Chao-Yuan Zhu

List of Publications by Year
in descending order

122	3,846	136885	143943
papers	citations	32 h-index	57 g-index

126	126	126	2910
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Bornâ€“Oppenheimer trajectories. Journal of Chemical Physics, 2004, 121, 7658.	1.2	288
2	Non-Bornâ^'Oppenheimer Molecular Dynamics. Accounts of Chemical Research, 2006, 39, 101-108.	7.6	197
3	Introductory lecture: Nonadiabatic effects in chemical dynamics. Faraday Discussions, 2004, 127, 1.	1.6	190
4	Non-Bornâ€“Oppenheimer trajectories with self-consistent decay of mixing. Journal of Chemical Physics, 2004, 120, 5543-5557.	1.2	150
5	Theory of nonadiabatic transition for general twoâ€state curve crossing problems. I. Nonadiabatic tunneling case. Journal of Chemical Physics, 1994, 101, 10630-10647.	1.2	147
6	Theory of nonadiabatic transition for general twoâ€state curve crossing problems. II. Landauâ€“Zener case. Journal of Chemical Physics, 1995, 102, 7448-7461.	1.2	135
7	Non-Born-Oppenheimer Liouville-von Neumann Dynamics. Evolution of a Subsystem Controlled by Linear and Population-Driven Decay of Mixing with Decoherent and Coherent Switching. Journal of Chemical Theory and Computation, 2005, 1, 527-540.	2.3	114
8	Trajectory-based nonadiabatic molecular dynamics without calculating nonadiabatic coupling in the avoided crossing case: trans â†" cis photoisomerization in azobenzene. Physical Chemistry Chemical Physics, 2014, 16, 25883-25895.	1.3	92
9	Intersystem Crossing Pathway in Quinolineâ€“Pyrazole Isomerism: A Time-Dependent Density Functional Theory Study on Excited-State Intramolecular Proton Transfer. Journal of Physical Chemistry A, 2015, 119, 6269-6274.	1.1	89
10	New implementation of the trajectory surface hopping method with use of the Zhuâ€“Nakamura theory. Journal of Chemical Physics, 2001, 115, 3031-3044.	1.2	83
11	The twoâ€state linear curve crossing problems revisited. II. Analytical approximations for the Stokes constant and scattering matrix: The Landauâ€“Zener case. Journal of Chemical Physics, 1992, 97, 8497-8514.	1.2	79
12	Semiclassical theory of multi-channel curve crossing problems: Landau-Zener case. Journal of Chemical Physics, 1997, 106, 2599-2611.	1.2	79
13	The twoâ€state linear curve crossing problems revisited. III. Analytical approximations for Stokes constant and scattering matrix: Nonadiabatic tunneling case. Journal of Chemical Physics, 1993, 98, 6208-6222.	1.2	76
14	Electron-Deficient Pyrimidine Adopted in Porphyrin Sensitizers: A Theoretical Interpretation of Ï€-Spacers Leading to Highly Efficient Photo-to-Electric Conversion Performances in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 9166-9179.	1.5	76
15	The twoâ€state linear curve crossing problems revisited. I. Analysis of Stokes phenomenon and expressions for scattering matrices. Journal of Chemical Physics, 1992, 97, 1892-1904.	1.2	68
16	Nonadiabatic transitions due to curve crossings: complete solutions of the landau-zener-stueckelberg problems and their applications. Advances in Chemical Physics, 2007, , 127-233.	0.3	65
17	Twoâ€state linear curve crossing problems revisited. IV. The best analytical formulas for scattering matrices. Journal of Chemical Physics, 1994, 101, 4855-4866.	1.2	58
18	The optical absorption and hydrogen production by water splitting of (Si,Fe)-codoped anatase TiO2 photocatalyst. International Journal of Hydrogen Energy, 2013, 38, 5209-5214.	3.8	58

#	Article	IF	Citations
19	Functional Supramolecular Polypeptides Involving Ï€â€“Ï€ Stacking and Strong Hydrogen-Bonding Interactions: A Conformation Study toward Carbon Nanotubes (CNTs) Dispersion. Macromolecules, 2016, 49, 5374-5385.	2.2	52
