Wensheng Bian

List of Publications by Year
in descending order

84	1,702	304743	330143
papers	citations	22 h-index	37 g-index

85	85	85	905
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	van der Waals Interactions in the Cl + HD Reaction. Science, 1999, 286, 1713-1716.	12.6	287
2	Global ab initio potential energy surfaces for the ClH2 reactive system. Journal of Chemical Physics, 2000, 112, 220-229.	3.0	140
3	Accurate quantum dynamics of electronically nonadiabatic chemical reactions in the DH2+ system. Journal of Chemical Physics, 2002, 116, 654-665.	3.0	76
4	Quantum-mechanical calculation of the thermal rate constant for the H2+Clâ†'H+HCl reaction. Chemical Physics Letters, 1999, 313, 647-654.	2.6	74
5	ACCURATE AND HIGHLY EFFICIENT CALCULATION OF THE O(1D)HCl VIBRATIONAL BOUND STATES, USING A COMBINATION OF METHODS. Journal of Theoretical and Computational Chemistry, 2003, 02, 583-597.	1.8	47
6	Influence of Solvent Polarity and Hydrogen Bonding on the Electronic Transition of Coumarin 120: A TDDFT Study. ChemPhysChem, 2008, 9, 1593-1602.	2.1	42
7	Dynamical importance of van der Waals saddle and excited potential surface in C(1D)+D2 complex-forming reaction. Nature Communications, 2017, 8, 14094.	12.8	40
8	Extensive theoretical study on electronically excited states and predissociation mechanisms of sulfur monoxide including spinâ€“orbit coupling. Journal of Computational Chemistry, 2011, 32, 1577-1588.	3.3	34
9	Accurate and highly efficient calculation of the highly excited pure OH stretching resonances of O(1D)HCl, using a combination of methods. Journal of Chemical Physics, 2004, 121, 4467-4478.	3.0	31
10	Efficient quantum calculations of vibrational states of vinylidene in full dimensionality: A scheme with combination of methods. Journal of Chemical Physics, 2008, 129, 024111.	3.0	31
11	Quasiclassical trajectory study of H+SiH ₄ reactions in full-dimensionality reveals atomic-level mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13180-13185.	7.1	29
12	Potential energy surface intersections in the C(D1)H2 reactive system. Journal of Chemical Physics, 2006, 125, 074306.	3.0	28
13	The hydrogen tunneling splitting in malonaldehyde: A full-dimensional time-independent quantum mechanical method. Journal of Chemical Physics, 2016, 145, 074309.	3.0	28
14	Investigation of the structures and electronic spectra for coumarin 6 through TD-DFT calculations including PCM solvation. Computational and Theoretical Chemistry, 2007, 818, 43-49.	1.5	27
15	Quantum reaction dynamics of the C(1D) + H2(D2) â†' CH(D) + H(D) on a new potential energy surface. Journal of Chemical Physics, 2013, 139, 014306.	3.0	27
16	Quantum mechanical differential and integral cross sections for the C(1D) + H2(Î½ = 0, j =) Tj ETQq0 0 0 rgBT /Overlock 1	3.0	27
17	Extensive theoretical study on electronically excited states of calcium monochloride: Molecular laser cooling and production of ultracold chlorine atoms. Journal of Chemical Physics, 2016, 144, 184302.	3.0	27
18	Conical intersectionâ€“regulated intermediates in bimolecular reactions: Insights from C(¹) Tj ETQq0 0 0 rgBT /Overlock 1	10.3	27

