Ming-Liang Wang

List of Publications by Year in Descending Order

67 papers	1,572 citations	19 h-index	38 g-index
70 ext. papers	1,706 ext. citations	4.2 avg, IF	4.36 L-index

#	Paper	IF	Citations
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		
66	Skin-Inspired Double-Hydrophobic-Coating Encapsulated Hydrogels with Enhanced Water Retention Capacity. *Advanced Functional Materials*, **2021**, 31, 2102433	15.6	23
65	Enhanced Thermoelectric Performance of a Donor–Acceptor-Based Two-Dimensional Conjugated Polymer with High Crystallinity. *ACS Applied Energy Materials*, **2021**, 4, 4662-4671	6.1	5
64	Cyclization mechanism and kinetics of poly(acrylonitrile-co-2-acrylamido-2-methylpropane sulfonic acid) copolymer investigated by FTIR spectroscopy. *Polymer Testing*, **2021**, 93, 106969	4.5	4
63	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	3.6	1
62	Feasibility of Predicting Static Dielectric Constants of Polymer Materials: A Density Functional Theory Method. *Polymers*, **2021**, 13,	4.5	2
61	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	3.9	4
60	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	3.6	5
59	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	19.4	21
58	Preparation, Stabilization and Carbonization of a Novel Polyacrylonitrile-Based Carbon Fiber Precursor. *Polymers*, **2019**, 11,	4.5	36
57	Effective degradation of refractory nitrobenzene in water by the natural 4-hydroxycoumarin under solar illumination. *Chemosphere*, **2019**, 215, 199-205	8.4	4
56	New comonomer for polyacrylonitrile-based carbon fiber: Density functional theory study and experimental analysis. *Polymer*, **2018**, 153, 369-377	3.9	11
55	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	3.6	11
54	DFT study on the hydrolysis of metsulfuron-methyl: A sulfonylurea herbicide. *Journal of Theoretical and Computational Chemistry*, **2018**, 17, 1850050	1.8	2
53	A novel boron-based ionic liquid electrolyte for high voltage lithium-ion batteries with outstanding cycling stability. *Electrochimica Acta*, **2018**, 283, 111-120	6.7	14
52	In-Situ Characterization and Cure Kinetics in NEPE Propellant/ HTPB Liner Interface by Microscopic FT-IR. *Propellants, Explosives, Pyrotechnics*, **2017**, 42, 410-416	1.7	4
51	DFT study on the ionic cyclization mechanism of copolymers of acrylonitrile-itaconic acid: Direct or autocatalytic?. *Chemical Physics Letters*, **2017**, 687, 158-162	2.5	13

50	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	5.1	2
49	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	8.9	53
48	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
47	Optical activity of SiC nanoparticles prepared from single-handed helical 4,4?-biphenylene-bridged polybissilsesquioxane nanotubes. *New Journal of Chemistry*, **2015**, 39, 8424-8429	3.6	4
46	First principle simulation on oxidation mechanism of diethyl ether by nitrogen dioxide. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550020	1.8	3
45	Photocleavage of DNA and adenine–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	3.1	5
44	Chiral carbonaceous nanotubes containing twisted carbonaceous nanoribbons, prepared by the carbonization of chiral organic self-assemblies. *Chemistry - an Asian Journal*, **2014**, 9, 2866-71	4.5	15
43	Proton Transfer in Reaction between 2,4-Diisocyanatotoluene and Amine Compounds. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2014**, 30, 34-42	3.8	5
42	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		8
41	Chirality of the 1,4-phenylene-silica nanoribbons at the nano and angstrom levels. *Nanotechnology*, **2013**, 24, 035603	3.4	18
40	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	5.1	10
39	A chirality indicator for the surfaces of the silica nanotubes. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 5732-5	1.3	7
38	Characterization of 4,4′-biphenylene-silicas and a chiral sensor for silicas. *Chemical Communications*, **2011**, 47, 11495-7	5.8	30
37	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	9
36	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	10
35	Construction of an implicit membrane environment for the lattice Monte Carlo simulation of transmembrane protein. *Biophysical Chemistry*, **2010**, 147, 35-41	3.5	3
34	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 = CNOIP, HPIP, DPPZ, TAPIP). *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 631-646	1.8	3
33	Molecular dynamics study on ion diffusion in LiFePO4 olivine materials. *Journal of Physical Chemistry A*, **2008**, 112, 5406-10	2.8	40