20	New implementation of the trajectory surface hopping method with use of the Zhuâ€“Nakamura theory. II. Application to the charge transfer processes in the 3D DH2+ system. Journal of Chemical Physics, 2002, 116, 3234-3247.	1.2	48
21	Probing the Ï€ â†' Ï€* photoisomerization mechanism of cis-azobenzene by multi-state ab initio on-the-fly trajectory dynamics simulation. Physical Chemistry Chemical Physics, 2015, 17, 17646-17660.	1.3	48
22	Algorithmic decoherence time for decay-of-mixing nonâ€“Bornâ€“Oppenheimer dynamics. Journal of Chemical Physics, 2008, 129, 024112.	1.2	47
23	A TDDFT study on the excited-state double proton transfer reaction of 8-hydroxyquinoline along a hydrogen-bonded bridge. New Journal of Chemistry, 2017, 41, 8437-8442.	1.4	47
24	Stokes constants for a certain class of secondâ€order ordinary differential equations. Journal of Mathematical Physics, 1992, 33, 2697-2717.	0.5	42
25	Characteristics of high-water-uptake activated carbon/Nafion hybrid membranes for proton exchange membrane fuel cells. Journal of Power Sources, 2013, 226, 87-93.	4.0	42
26	C/B codoping effect on band gap narrowing and optical performance of TiO2 photocatalyst: a spin-polarized DFT study. Journal of Materials Chemistry A, 2013, 1, 4516.	5.2	42
27	Significant improvement of the trajectory surface hopping method by the Zhuâ€“Nakamura theory. Journal of Chemical Physics, 2001, 115, 11036-11039.	1.2	40
28	Benchmark Performance of Global Switching versus Local Switching for Trajectory Surface Hopping Molecular Dynamics Simulation: Cisâ†"Trans Azobenzene Photoisomerization. ChemPhysChem, 2017, 18, 1274-1287.	1.0	39
29	Intersystem crossing-branched excited-state intramolecular proton transfer for o-nitrophenol: An ab initio on-the-fly nonadiabatic molecular dynamic simulation. Scientific Reports, 2016, 6, 26768.	1.6	37
30	Visible-light photocatalytic activity of Ni-doped TiO2 from ab initio calculations. Materials Chemistry and Physics, 2012, 133, 746-750.	2.0	35
31	Performance of TDDFT with and without spin-flip in trajectory surface hopping dynamics: cisâ€"trans azobenzene photoisomerization. Physical Chemistry Chemical Physics, 2018, 20, 24123-24139.	1.3	35
32	Semiclassical theory of multi-channel curve crossing problems: Nonadiabatic tunneling case. Journal of Chemical Physics, 1997, 107, 7839-7848.	1.2	34
33	Transparent Heat-Resistant PMMA Copolymers for Packing Light-Emitting Diode Materials. Polymers, 2015, 7, 1379-1388.	2.0	33
34	Orientation hydrogen-bonding effect on vibronic spectra of isoquinoline in water solvent: Franck-Condon simulation and interpretation. Journal of Chemical Physics, 2016, 145, 164314.	1.2	33
35	Franck-Condon simulation of vibrationally resolved optical spectra for zinc complexes of phthalocyanine and tetrabenzoporphyrin including the Duschinsky and Herzberg-Teller effects. Journal of Chemical Physics, 2012, 136, 144313.	1.2	32
36	A cross-linkable triphenylamine derivative as a hole injection/transporting material in organic light-emitting diodes. Polymer Chemistry, 2015, 6, 6227-6237.	1.9	31

#	Article	IF	Citations
37	Ternary polybenzoxazine/POSS/SWCNT hybrid nanocomposites stabilized through supramolecular interactions. Soft Matter, 2016, 12, 1847-1858.	1.2	31
38	Photo-Crosslinking of Pendent Uracil Units Provides Supramolecular Hole Injection/Transport Conducting Polymers for Highly Efficient Light-Emitting Diodes. Polymers, 2015, 7, 804-818.	2.0	30
39	A solvent-resistant azide-based hole injection/transporting conjugated polymer for fluorescent and phosphorescent light-emitting diodes. Journal of Materials Chemistry C, 2015, 3, 8142-8151.	2.7	29
40	A nonlinear optical switch induced by an external electric field: inorganic alkalineâ€“earth alkalide. RSC Advances, 2019, 9, 16718-16728.	1.7	27
