HS+OH reaction: A theoretical study. Journal of Chemical Physics, 1996, 104, 1953-1957.	1.2	4
83	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
84	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
85	The photodissociation dynamics of dichloroethenes at 214 and 220 nm. Journal of Chemical Physics, 1993, 99, 1703-1709.	1.2	19
86	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
87	Metastable dissociation of multiphoton-ionized xenon clusters. Rapid Communications in Mass Spectrometry, 1991, 5, 303-306.	0.7	1