32	Self-assembly of polymer and molybdenum oxide into lamellar hybrid materials. *Journal of Colloid and Interface Science*, **2008**, 320, 445-51	9.3	14
31	Efficient quantum mechanical calculation of solvation free energies based on density functional theory, numerical atomic orbitals and Poisson□Boltzmann equation. *Chemical Physics Letters*, **2007**, 442, 464-467	2.5	10
30	Rank-ordering protein-ligand binding affinity by a quantum mechanics/molecular mechanics/Poisson-Boltzmann-surface area model. *Journal of Chemical Physics*, **2007**, 126, 026101	3.9	19
29	Nuclear quantum effects on an enzyme-catalyzed reaction with reaction path potential: proton transfer in triosephosphate isomerase. *Journal of Chemical Physics*, **2006**, 124, 124516	3.9	46
28	Calculation of solvation free energy from quantum mechanical charge density and continuum dielectric theory. *Journal of Physical Chemistry A*, **2006**, 110, 4873-9	2.8	16
27	Designing molecules by optimizing potentials. *Journal of the American Chemical Society*, **2006**, 128, 3228-32	13.4	121
26	First principles quantum dynamics study reveals subtle resonance in polyatomic reaction: The case of F + CH4 -jHF + CH3. *Chemical Physics Letters*, **2006**, 424, 243-246	2.5	19
25	Effect of entrance channel topology on reaction dynamics: O(3P) + CH4 -jCH3 + OH. *Chemical Physics Letters*, **2005**, 410, 115-119	2.5	9
24	Transmission coefficient calculation for proton transfer in triosephosphate isomerase based on the reaction path potential method. *Journal of Chemical Physics*, **2004**, 121, 101-7	3.9	17
23	MIXED QUANTUM-CLASSICAL SEMI-RIGID VIBRATING ROTOR TARGET MODEL FOR ATOM-POLYATOM REACTION: O(3P) + CH4 -jCH3 + OH. *Journal of Theoretical and Computational Chemistry*, **2003**, 02, 351-356	1.8	
22	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	2.8	6
21	Quantum dynamics study of isotope effect for H+CH4 reaction using the SVRT model. *Journal of Chemical Physics*, **2003**, 118, 9266-9271	3.9	25
20	Ab initio quantum dynamics study of rotationally inelastic scattering of glycine by hydrogen atom. *Journal of Chemical Physics*, **2003**, 118, 2716	3.9	1
19	Mixed quantum-classical study of energy transfer between H2O and a dipeptide. *Journal of Chemical Physics*, **2003**, 119, 11152-11158	3.9	4
18	Comparison of quantum and mixed quantum□classical semirigid vibrating rotor target studies for isotopic reactions H(D,T)+CH4-JHH(D,T)+CH3. *Journal of Chemical Physics*, **2003**, 119, 9455-9460	3.9	9
17	Mixed quantum-classical study of energy transfer in a Na+ collision with a peptide. *Journal of Chemical Physics*, **2003**, 118, 7846-7856	3.9	3
16	Time-dependent quantum wave packet study of H+HCN-JH2+CN reaction. *Journal of Chemical Physics*, **2002**, 117, 172-176	3.9	14
15	Stereodynamics and rovibrational effect for H+CH4(v,j,K,n)-JH2+CH3 reaction. *Journal of Chemical Physics*, **2002**, 116, 6497-6504	3.9	42

14	Generalized semirigid vibrating rotor target model for atom poly reaction: Inclusion of umbrella mode for H+CH4 reaction. *Journal of Chemical Physics*, **2002**, 117, 3081-3087	3.9	49
13	Semirigid vibrating rotor target calculation for reaction H+HOD-H2+OD, HD+OH. *Journal of Chemical Physics*, **2001**, 114, 7013-7017	3.9	19
12	Application of Semirigid Vibrating Rotor Target Model to the Reaction of O(3P) + CH4 -jCH3 + OH *Journal of Physical Chemistry A*, **2001**, 105, 2530-2534	2.8	40
11	Application of semirigid vibrating rotor target model to reaction of H+CH4-CH3+H2. *Journal of Chemical Physics*, **2000**, 113, 1802-1806	3.9	94
10	Product rotational polarization: Stereodynamics of the reaction Cl(2P3/2)+CD4(v=0,j=0)-DCl(v?=0,j?=1)+CD3. *Journal of Chemical Physics*, **2000**, 112, 3710-3716	3.9	37
9	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	2.5	46
8	Transition-state spectroscopy of Cl+Na2-[NaNaCl]-NaCl+Na*.: Theoretical model. *Chemical Physics Letters*, **1998**, 284, 200-204	2.5	6
7	Rotational alignment from the reactions and CHCl3. *Chemical Physics*, **1998**, 236, 387-392	2.3	14
6	Rotational alignment from the Sr(3PJ)+CH2ClI chemiluminescent reaction. *Chemical Physics*, **1998**, 238, 481-485	2.3	15
5	Product Rotational Polarization in Photo-initiated Bimolecular Reactions A+BC: Dependence on the Character of the Potential Energy Surface for Different Mass Combinations. *Journal of Physical Chemistry A*, **1998**, 102, 10204-10210	2.8	178
4	Rotational alignment of products from NOCl+Sr chemiluminescent reaction. *Journal of Chemical Physics*, **1998**, 109, 1819-1823	3.9	7
3	Product rotational polarization in the photoinitiated bimolecular reaction A+BC-AB+C on attractive, mixed and repulsive surfaces. *Journal of Chemical Physics*, **1998**, 109, 5446-5454	3.9	226
2	Theoretical Studies of the Relative Cross Sections and Transition State Spectroscopy of Cl+Na2(3 v? 19) -j[NaNaCl]*-jNaCl+Na*. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1997**, 101, 1527-1530		10
1	Reaction dynamics of the Sr(3RJ) + RI -jSrI* + R (R = CH3, CH3CH2) systems: rotational alignment, electronic state branching ratio and vibrational state population of products. *Chemical Physics Letters*, **1997**, 278, 307-312	2.5	55