41	Theoretical treatment of anharmonic effect on molecular absorption, fluorescence spectra, and electron transfer. Chemical Physics, 2009, 358, 137-146.	0.9	26
42	Photo-induced 1,3-cyclohexadiene ring opening reaction: Ab initio on-the-fly nonadiabatic molecular dynamics simulation. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 317, 39-49.	2.0	26
43	IRâ€“VUV spectroscopy of pyridine dimers, trimers and pyridineâ€“ammonia complexes in a supersonic jet. Physical Chemistry Chemical Physics, 2020, 22, 21520-21534.	1.3	26
44	Exploring the role of varied-length spacers in charge transfer: a theoretical investigation on pyrimidine-bridged porphyrin dyes. RSC Advances, 2013, 3, 17515.	1.7	25
45	Remarkable nonlinear optical response of excess electron compounds: theoretically designed alkali-doped aziridine Mâ€“(C₂NH₅)_n. Physical Chemistry Chemical Physics, 2017, 19, 23951-23959.	1.3	25
46	Electronic and optical performances of Si and Fe-codoped TiO2 nanoparticles: A photocatalyst for the degradation of methylene blue. Applied Catalysis B: Environmental, 2013, 142-143, 38-44.	10.8	24
47	Molecular Orbital Imaging of the AcetoneS2Excited State Using Time-Resolved (e,2e) Electron Momentum Spectroscopy. Physical Review Letters, 2015, 114, 103005.	2.9	24
48	A phenothiazine-based colorimetric chemodosimeter for the rapid detection of cyanide anions in organic and aqueous media. RSC Advances, 2014, 4, 36344.	1.7	22
49	The electronic structure, optical absorption and photocatalytic water splitting of (FeÂ+ÂNi)-codoped TiO2: A DFT +U study. International Journal of Hydrogen Energy, 2017, 42, 4966-4976.	3.8	22
50	Probing the Ï€ â†' Ï€* photoisomerization mechanism of trans-azobenzene by multi-state ab initio on-the-fly trajectory dynamics simulations. Physical Chemistry Chemical Physics, 2018, 20, 23885-23897.	1.3	22
51	Anharmonic Franckâ^'Condon Simulation of the Absorption and Fluorescence Spectra for the Low-Lying S₁ and S₂ Excited States of Pyridine. Journal of Physical Chemistry A, 2009, 113, 14407-14414.	1.1	21
52	Enhanced optical absorption and photocatalytic activity of anatase TiO₂ through (Si,Ni) codoping. Applied Physics Letters, 2012, 101, 062106.	1.5	21
53	The structure, electronic, and optical properties of (Sm,N)-codoped anatase TiO2 photocatalyst: A density functional study. Journal of Catalysis, 2014, 309, 115-120.	3.1	21
54	Landscapes of Four-Enantiomer Conical Intersections for Photoisomerization of Stilbene: CASSCF Calculation. Journal of Physical Chemistry A, 2014, 118, 9021-9031.	1.1	21

#	Article	IF	Citations
55	Stimuli-responsive supramolecular materials: photo-tunable properties and molecular recognition behavior. Polymer Chemistry, 2016, 7, 795-806.	1.9	20
56	Exact analytical solution for coupled time-independent SchrÃ¶dinger equations with certain model potentials. Journal of Physics A, 1996, 29, 1293-1303.	1.6	19
57	Ultrafast intersystem crossing for nitrophenols: ab initio nonadiabatic molecular dynamics simulation. Physical Chemistry Chemical Physics, 2018, 20, 5606-5616.	1.3	19
58	Ab initio studies of excited electronic state S2 of pyrazine and Franckâ€“Condon simulation of its absorption spectrum. Chemical Physics Letters, 2009, 476, 19-24.	1.2	18
59	A Density Functional Theory Study on Nonlinear Optical Properties of Double Cage Excess Electron Compounds: Theoretically Design M[Cu(Ag)@(NH 3) n](Mâ€‰=â€‰Be, Mg and Ca; n â€‰=â€‰1â€“3). Journal of Computational Chemistry, 2019, 40, 971-979.	1.5	18
60	Insight into the Expanded Mislinked Porphyrins with High Second Order Nonlinear Optical Response. Journal of Physical Chemistry A, 2020, 124, 955-965.	1.1	18
61	Quantum yields of singlet and triplet chemiexcitation of dimethyl 1,2-dioxetane: ab initio nonadiabatic molecular dynamic simulations. Physical Chemistry Chemical Physics, 2020, 22, 11440-11451.	1.3	17
