Ming-Liang Wang

List of Publications by Year
in descending order

68 papers	1,871 citations	361388 20 h-index	265191 42 g-index
70 all docs	70 docs citations	70 times ranked	1372 citing authors

#	Article	IF	Citations
1	Product rotational polarization in the photoinitiated bimolecular reaction A+BCâ†'AB+C on attractive, mixed and repulsive surfaces. Journal of Chemical Physics, 1998, 109, 5446-5454.	3.0	233
2	Product Rotational Polarization in Photo-initiated Bimolecular Reactions A+BC:Â Dependence on the Character of the Potential Energy Surface for Different Mass Combinations. Journal of Physical Chemistry A, 1998, 102, 10204-10210.	2.5	182
3	Designing Molecules by Optimizing Potentials. Journal of the American Chemical Society, 2006, 128, 3228-3232.	13.7	138
4	Application of semirigid vibrating rotor target model to reaction of H+CH4â†'CH3+H2. Journal of Chemical Physics, 2000, 113, 1802-1806.	3.0	98
5	Skinâ€Inspired Doubleâ€Hydrophobicâ€Coating Encapsulated Hydrogels with Enhanced Water Retention Capacity. Advanced Functional Materials, 2021, 31, 2102433.	14.9	96
6	Improving the electrochemical performance of high voltage spinel cathode at elevated temperature by a novel electrolyte additive. Journal of Power Sources, 2016, 303, 41-48.	7.8	62
7	Selective etching of C-N bonds for preparation of porous carbon with ultrahigh specific surface area and superior capacitive performance. Energy Storage Materials, 2020, 24, 486-494.	18.0	60
8	Preparation, Stabilization and Carbonization of a Novel Polyacrylonitrile-Based Carbon Fiber Precursor. Polymers, 2019, 11, 1150.	4.5	59
9	Reaction dynamics of the Sr(3RJ) + RI â†' SrIâ^— + R (R = CH3, CH3CH2) systems: rotational alignment, electronic state branching ratio and vibrational state population of products. Chemical Physics Letters, 1997, 278, 307-312.	2.6	57
10	Generalized semirigid vibrating rotor target model for atomâ€"poly reaction: Inclusion of umbrella mode for H+CH4 reaction. Journal of Chemical Physics, 2002, 117, 3081-3087.	3.0	52
11	Nuclear quantum effects on an enzyme-catalyzed reaction with reaction path potential: Proton transfer in triosephosphate isomerase. Journal of Chemical Physics, 2006, 124, 124516.	3.0	49
12	Theoretical studies of scattering-angle resolved product rotational alignment for the reaction of Cl with vibrationally excited methane. Chemical Physics Letters, 1999, 301, 303-308.	2.6	47
13	Stereodynamics and rovibrational effect for H+CH4(v,j,K,n)â†'H2+CH3 reaction. Journal of Chemical Physics, 2002, 116, 6497-6504.	3.0	44
14	Molecular Dynamics Study on Ion Diffusion in LiFePO₄ Olivine Materials. Journal of Physical Chemistry A, 2008, 112, 5406-5410.	2.5	43
15	Application of Semirigid Vibrating Rotor Target Model to the Reaction of O(3P) + CH4â†' CH3+ OHâ€. Journal of Physical Chemistry A, 2001, 105, 2530-2534.	2.5	41
16	Product rotational polarization: Stereodynamics of the reaction Cl(2P3/2)+CD4(v=0,j=0)â†'DCl(vâ€²=0,jâ€²=1)+CD3. Journal of Chemical Physics, 2000, 112, 3710-3716.	3.0	38
17	Characterization of 4,4â€²-biphenylene-silicas and a chiral sensor for silicas. Chemical Communications, 2011, 47, 11495.	4.1	32
18	Quantum dynamics study of isotope effect for H+CH4 reaction using the SVRT model. Journal of Chemical Physics, 2003, 118, 9266-9271.	3.0	28