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19	A Theoretical Study of the Reaction of O(3P) with Isobutene. Journal of Physical Chemistry A, 2006, 110, 7858-7866.	2.5	25
20	Full-dimensional quantum dynamics study of vinylideneâ€“acetylene isomerization: a scheme using the normal mode Hamiltonian. Physical Chemistry Chemical Physics, 2011, 13, 2052-2061.	2.8	24
21	Electronically excited-state properties and predissociation mechanisms of phosphorus monofluoride: A theoretical study including spinâ€“orbit coupling. Journal of Chemical Physics, 2012, 137, 014313.	3.0	24
22	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM I.. Journal of Theoretical and Computational Chemistry, 2002, 01, 263-273.	1.8	23
23	Global analytical ab initio ground-state potential energy surface for the C(1D)+H2 reactive system. Journal of Chemical Physics, 2014, 140, 234301.	3.0	20
24	Quasiclassical Trajectory Study of the C(¹D) + H₂ â†' CH + H Reaction on a New Global ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2014, 118, 4235-4242.	2.5	20
25	The dynamics of the C(1D)+H2/D2/HD reactions at low temperature. Journal of Chemical Physics, 2018, 148, 234305.	3.0	20
26	Theoretical Investigation of the Reaction of Co+with OCS. Journal of Physical Chemistry A, 2003, 107, 8618-8622.	2.5	19
27	Mode-Specific Tunneling Splittings for a Sequential Double-Hydrogen Transfer Case: An Accurate Quantum Mechanical Scheme. Journal of Physical Chemistry Letters, 2015, 6, 1824-1829.	4.6	19
28	Ultrafast Deep-Ultraviolet Laser Ionization Mass Spectrometry Applicable To Identify Phenylenediamine Isomers. Analytical Chemistry, 2018, 90, 10635-10640.	6.5	19
29	Theoretical Study of the Reactivity of Fe+ toward OCS. Journal of Physical Chemistry A, 2003, 107, 8955-8960.	2.5	18
30	Efficient quantum calculation of the vibrational states of acetylene. Chemical Physics, 2012, 400, 1-7.	1.9	18
31	Accurate Quantum Dynamics Study on the Resonance Decay of Vinylidene. ChemPhysChem, 2011, 12, 2419-2422.	2.1	17
32	Extensive Theoretical Study on Various Low-Lying Electronic States of Silicon Monochloride Cation Including Spinâ^'Orbit Coupling. Journal of Physical Chemistry A, 2009, 113, 1678-1685.	2.5	16
33	Laser cooling of CaBr molecules and production of ultracold Br atoms: A theoretical study including spinâ€“orbit coupling. Journal of Chemical Physics, 2017, 146, 134309.	3.0	16
34	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM II.. Journal of Theoretical and Computational Chemistry, 2002, 01, 275-284.	1.8	15
35	Accurate quantum mechanical study of the Renner-Teller effect in the singlet CH2. Journal of Chemical Physics, 2011, 135, 154303.	3.0	15
36	Double Proton Transfer in the Dimer of Formic Acid: An Efficient Quantum Mechanical Scheme. Frontiers in Chemistry, 2019, 7, 676.	3.6	15

