Xing Gao

List of Publications by Year in descending order

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30	1,540	471509 17	477307 29
papers	citations	h-index	g-index

31	31	31	1578
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theory of Excited State Decays and Optical Spectra: Application to Polyatomic Molecules. Journal of Physical Chemistry A, 2010, 114, 7817-7831.	2.5	363
2	Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods. Journal of Chemical Theory and Computation, 2017, 13, 515-524.	5.3	249
3	Correlation Function Formalism for Triplet Excited State Decay: Combined Spinâ€“Orbit and Nonadiabatic Couplings. Journal of Chemical Theory and Computation, 2013, 9, 1132-1143.	5.3	198
4	Theoretical Insights into the Aggregation-Induced Emission by Hydrogen Bonding: A QM/MM Study. Journal of Physical Chemistry A, 2012, 116, 3881-3888.	2.5	88
5	Nickel-Catalyzed Carbonylation of Difluoroalkyl Bromides with Arylboronic Acids. Organic Letters, 2019, 21, 1031-1036.	4.6	65
6	Copperâ€Catalyzed Highly Stereoselective Trifluoromethylation and Difluoroalkylation of Secondary Propargyl Sulfonates. Angewandte Chemie - International Edition, 2018, 57, 3187-3191.	13.8	55
7	Theoretical insight into the aggregation induced emission phenomena of diphenyldibenzofulvene: a nonadiabatic molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 14207.	2.8	50
8	Highly Î³â€Selective Arylation and Carbonylative Arylation of 3â€Bromoâ€3,3â€difluoropropene via Nickel Catalysis. Angewandte Chemie - International Edition, 2021, 60, 12386-12391.	13.8	47
9	Benchmarking Quasiclassical Mapping Hamiltonian Methods for Simulating Electronically Nonadiabatic Molecular Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 2883-2895.	5.3	44
10	Theoretical design of polythienylenevinylene derivatives for improvements of light-emitting and photovoltaic performances. Journal of Materials Chemistry, 2012, 22, 4491.	6.7	41
11	Non-Hermitian surface hopping. Physical Review E, 2017, 95, 013308.	2.1	31
12	Nonadiabatic Molecular Dynamics Modeling of the Intrachain Charge Transport in Conjugated Diketopyrrolo-pyrrole Polymers. Journal of Physical Chemistry C, 2014, 118, 6631-6640.	3.1	30
13	Combining the mapping Hamiltonian linearized semiclassical approach with the generalized quantum master equation to simulate electronically nonadiabatic molecular dynamics. Journal of Chemical Physics, 2019, 151, 074103.	3.0	30
14	A Nonperturbative Methodology for Simulating Multidimensional Spectra of Multiexcitonic Molecular Systems via Quasiclassical Mapping Hamiltonian Methods. Journal of Chemical Theory and Computation, 2020, 16, 6491-6502.	5.3	26
15	Charge transfer rate constants for the carotenoid-porphyrin-C60 molecular triad dissolved in tetrahydrofuran: The spin-boson model vs the linearized semiclassical approximation. Journal of Chemical Physics, 2020, 153, 044105.	3.0	25
16	Simulating Absorption Spectra of Multiexcitonic Systems via Quasiclassical Mapping Hamiltonian Methods. Journal of Chemical Theory and Computation, 2020, 16, 6465-6480.	5.3	25
17	Electronic Dynamics through Conical Intersections via Quasiclassical Mapping Hamiltonian Methods. Journal of Chemical Theory and Computation, 2020, 16, 4479-4488.	5.3	25
18	Simulating energy transfer dynamics in the Fennaâ€“Matthewsâ€“Olson complex via the modified generalized quantum master equation. Journal of Chemical Physics, 2021, 154, 204109.	3.0	19

#	ARTICLE	IF	CITATIONS
19	Copper-Catalyzed Enantioselective Trifluoromethylthiolation of Secondary Propargyl Sulfonates. CCS Chemistry, 2021, 3, 1463-1471.	7.8	17
20	Using Chlorotrifluoroethane for Trifluoroethylation of (Hetero)aryl Bromides and Chlorides via Nickel Catalysis. Organic Letters, 2021, 23, 1400-1405.	4.6	16
21	Promoting Intersystem Crossing of a Fluorescent Molecule via Single Functional Group Modification. Journal of Physical Chemistry Letters, 2019, 10, 1388-1393.	4.6	15
22	Near-Field Spectroscopy of Nanoscale Molecular Aggregates. Journal of Physical Chemistry Letters, 2018, 9, 6003-6010.	4.6	13
23	Nickelâ€Catalyzed Difluoroalkylation of (Hetero)aryl Bromides with Unactivated 1â€Bromoâ€1,1â€difluoroalkanes. Chinese Journal of Chemistry, 2018, 36, 1059-1062.	4.9	13
24	Excitonic Wave Function Reconstruction from Near-Field Spectra Using Machine Learning Techniques. Physical Review Letters, 2019, 123, 163202.	7.8	13
25	Improving the Accuracy of Quasiclassical Mapping Hamiltonian Methods by Treating the Window Function Width as an Adjustable Parameter. Journal of Physical Chemistry A, 2020, 124, 11006-11016.	2.5	12
26	Copperâ€Catalyzed Highly Stereoselective Trifluoromethylation and Difluoroalkylation of Secondary Propargyl Sulfonates. Angewandte Chemie, 2018, 130, 3241-3245.	2.0	10
27	Non-Markovian stochastic SchrÃ¶dinger equation: Matrix-product-state approach to the hierarchy of pure states. Physical Review A, 2022, 105, .	2.5	9
28	Charge and energy transfer in large molecular assemblies: Quantum state diffusion with an adaptive basis. Journal of Chemical Physics, 2019, 150, 234115.	3.0	8
29	Theoretical Understanding of AIE Phenomena Through Computational Chemistry. , 2013, , 357-398.		2
30	Highly Î³â€Selective Arylation and Carbonylative Arylation of 3â€Bromoâ€3,3â€difluoropropene via Nickel Catalysis. Angewandte Chemie, 2021, 133, 12494-12499.	2.0	1