62	Franckâ€“Condon simulation of the A 1B2 â† X 1A1 dispersed fluorescence spectrum of fluorobenzene and its rate of the internal conversion. Journal of Chemical Physics, 2011, 134, 094313.	1.2	16
63	Absorption and fluorescence spectra of the neutral and anionic green fluorescent protein chromophore: Franckâ€“Condon simulation. Chemical Physics Letters, 2012, 541, 110-116.	1.2	16
64	Poly(ethylene glycol) modified activated carbon for high performance proton exchange membrane fuel cells. International Journal of Hydrogen Energy, 2013, 38, 11331-11339.	3.8	16
65	Multicomponent Reactions of Phosphines, Enynedioates and Cinnamaldimines Give Î³â€Lactams with a 1,3,5â€Hexatriene Moiety for Facile 6Ï€ Electrocyclization: Access to Oxindoles, Isatins and Isoxazolinones. Advanced Synthesis and Catalysis, 2015, 357, 1453-1462.	2.1	16
66	Photoisomerization Reaction Mechanisms of o-Nitrophenol Revealed by Analyzing Intersystem Crossing Network at the MRCI Level. Journal of Physical Chemistry A, 2015, 119, 10441-10450.	1.1	16
67	Restoring electronic coherence/decoherence for a trajectory-based nonadiabatic molecular dynamics. Scientific Reports, 2016, 6, 24198.	1.6	16
68	Theoretical study of the substituent effect controlling the radiative and non-radiative decay processes of platinum(ii) complexes. Physical Chemistry Chemical Physics, 2017, 19, 23532-23540.	1.3	16
69	Facially Polarized Molecule for Alkalides and Superalkalides with Considerable Nonlinear Optical Response. ChemistrySelect, 2018, 3, 12782-12790.	0.7	16
70	Two-by-two diabatic approach for multi-channel curve crossing problems. Chemical Physics Letters, 1996, 258, 342-347.	1.2	15
71	Anharmonic Franckâ€“Condon simulation of the absorption and fluorescence spectra for the low-lying S1 and S2 excited states of pyrimidine. Chemical Physics, 2012, 400, 126-136.	0.9	15
72	Photoisomerization mechanisms from trans, trans-1,4-diphenyl-1,3-butadiene: CASSCF on-the-fly trajectory surface hopping dynamic simulations. Physical Chemistry Chemical Physics, 2016, 18, 8971-8979.	1.3	15

#	Article	IF	Citations
73	Semiclassical analysis of resonance states induced by a conical intersection. Journal of Chemical Physics, 1996, 104, 7059-7067.	1.2	14
74	Improvement of the adiabatic phase integral for the Landauâ€“Zener-type curve crossing. Journal of Chemical Physics, 1998, 109, 4689-4690.	1.2	14
75	Franck-Condon factors perturbed by damped harmonic oscillators: Solvent enhanced X 1Ag â†" A1B1u absorption and fluorescence spectra of perylene. Journal of Chemical Physics, 2014, 141, 084106.	1.2	14
76	Electronically adiabatic chemical reactions analyzed by the semiclassical theory of nonadiabatic transition. Physical Chemistry Chemical Physics, 2000, 2, 557-570.	1.3	13
77	Unified semiclassical theory for the twoâ€state system: Analytical solutions for scattering matrices. Journal of Chemical Physics, 1996, 105, 4159-4172.	1.2	12
78	Franckâ€“Condon simulation for unraveling vibronic origin in solvent enhanced absorption and fluorescence spectra of rubrene. RSC Advances, 2017, 7, 12407-12418.	1.7	12
79	The Role of the nÏ€* ¹A_u State in the Photoabsorption and Relaxation of Pyrazine. Chemistry - an Asian Journal, 2011, 6, 2977-2985.	1.7	11
80	Highly hydrated Nafion/activated carbon hybrids. Polymer, 2012, 53, 4927-4930.	1.8	11
81	Topology of conical/surface intersections among five low-lying electronic states of CO2: Multireference configuration interaction calculations. Journal of Chemical Physics, 2013, 139, 154302.	1.2	11
82	Theoretical Study on Structure and Sum-Frequency Generation (SFG) Spectroscopy of Styreneâ€“Graphene Adsorption System. Journal of Physical Chemistry C, 2013, 117, 1754-1760.	1.5	11