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37	van der Waals interactions in bimolecular reactions. Chinese Journal of Chemical Physics, 2019, 32, 157-166.	1.3	15
38	Investigation of the structures and electronic spectra of two coumarins with heterocyclic substituents through TD-DFT calculations. Computational and Theoretical Chemistry, 2008, 859, 73-78.	1.5	14
39	Theoretical Study on the Photodegradation Mechanism of Nonaâ€BDEs in Methanol. ChemPhysChem, 2013, 14, 1264-1271.	2.1	13
40	Direct solution of the many-body SchrÃ¶dinger equation in the hyperspherical formalism: Formulation of theCFHH-GLFmethod. International Journal of Quantum Chemistry, 1994, 51, 285-291.	2.0	12
41	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM III.. Journal of Theoretical and Computational Chemistry, 2002, 01, 285-293.	1.8	12
42	Quasiclassical trajectory study of the C(¹D) + HD reaction. RSC Advances, 2017, 7, 34348-34355.	3.6	12
43	A Theoretical Study on Laser Cooling Feasibility of Group IVA Hydrides XH (X = Si, Ge, Sn, and Pb): The Role of Electronic State Crossing. Frontiers in Chemistry, 2020, 8, 20.	3.6	12
44	Theoretical study of rate constants and kinetic isotope effects for reactions in the ClH2 system using variational transition state theory. Chemical Physics Letters, 2004, 391, 354-360.	2.6	11
45	The Effect of Explicit Solvent on Photodegradation of Decabromodiphenyl Ether in Toluene: Insights from Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 5291-5298.	2.5	11
46	Laser cooling of copper monofluoride: a theoretical study including spinâ€“orbit coupling. RSC Advances, 2016, 6, 100568-100576.	3.6	11
47	A theoretical study on laser cooling of silicon monofluoride. Chemical Physics, 2017, 485-486, 29-34.	1.9	11
48	Direct solution of the many-body schrï¿½udinger equation in the hyperspherical formalism: Application of the HH-GLF method to the positronium ione+e?e+. International Journal of Quantum Chemistry, 1994, 50, 395-400.	2.0	10
49	Cl+HD reaction dynamics from quasiclassical trajectory calculation on a new ab initio potential energy surface. Chemical Physics, 2001, 272, 61-68.	1.9	10
50	PARTIAL POTENTIAL ENERGY SURFACE AND ITS APPLICATIONS IN REACTIVE RESONANCES. Journal of Theoretical and Computational Chemistry, 2004, 03, 543-553.	1.8	10
51	Study of electronic and spectroscopic properties on a newly synthesized red fluorescent material. Journal of Chemical Physics, 2006, 124, 174711.	3.0	10
52	Extensive theoretical study on the low-lying electronic states of silicon monofluoride cation including spin-orbit coupling. Journal of Computational Chemistry, 2008, 29, 256-265.	3.3	10
53	Quasiclassical trajectory study of the SiH4+Hâ†'SiH3+H2 reaction on a global ab initio potential energy surface. Journal of Chemical Physics, 2008, 129, 084309.	3.0	10
54	A theoretical study on the reaction mechanisms of O(³P)+1â€butene. International Journal of Quantum Chemistry, 2012, 112, 858-872.	2.0	10