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19	Rank-ordering protein-ligand binding affinity by a quantum mechanics/molecular mechanics/Poisson-Boltzmann-surface area model. Journal of Chemical Physics, 2007, 126, 026101.	3.0	24
20	A novel boron-based ionic liquid electrolyte for high voltage lithium-ion batteries with outstanding cycling stability. Electrochimica Acta, 2018, 283, 111-120.	5.2	23
21	Chirality of the 1,4-phenyleneâ€“silica nanoribbons at the nano and angstrom levels. Nanotechnology, 2013, 24, 035603.	2.6	21
22	Semirigid vibrating rotor target calculation for reaction H+HODâ†'H2+OD, HD+OH. Journal of Chemical Physics, 2001, 114, 7013-7017.	3.0	20
23	First principles quantum dynamics study reveals subtle resonance in polyatomic reaction: The case of F+CH4â†'HF+CH3. Chemical Physics Letters, 2006, 424, 243-246.	2.6	19
24	Calculation of Solvation Free Energy from Quantum Mechanical Charge Density and Continuum Dielectric Theory. Journal of Physical Chemistry A, 2006, 110, 4873-4879.	2.5	18
25	Transmission coefficient calculation for proton transfer in triosephosphate isomerase based on the reaction path potential method. Journal of Chemical Physics, 2004, 121, 101.	3.0	17
26	Enhanced Thermoelectric Performance of a Donorâ€“Acceptor-Based Two-Dimensional Conjugated Polymer with High Crystallinity. ACS Applied Energy Materials, 2021, 4, 4662-4671.	5.1	17
27	Chiral Carbonaceous Nanotubes Containing Twisted Carbonaceous Nanoribbons, Prepared by the Carbonization of Chiral Organic Selfâ€Assemblies. Chemistry - an Asian Journal, 2014, 9, 2866-2871.	3.3	16
28	New comonomer for polyacrylonitrile-based carbon fiber: Density functional theory study and experimental analysis. Polymer, 2018, 153, 369-377.	3.8	16
29	A long lasting sunscreen controversy of 4-aminobenzoic acid and 4-dimethylaminobenzaldehyde derivatives resolved by ultrafast spectroscopy combined with density functional theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 8006-8020.	2.8	16
30	Rotational alignment from the Sr()+CH2ClI chemiluminescent reaction. Chemical Physics, 1998, 238, 481-485.	1.9	15
31	Rotational alignment from the reactions and CHCl3. Chemical Physics, 1998, 236, 387-392.	1.9	14
32	Time-dependent quantum wave packet study of H+HCNâ†'H2+CN reaction. Journal of Chemical Physics, 2002, 117, 172-176.	3.0	14
33	Self-assembly of polymer and molybdenum oxide into lamellar hybrid materials. Journal of Colloid and Interface Science, 2008, 320, 445-451.	9.4	14
34	DFT study on the ionic cyclization mechanism of copolymers of acrylonitrile-itaconic acid: Direct or autocatalytic?. Chemical Physics Letters, 2017, 687, 158-162.	2.6	14
35	Feasibility of Predicting Static Dielectric Constants of Polymer Materials: A Density Functional Theory Method. Polymers, 2021, 13, 284.	4.5	14
36	DFT Study of the Proton Transfer in the Urethane Formation between 2,4-Diisocyanatotoluene and Methanol. Bulletin of the Chemical Society of Japan, 2013, 86, 255-265.	3.2	13

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37	SUPPLEMENTING THE PBSA APPROACH WITH QUANTUM MECHANICS TO STUDY THE BINDING BETWEEN CDK2 AND N²-SUBSTITUTED O⁶-CYCLOHEXYLMETHOXYGUANINE INHIBITORS. Journal of Theoretical and Computational Chemistry, 2010, 09, 543-559.	1.8	12
38	Inâ€“situ Characterization and Cure Kinetics in NEPE Propellant/ HTPB Liner Interface by Microscopic FTâ€IR. Propellants, Explosives, Pyrotechnics, 2017, 42, 410-416.	1.6	12
39	Nonradiative dynamics determined by charge transfer induced hydrogen bonding: a combined femtosecond time-resolved fluorescence and density functional theoretical study of methyl dimethylaminobenzoate in water. Physical Chemistry Chemical Physics, 2018, 20, 1240-1251.	2.8	12
40	Efficient quantum mechanical calculation of solvation free energies based on density functional theory, numerical atomic orbitals and Poissonâ€“Boltzmann equation. Chemical Physics Letters, 2007, 442, 464-467.	2.6	11
41	RANK-ORDERING THE BINDING AFFINITY FOR FKBP12 AND H1N1 NEURAMINIDASE INHIBITORS IN THE COMBINATION OF A PROTEIN MODEL WITH DENSITY FUNCTIONAL THEORY. Journal of Theoretical and Computational Chemistry, 2011, 10, 541-565.	1.8	11
42	Theoretical Studies of the Relative Cross Sections and Transition State Spectroscopy of Cl+Na₂(3 â‰ vâ€³ â‰ 19) â†' [NaNaCl]â€¡ *â†' NaCl+Na*. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 1527-1530.	0.9	10
43	Effective degradation of refractory nitrobenzene in water by the natural 4-hydroxycoumarin under solar illumination. Chemosphere, 2019, 215, 199-205.	8.2	10
44	Cyclization mechanism and kinetics of poly(acrylonitrile-co-2-acrylamido-2-methylpropane sulfonic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	4.8	10
45	Comparison of quantum and mixed quantumâ€“classical semirigid vibrating rotor target studies for isotopic reactions H(D,T)+CH4â†'HH(D,T)+CH3. Journal of Chemical Physics, 2003, 119, 9455-9460.	3.0	9
46	Effect of entrance channel topology on reaction dynamics: O(3P) + CH4â†' CH3+ OH. Chemical Physics Letters, 2005, 410, 115-119.	2.6	9
47	DFT Study of the Catalytic Mechanism for Urethane Formation in the Presence of Basic Catalyst 1,4-diazabicyclo[2.2.2]octane. Communications in Computational Chemistry, 2014, 2, 22-35.	1.0	9
48	Rotational alignment of products from NOCl+Sr chemiluminescent reaction. Journal of Chemical Physics, 1998, 109, 1819-1823.	3.0	7
49	A Chirality Indicator for the Surfaces of the Silica Nanotubes. Journal of Nanoscience and Nanotechnology, 2013, 13, 5732-5735.	0.9	7
50	Transition-state spectroscopy of Cl+Na2â†'[NaNaCl]â€¡*â†'NaCl+Na*.. Chemical Physics Letters, 1998, 284, 200-204.	2.6	6
51	Quantum Dynamics Study of Torsional Excitation of Glycine in Collision with Hydrogen Atom on ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2003, 107, 7106-7111.	2.5	6
52	Optical activity of SiC nanoparticles prepared from single-handed helical 4,4â€²-biphenylene-bridged polybissilsesquioxane nanotubes. New Journal of Chemistry, 2015, 39, 8424-8429.	2.8	6
53	Investigation of the Cyclization Mechanism of Poly(acrylonitrile-co-ethylenesulfonic acid) Copolymer during Thermal Oxidative Stabilization by In Situ Infrared Spectroscopy. Industrial & Engineering Chemistry Research, 2020, 59, 9519-9531.	3.7	6
54	Proton Transfer in Reaction between 2,4-Diisocyanatotoluene and Amine Compounds. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2014, 30, 34-42.	4.9	5

