Shaohong L Li

List of Publications by Year
in descending order

15 papers	1,469 citations	686830 13 h-index	940134 16 g-index
16 all docs	16 docs citations	16 times ranked	2086 citing authors

#	Article	IF	Citations
1	Direct diabatization and analytic representation of coupled potential energy surfaces and couplings for the reactive quenching of the excited 2Î£+ state of OH by molecular hydrogen. Journal of Chemical Physics, 2019, 151, 104311.	1.2	27
2	Full-dimensional ground- and excited-state potential energy surfaces and state couplings for photodissociation of thioanisole. Journal of Chemical Physics, 2017, 146, 064301.	1.2	27
3	Franckâ€“Condon Models for Simulating the Band Shape of Electronic Absorption Spectra. Journal of Chemical Theory and Computation, 2017, 13, 2823-2830.	2.3	23
4	Full-dimensional multi-state simulation of the photodissociation of thioanisole. Journal of Chemical Physics, 2017, 147, 044311.	1.2	16
5	Perspective: Kohn-Sham density functional theory descending a staircase. Journal of Chemical Physics, 2016, 145, 130901.	1.2	243
6	MN15: A Kohnâ€“Sham global-hybrid exchangeâ€“correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. Chemical Science, 2016, 7, 5032-5051.	3.7	858
7	Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole. Physical Chemistry Chemical Physics, 2015, 17, 20093-20099.	1.3	16
8	Improving Rydberg Excitations within Time-Dependent Density Functional Theory with Generalized Gradient Approximations: The Exchange-Enhancement-for-Large-Gradient Scheme. Journal of Chemical Theory and Computation, 2015, 11, 3123-3130.	2.3	28
9	Model space diabatization for quantum photochemistry. Journal of Chemical Physics, 2015, 142, 064106.	1.2	42
10	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. Journal of Physical Chemistry Letters, 2015, 6, 3352-3359.	2.1	17
11	Testing time-dependent density functional theory with depopulated molecular orbitals for predicting electronic excitation energies of valence, Rydberg, and charge-transfer states and potential energies near a conical intersection. Journal of Chemical Physics, 2014, 141, 104106.	1.2	13
12	Configuration Interaction-Corrected Tammâ€“Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. Journal of Physical Chemistry Letters, 2014, 5, 322-328.	2.1	45
13	Modeling the Partial Atomic Charges in Inorganometallic Molecules and Solids and Charge Redistribution in Lithium-Ion Cathodes. Journal of Chemical Theory and Computation, 2014, 10, 5640-5650.	2.3	73
14	Near-field for electrodynamics at sub-wavelength scales: Generalizing to an arbitrary number of dielectrics. Journal of Chemical Physics, 2012, 136, 234104.	1.2	8
15	Simulate the diffusion of hydrated ions by nanofiltration membrane process with random walk. Molecular Simulation, 2012, 38, 491-497.	0.9	6