

# Wensheng Bian

## List of Publications by Year in descending order

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84  
papers

1,702  
citations

304743

22  
h-index

330143

37  
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85  
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85  
docs citations

85  
times ranked

905  
citing authors

#	ARTICLE	IF	CITATIONS
1	A theoretical study on laser cooling feasibility of XH (X = As, Sb and Bi): effects of intersystem crossings and spin-orbit couplings. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10114-10123.	2.8	7
2	Accurate quantum dynamics of the simplest isomerization system involving double-H transfer. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 185-192.	1.3	3
3	Dynamics and kinetics of the Si( <sup>1</sup> D) + H <sub>2</sub> /D <sub>2</sub> reactions on a new global <i>ab initio</i> potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6141-6153.	2.8	8
4	Production of ultracold CaCCH and SrCCH molecules by direct laser cooling: A theoretical study based on accurate <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2021, 155, 204304.	3.0	3
5	Excellent Ultracold Molecular Candidates From Group VA Hydrides: Whether Do Nearby Electronic States Interfere?. <i>Frontiers in Chemistry</i> , 2021, 9, 778292.	3.6	4
6	Efficient Quantum Mechanical Calculations of Mode-Specific Tunneling Splittings upon Fundamental Excitation in the Dimer of Formic Acid. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6536-6543.	2.5	9
7	Accurate quantum mechanical calculations on deuterated vinylidene isomerization. <i>Journal of Chemical Physics</i> , 2020, 153, 054309.	3.0	5
8	Quantum Dynamics Study of the C( <sup>1</sup> D) + HD Reaction on the $\tilde{X}^1A'$ and $\tilde{b}^1A'$ Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2020, 124, 801-809.	2.5	8
9	A Theoretical Study on Laser Cooling Feasibility of Group IVA Hydrides XH (X = Si, Ge, Sn, and Pb): The Role of Electronic State Crossing. <i>Frontiers in Chemistry</i> , 2020, 8, 20.	3.6	12
10	Double Proton Transfer in the Dimer of Formic Acid: An Efficient Quantum Mechanical Scheme. <i>Frontiers in Chemistry</i> , 2019, 7, 676.	3.6	15
11	van der Waals interactions in bimolecular reactions. <i>Chinese Journal of Chemical Physics</i> , 2019, 32, 157-166.	1.3	15
12	Conical intersection-regulated intermediates in bimolecular reactions: Insights from C( <sup>1</sup> D) + H <sub>2</sub> /D <sub>2</sub> reactions. <i>Journal of Chemical Physics</i> , 2019, 150, 103207.	10.3	27
13	<sup>1</sup> H NMR relaxation and theoretical calculation study on Tris(pentafluorophenyl)borane as a catalyst in preparation of Poly(carborane-siloxane) polymers. <i>Polymer Testing</i> , 2019, 73, 412-417.	4.8	1
14	The dynamics of the C( <sup>1</sup> D)+H <sub>2</sub> /D <sub>2</sub> /HD reactions at low temperature. <i>Journal of Chemical Physics</i> , 2018, 148, 234305.	3.0	20
15	Ultrafast Deep-Ultraviolet Laser Ionization Mass Spectrometry Applicable To Identify Phenylenediamine Isomers. <i>Analytical Chemistry</i> , 2018, 90, 10635-10640.	6.5	19
16	Dynamical importance of van der Waals saddle and excited potential surface in C( <sup>1</sup> D)+D <sub>2</sub> complex-forming reaction. <i>Nature Communications</i> , 2017, 8, 14094.	12.8	40
17	A theoretical study on laser cooling of silicon monofluoride. <i>Chemical Physics</i> , 2017, 485-486, 29-34.	1.9	11
18	Laser cooling of CaBr molecules and production of ultracold Br atoms: A theoretical study including spin-orbit coupling. <i>Journal of Chemical Physics</i> , 2017, 146, 134309.	3.0	16