83	Multi-state nonadiabatic deactivation mechanism of coumarin revealed by ab initio on-the-fly trajectory surface hopping dynamic simulation. Physical Chemistry Chemical Physics, 2017, 19, 12094-12106.	1.3	11
84	Electronic State and Photophysics of 2-Ethylhexyl-4-methoxycinnamate as UV-B Sunscreen under Jet-Cooled Condition. Journal of Physical Chemistry A, 2020, 124, 1272-1278.	1.1	11
85	Unified semiclassical theory for the two-state system: An analytical solution for general nonadiabatic tunneling. Journal of Chemical Physics, 2006, 125, 044104.	1.2	10
86	Chiral conversion and periodical decay in bridged-azobenzene photoisomerization: an ab initio on-the-fly nonadiabatic dynamics simulation. RSC Advances, 2016, 6, 39542-39552.	1.7	10
87	Functional and Basis Set Dependence for Timeâ€Dependent Density Functional Theory Trajectory Surface Hopping Molecular Dynamics: Cisâ€Azobenzene Photoisomerization. Journal of Computational Chemistry, 2020, 41, 635-645.	1.5	10
88	Numerical method for the two-state linear curve crossing: nonadiabatic tunneling case. Computer Physics Communications, 1993, 74, 9-17.	3.0	9
89	Usefulness of the newly completed semiclassical theory of curve crossing: multi-channel resonant scattering. Chemical Physics Letters, 1997, 274, 205-212.	1.2	9
90	The absorption and fluorescence spectra of 4-(3-methoxybenzylidene)-2-methyl-oxazalone interpreted by Franckâ€“Condon simulation in various pH solvent environments. Physical Chemistry Chemical Physics, 2020, 22, 17559-17566.	1.3	9

#	Article	IF	Citations
91	Electronic States and Nonradiative Decay of Cold Gas-Phase Cinnamic Acid Derivatives Studied by Laser Spectroscopy with a Laser-Ablation Technique. Journal of Physical Chemistry A, 2020, 124, 5580-5589.	1.1	9
92	Excited-state E â†' Z photoisomerization mechanism unveiled by ab initio nonadiabatic molecular dynamics simulation for hemithioindigoâ€"hemistilbene. Physical Chemistry Chemical Physics, 2017, 19, 12185-12198.	1.3	8
93	Dioxygen Activation by Iron Complexes: The Catalytic Role of Intersystem Crossing Dynamics for a Heme-Related Model. Journal of Physical Chemistry C, 2018, 122, 2821-2831.	1.5	8
94	Methyl substitution enhanced photoisomerization of trans,trans-1,4-diphenyl-1,3-butadiene: direct ab initio trajectory surface hopping dynamic simulations. Physical Chemistry Chemical Physics, 2018, 20, 2260-2273.	1.3	7
95	Theoretical Studies on Catalysis Mechanisms of Serum Paraoxonase 1 and Phosphotriesterase Diisopropyl Fluorophosphatase Suggest the Alteration of Substrate Preference from Paraoxonase to DFP. Molecules, 2018, 23, 1660.	1.7	7
96	Theoretical study on S1(1B3u) state electronic structure and absorption spectrum of pyrazine. Science in China Series B: Chemistry, 2008, 51, 1166-1173.	0.8	6
97	Constraint Trajectory Surface-Hopping Molecular Dynamics Simulation of the Photoisomerization of Stilbene. International Journal of Photoenergy, 2014, 2014, 1-18.	1.4	5
98	TDDFT studies for electronic excitations of the intermediates and radicals in the pyrolysis of 2,5-dimethylfuran. AIP Advances, 2018, 8, .	0.6	5
99	Extremely solvent-enhanced absorbance and fluorescence of carbazole interpreted using a damped Franckâ€"Condon simulation. Journal of Chemical Physics, 2020, 152, 104106.	1.2	5
100	Aggregation-induced emission spectra of triphenylamine salicylaldehyde derivatives via excited-state intramolecular proton transfer revealed by molecular spectral and dynamics simulations. RSC Advances, 2021, 11, 37171-37180.	1.7	5
101	Analytical semiclassical theory for general non-adiabatic transition and tunneling. Physica Scripta, 2009, 80, 048114.	1.2	4
