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	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
2	Perspective: Kohn-Sham density functional theory descending a staircase. Journal of Chemical Physics, 2016, 145, 130901.	1.2	243
3	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
4	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
5	Model space diabatization for quantum photochemistry. Journal of Chemical Physics, 2015, 142, 064106.	1.2	42
6	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
7	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
8	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
9	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
10	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. Journal of Physical Chemistry Letters, 2015, 6, 3352-3359.	2.1	17
11	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
12	Full-dimensional multi-state simulation of the photodissociation of thioanisole. Journal of Chemical Physics, 2017, 147, 044311.	1.2	16
13	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
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