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55	A global 12-dimensional ab initio potential energy surface and dynamical studies for the SiH4+Hâ†'SiH3+H2 reaction. Journal of Chemical Physics, 2006, 124, 234311.	3.0	9
56	Kinetic study on the H+SiH4 abstraction reaction using an ab initio potential energy surface. Journal of Chemical Physics, 2011, 134, 024315.	3.0	9
57	Efficient Quantum Mechanical Calculations of Mode-Specific Tunneling Splittings upon Fundamental Excitation in the Dimer of Formic Acid. Journal of Physical Chemistry A, 2020, 124, 6536-6543.	2.5	9
58	Novel insight into the mechanism of the reaction of Fe+ with ethane. Computational and Theoretical Chemistry, 2003, 635, 239-245.	1.5	8
59	Quantum Dynamics Study of the C(¹D) + HD Reaction on the Ã£¹Aâ€² and bÌƒ¹Aâ€³ Potential Energy Surfaces. Journal of Physical Chemistry A, 2020, 124, 801-809.	2.5	8
60	Dynamics and kinetics of the Si(¹D) + H₂/D₂ reactions on a new global ab initio potential energy surface. Physical Chemistry Chemical Physics, 2021, 23, 6141-6153.	2.8	8
61	A Theoretical Study of the Mechanism and Kinetics of F+N3 Reactions. ChemPhysChem, 2006, 7, 1786-1794.	2.1	7
62	A theoretical study on laser cooling feasibility of XH (X = As, Sb and Bi): effects of intersystem crossings and spinâ€“orbit couplings. Physical Chemistry Chemical Physics, 2022, 24, 10114-10123.	2.8	7
63	Reaction Cross Sections and Rate Constants for the Cl + H2 Reaction from Quasiclassical Trajectory Calculation on Two New ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2002, 106, 176-180.	2.5	5
64	The density functional theory study on the 1,3-dipolar cycloaddition of carbon-methyl nitrone with acrlonitrile. Computational and Theoretical Chemistry, 2004, 679, 73-87.	1.5	5
65	New ab Initio Potential Energy Surfaces for the Renner-Teller Coupled <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M1"><mml:msup><mml:mrow><mml:mn mathvariant="bold">1</mml:mn></mml:mrow><mml:mrow><mml:mn mathvariant="bold">1</mml:mn></mml:mrow></mml:msup><mml:msup><mml:mrow><mml:mi>A</mml:mi></mml:mrow><mml:mr and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" id="M2"><mml:msup><mml:mrow><mml:mn>1</mml:mn> Advances in Physical Chemistry, 2012, 2012, 1-12.	2.0	5
66	Theoretical Study on Mechanism and Kinetics of Reaction of O(3P) with Propane. Chinese Journal of Chemical Physics, 2016, 29, 430-436.	1.3	5
67	Accurate quantum mechanical calculations on deuterated vinylidene isomerization. Journal of Chemical Physics, 2020, 153, 054309.	3.0	5
68	Direct solution of the many-body SchrÃ¶dinger equation in the hyperspherical formalism: Application of the CFHH-GLF method to a set of He-like systems. International Journal of Quantum Chemistry, 1995, 54, 273-279.	2.0	4
69	Direct solution of the SchrÃ¶dinger equation for some muonic molecules. Chemical Physics, 1999, 242, 195-202.	1.9	4
70	The effect of metal electron cloud on the luminescence characteristics of organic ligands: An experimental and theoretical investigation. Science Bulletin, 2011, 56, 479-483.	1.7	4
71	Quantum dynamics study of resonance states of vinylidene using normal mode Hamiltonian. AIP Conference Proceedings, 2012, , .	0.4	4
72	Excellent Ultracold Molecular Candidates From Group VA Hydrides: Whether Do Nearby Electronic States Interfere?. Frontiers in Chemistry, 2021, 9, 778292.	3.6	4

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73	Fourier transform approach to potential harmonics. International Journal of Quantum Chemistry, 1997, 63, 5-14.	2.0	3
74	Structure and electronic properties for a newly synthesized red fluorescent material. Computational and Theoretical Chemistry, 2006, 770, 73-77.	1.5	3
75	Direct solution of H. Theoretica Chimica Acta, 1995, 92, 135.	0.8	3
76	Production of ultracold CaCCH and SrCCH molecules by direct laser cooling: A theoretical study based on accurate ab initio calculations. Journal of Chemical Physics, 2021, 155, 204304.	3.0	3
77	Accurate quantum dynamics of the simplest isomerization system involving double-H transfer. Chinese Journal of Chemical Physics, 2022, 35, 185-192.	1.3	3
78	A potential harmonic method for the three-body coulomb problem. Theoretical Chemistry Accounts, 1997, 98, 110-116.	1.4	2
79	Theoretical study on the photodegradation reaction of deca-BDE in THF in the presence of furan. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	2
80	Ring polymer molecular dynamics of the C(1D)+H2 reaction on the most recent potential energy surfaces. Chinese Journal of Chemical Physics, 0, , .	1.3	2
81	A fullyab initio potential energy surface for ClH2 reactive system. Science in China Series B: Chemistry, 2000, 43, 396-404.	0.8	1
82	1H NMR relaxation and theoretical calculation study on Tris(pentafluorophenyl)borane as a catalyst in preparation of Poly(carborane-siloxane) polymers. Polymer Testing, 2019, 73, 412-417.	4.8	1
83	Direct solution of H 2 + Schrï¿½dinger equation using the hyperspherical coordinate. Theoretica Chimica Acta, 1995, 92, 135-147.	0.8	0
84	An ab initio study of the potential energy surfaces for the collision between a Cs atom and an I2 molecule. Canadian Journal of Chemistry, 2004, 82, 1216-1222.	1.1	0