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19	Quasiclassical trajectory study of the C( <sup>1</sup> D) + HD reaction. RSC Advances, 2017, 7, 34348-34355.	3.6	12
20	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
21	Laser cooling of copper monofluoride: a theoretical study including spin-orbit coupling. RSC Advances, 2016, 6, 100568-100576.	3.6	11
22	The hydrogen tunneling splitting in malonaldehyde: A full-dimensional time-independent quantum mechanical method. Journal of Chemical Physics, 2016, 145, 074309.	3.0	28
23	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
24	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
25	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
26	Quantum mechanical differential and integral cross sections for the C(1D) + H <sub>2</sub> ( <sup>1</sup> / <sub>2</sub> ) = 0, <sup>1</sup> / <sub>2</sub> => Tj ETQq0,0,0 rgBT /Overlock 1	3.0	27
27	Global analytical <i>ab initio</i> ground-state potential energy surface for the C(1D)+H <sub>2</sub> reactive system. Journal of Chemical Physics, 2014, 140, 234301.	3.0	20
28	Quasiclassical Trajectory Study of the C( <sup>1</sup> D) + H <sub>2</sub> → CH + H Reaction on a New Global <i>ab initio</i> Potential Energy Surface. Journal of Physical Chemistry A, 2014, 118, 4235-4242.	2.5	20
29	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
30	Theoretical Study on the Photodegradation Mechanism of Nonabrominated BDEs in Methanol. ChemPhysChem, 2013, 14, 1264-1271.	2.1	13
31	Quantum reaction dynamics of the C(1D) + H <sub>2</sub> (D <sub>2</sub> ) → CH(D) + H(D) on a new potential energy surface. Journal of Chemical Physics, 2013, 139, 014306.	3.0	27
32	Electronically excited-state properties and predissociation mechanisms of phosphorus monofluoride: A theoretical study including spin-orbit coupling. Journal of Chemical Physics, 2012, 137, 014313.	3.0	24
33	New <i>ab initio</i> Potential Energy Surfaces for the Renner-Teller Coupled $\text{C}(\text{1D}) + \text{H}_2$ and $\text{C}(\text{1D}) + \text{D}_2$ Reaction. <i>Advances in Physical Chemistry</i> , 2012, 2012, 1-12.	2.0	5
34	Quantum dynamics study of resonance states of vinylidene using normal mode Hamiltonian. AIP Conference Proceedings, 2012, , .	0.4	4
35	A theoretical study on the reaction mechanisms of O( <sup>3</sup> P)+1-butene. International Journal of Quantum Chemistry, 2012, 112, 858-872.	2.0	10
36	Efficient quantum calculation of the vibrational states of acetylene. Chemical Physics, 2012, 400, 1-7.	1.9	18

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37	Full-dimensional quantum dynamics study of vinylidene's acetylene isomerization: a scheme using the normal mode Hamiltonian. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2052-2061.	2.8	24
38	The effect of metal electron cloud on the luminescence characteristics of organic ligands: An experimental and theoretical investigation. <i>Science Bulletin</i> , 2011, 56, 479-483.	1.7	4
39	Accurate Quantum Dynamics Study on the Resonance Decay of Vinylidene. <i>ChemPhysChem</i> , 2011, 12, 2419-2422.	2.1	17
40	Extensive theoretical study on electronically excited states and predissociation mechanisms of sulfur monoxide including spin-orbit coupling. <i>Journal of Computational Chemistry</i> , 2011, 32, 1577-1588.	3.3	34
41	Kinetic study on the H+SiH <sub>4</sub> abstraction reaction using an <i>ab initio</i> potential energy surface. <i>Journal of Chemical Physics</i> , 2011, 134, 024315.	3.0	9
42	Accurate quantum mechanical study of the Renner-Teller effect in the singlet CH <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2011, 135, 154303.	3.0	15
43	Quasiclassical trajectory study of H+SiH <sub>4</sub> reactions in full-dimensionality reveals atomic-level mechanisms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 13180-13185.	7.1	29
44	Extensive Theoretical Study on Various Low-Lying Electronic States of Silicon Monochloride Cation Including Spin-Orbit Coupling. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1678-1685.	2.5	16
45	Investigation of the structures and electronic spectra of two coumarins with heterocyclic substituents through TD-DFT calculations. <i>Computational and Theoretical Chemistry</i> , 2008, 859, 73-78.	1.5	14
46	Influence of Solvent Polarity and Hydrogen Bonding on the Electronic Transition of Coumarin 120: A TDDFT Study. <i>ChemPhysChem</i> , 2008, 9, 1593-1602.	2.1	42
47	Extensive theoretical study on the low-lying electronic states of silicon monofluoride cation including spin-orbit coupling. <i>Journal of Computational Chemistry</i> , 2008, 29, 256-265.	3.3	10
48	Efficient quantum calculations of vibrational states of vinylidene in full dimensionality: A scheme with combination of methods. <i>Journal of Chemical Physics</i> , 2008, 129, 024111.	3.0	31
49	Quasiclassical trajectory study of the SiH <sub>4</sub> +H <sup>+</sup> SiH <sub>3</sub> +H <sub>2</sub> reaction on a global <i>ab initio</i> potential energy surface. <i>Journal of Chemical Physics</i> , 2008, 129, 084309.	3.0	10
50	Investigation of the structures and electronic spectra for coumarin 6 through TD-DFT calculations including PCM solvation. <i>Computational and Theoretical Chemistry</i> , 2007, 818, 43-49.	1.5	27
51	A Theoretical Study of the Reaction of O(3P) with Isobutene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7858-7866.	2.5	25
52	Structure and electronic properties for a newly synthesized red fluorescent material. <i>Computational and Theoretical Chemistry</i> , 2006, 770, 73-77.	1.5	3
53	A Theoretical Study of the Mechanism and Kinetics of F+N <sub>3</sub> Reactions. <i>ChemPhysChem</i> , 2006, 7, 1786-1794.	2.1	7
54	Study of electronic and spectroscopic properties on a newly synthesized red fluorescent material. <i>Journal of Chemical Physics</i> , 2006, 124, 174711.	3.0	10