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55	Photocleavage of DNA and adenineâ€“thymine inclined binding by a novel ruthenium(II) complex with 3,4-dibromo-imidazo[4,5-f][1,10]phenanthroline ligand. Inorganic Chemistry Communication, 2015, 55, 30-35.	3.9	5
56	Mixed quantum-classical study of energy transfer between H2O and a dipeptide. Journal of Chemical Physics, 2003, 119, 11152-11158.	3.0	4
57	DFT study on the hydrolysis of metsulfuron-methyl: A sulfonylurea herbicide. Journal of Theoretical and Computational Chemistry, 2018, 17, 1850050.	1.8	4
58	Mixed quantum-classical study of energy transfer in a Na+ collision with a peptide. Journal of Chemical Physics, 2003, 118, 7846-7856.	3.0	3
59	DENSITY FUNCTIONAL THEORY/TIME-DEPENDENT DENSITY FUNCTIONAL THEORY STUDY ON THE STRUCTURES AND SOLVENT EFFECTS ON THE ELECTRONIC SPECTRA OF Ru(II) POLYPYRIDYL COMPLEXES: [Ru(bpy)₂(L)]²⁺ (L =) Tj ETQq1 1 0.784314 rgBT	1.8	3
60	Construction of an implicit membrane environment for the lattice Monte Carlo simulation of transmembrane protein. Biophysical Chemistry, 2010, 147, 35-41.	2.8	3
61	First principle simulation on oxidation mechanism of diethyl ether by nitrogen dioxide. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550020.	1.8	3
62	Catalytic Effects of Water Clusters on the Hydrolysis of Toluene-2,4-diisocyanate: A DFT Study. Bulletin of the Chemical Society of Japan, 2016, 89, 74-91.	3.2	3
63	Ab initio quantum dynamics study of rotationally inelastic scattering of glycine by hydrogen atom. Journal of Chemical Physics, 2003, 118, 2716.	3.0	2
64	A DFT study on the mechanism of reaction between 2, 4-diisocyanatotolune and cellulose. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650012.	1.8	2
65	Long living excited state of protonated adenosine unveiled by ultrafast fluorescence spectroscopy and density functional theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 6472-6480.	2.8	2
66	Study on characterization of light aging of RGB LED packaging materials. , 2018, , .		1
67	High Activity and Easily Hydrolyzable Sulfonylurea Inhibitor Design Based on Density Functional Theory Calculations. Journal of Computational Biophysics and Chemistry, 2021, 20, 41-52.	1.7	1
68	MIXED QUANTUM-CLASSICAL SEMI-RIGID VIBRATING ROTOR TARGET MODEL FOR ATOM-POLYATOM REACTION: O(3P) + CH4 â†' CH3 + OH. Journal of Theoretical and Computational Chemistry, 2003, 02, 351-356.	1.8	0