102	Excited State ab Initio and Franckâ€"Condon Simulation of S₁ â†' S₀ Fluorescence Excitation Spectra of p-, m-, and o-Difluorobenzenes. Journal of Physical Chemistry A, 2011, 115, 14022-14033.	1.1	4
103	Quantum Chemical Calculations of Intramolecular Vibrational Redistribution and Energy Transfer of Dipeptides (GlyTyr and LeuTyr) and Applications to the RRKM Theory. Journal of the Chinese Chemical Society, 2013, 60, 974-985.	0.8	4
104	Enhanced photovoltaic performance of dye-sensitized solar cells by the adsorption of Zn-porphyrin dye molecule on TiO2 surfaces. Journal of Alloys and Compounds, 2019, 794, 35-44.	2.8	4
105	Nonadiabatic molecular dynamics simulation for the ultrafast photoisomerization of dMe-OMe-NAIP based on TDDFT on-the-fly potential energy surfaces. Physical Chemistry Chemical Physics, 2021, 23, 5236-5243.	1.3	4
106	New Implementation of Semi-classical Dynamic Simulation on the Photoisomerization ofcis- and trans-Isomers of Free Stilbene. Acta Chimica Sinica, 2012, 70, 1869.	0.5	4
107	Trajectory surface hopping molecular dynamics simulations for retinal protonated Schiff-base photoisomerization. Physical Chemistry Chemical Physics, 2021, 23, 23861-23874.	1.3	4
108	Excited-state intramolecular proton transfer with and without the assistance of vibronic-transition-induced skeletal deformation in phenolâ€"quinoline. RSC Advances, 2021, 11, 37299-37306.	1.7	4

#	Article	IF	Citations
109	Nonlinear responses of degenerate two-level systems to intense few-cycle pulses. Journal of Chemical Physics, 2007, 127, 094304.	1.2	3
110	DIELECTRIC CONSTANT AND SEEBECK COEFFICIENT FOR SEMICONDUCTORS: THERMODYNAMIC AND DFT STUDIES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1350057.	1.8	3
111	An excited-state Wolff rearrangement reaction of 5-diazo Meldrum's acid: anab initioon-the-fly nonadiabatic dynamics simulation. Physical Chemistry Chemical Physics, 2018, 20, 22681-22688.	1.3	3
112	Strong Hydrogen Bonding with Inorganic Pendant Polyhedral Oligomeric Silsesquioxane Nanoparticles Provides High Glass Transition Temperature Poly(methyl methacrylate) Copolymers. Journal of Nanoscience and Nanotechnology, 2018, 18, 188-194.	0.9	3
113	First-principles study on sum-frequency generation spectroscopy of methanol adsorbed on TiO2(110) surface: Effects of substrate and molecular coverages. Journal of Chemical Physics, 2019, 150, 184112.	1.2	3
114	Photorelaxation Pathways of 4-(N,N-Dimethylamino)-4â€²-nitrostilbene Upon S1 Excitation Revealed by Conical Intersection and Intersystem Crossing Networks. Molecules, 2020, 25, 2230.	1.7	2
115	Photoisomerization-mechanism-associated excited-state hydrogen transfer in 2â€²-hydroxychalcone revealed by on-the-fly trajectory surface-hopping molecular dynamics simulation. Physical Chemistry Chemical Physics, 2021, 23, 4300-4310.	1.3	2
116	Absorption and fluorescence spectra of conjugated polymers poly(propylene oxide)â€“poly(phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 T e4261.	0.9	2
117	Semiclassical treatment of resonances in the collinear O + HO exchange reaction. Chemical Physics Letters, 1998, 293, 448-454.	1.2	1
118	Unified Semiclassical Theory for the Nonadiabatic Transition. Journal of the Chinese Chemical Society, 2003, 50, 777-783.	0.8	1
119	Thermodynamical Study of the Thermoelectric Effect for Magnesium Silicideâ€. Journal of Physical Chemistry A, 2007, 111, 9362-9366.	1.1	1
120	Molecular Orbital Imaging of Excited States Using Time-Resolved (e, 2e) Electron Momentum Spectroscopy. , 2016, , .		1
121	A QUASICLASSICAL TRAJECTORY STUDY OF REACTIVE SCATTERING ON AN ANALYTICAL POTENTIAL ENERGY SURFACE FOR GeH2 SYSTEM. Journal of Theoretical and Computational Chemistry, 2011, 10, 147-163.	1.8	0
122	Density matrix method and ultrafast processes. Science China Chemistry, 2012, 55, 579-593.	4.2	0