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55	A global 12-dimensional ab initio potential energy surface and dynamical studies for the SiH <sub>4</sub> +H <sup>+</sup> SiH <sub>3</sub> +H <sub>2</sub> reaction. Journal of Chemical Physics, 2006, 124, 234311.	3.0	9
56	Potential energy surface intersections in the C(D1)H <sub>2</sub> reactive system. Journal of Chemical Physics, 2006, 125, 074306.	3.0	28
57	An ab initio study of the potential energy surfaces for the collision between a Cs atom and an I <sub>2</sub> molecule. Canadian Journal of Chemistry, 2004, 82, 1216-1222.	1.1	0
58	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
59	PARTIAL POTENTIAL ENERGY SURFACE AND ITS APPLICATIONS IN REACTIVE RESONANCES. Journal of Theoretical and Computational Chemistry, 2004, 03, 543-553.	1.8	10
60	The density functional theory study on the 1,3-dipolar cycloaddition of carbon-methyl nitrene with acrylonitrile. Computational and Theoretical Chemistry, 2004, 679, 73-87.	1.5	5
61	Theoretical study of rate constants and kinetic isotope effects for reactions in the CH <sub>2</sub> system using variational transition state theory. Chemical Physics Letters, 2004, 391, 354-360.	2.6	11
62	Novel insight into the mechanism of the reaction of Fe <sup>+</sup> with ethane. Computational and Theoretical Chemistry, 2003, 635, 239-245.	1.5	8
63	Theoretical Study of the Reactivity of Fe <sup>+</sup> toward OCS. Journal of Physical Chemistry A, 2003, 107, 8955-8960.	2.5	18
64	Theoretical Investigation of the Reaction of Co <sup>+</sup> with OCS. Journal of Physical Chemistry A, 2003, 107, 8618-8622.	2.5	19
65	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
66	Accurate quantum dynamics of electronically nonadiabatic chemical reactions in the DH <sub>2</sub> <sup>+</sup> system. Journal of Chemical Physics, 2002, 116, 654-665.	3.0	76
67	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM II.. Journal of Theoretical and Computational Chemistry, 2002, 01, 275-284.	1.8	15
68	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM I.. Journal of Theoretical and Computational Chemistry, 2002, 01, 263-273.	1.8	23
69	CHEMICAL REACTIONS IN THE O(1D) + HCl SYSTEM III.. Journal of Theoretical and Computational Chemistry, 2002, 01, 285-293.	1.8	12
70	Reaction Cross Sections and Rate Constants for the Cl + H <sub>2</sub> 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
71	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
72	A fully ab initio potential energy surface for CH <sub>2</sub> reactive system. Science in China Series B: Chemistry, 2000, 43, 396-404.	0.8	1

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73	Global ab initio potential energy surfaces for the CH <sub>2</sub> reactive system. Journal of Chemical Physics, 2000, 112, 220-229.	3.0	140
74	Direct solution of the Schrödinger equation for some muonic molecules. Chemical Physics, 1999, 242, 195-202.	1.9	4
75	Quantum-mechanical calculation of the thermal rate constant for the H <sub>2</sub> +Cl <sup>+</sup> H+HCl reaction. Chemical Physics Letters, 1999, 313, 647-654.	2.6	74
76	van der Waals Interactions in the Cl+HD Reaction. Science, 1999, 286, 1713-1716.	12.6	287
77	A potential harmonic method for the three-body coulomb problem. Theoretical Chemistry Accounts, 1997, 98, 110-116.	1.4	2
78	Fourier transform approach to potential harmonics. International Journal of Quantum Chemistry, 1997, 63, 5-14.	2.0	3
79	Direct solution of the many-body Schrödinger 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
80	Direct solution of H <sub>2</sub> + Schrödinger equation using the hyperspherical coordinate. Theoretica Chimica Acta, 1995, 92, 135-147.	0.8	0
81	Direct solution of H. Theoretica Chimica Acta, 1995, 92, 135.	0.8	3
82	Direct solution of the many-body Schrödinger equation in the hyperspherical formalism: Application of the HH-GLF method to the positronium ion+e <sup>-</sup> e <sup>+</sup> . International Journal of Quantum Chemistry, 1994, 50, 395-400.	2.0	10
83	Direct solution of the many-body Schrödinger equation in the hyperspherical formalism: Formulation of the CFHH-GLF method. International Journal of Quantum Chemistry, 1994, 51, 285-291.	2.0	12
84	Ring polymer molecular dynamics of the C(1D)+H <sub>2</sub> reaction on the most recent potential energy surfaces. Chinese Journal of Chemical Physics, 0, , .	1.3	2