Zhiyong Zhang

List of Publications by Year
in descending order

17	2,101	567281 15	888059 17
papers	citations	h-index	g-index

17	17	17	2731
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
2	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
3	Spinâ€“orbit DFT with analytic gradients and applications to heavy element compounds. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
4	Dynamic Mechanisms for Ammonia Borane Thermolysis in Solvent: Deviation from Gas-Phase Minimum-Energy Pathways. Journal of Physical Chemistry Letters, 2011, 2, 276-281.	4.6	27
5	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO₂ Reduction. Inorganic Chemistry, 2010, 49, 8724-8728.	4.0	70
6	The Role of Free Nâ€Heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammoniaâ€“Borane in the Nickel NHC System. Angewandte Chemie - International Edition, 2009, 48, 2201-2205.	13.8	115
7	Oligomerization and Autocatalysis of NH2BH2 with Ammoniaâˆ’Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	4.0	108
8	Energetics of Câˆ’H Bonds Formed at Single-Walled Carbon Nanotubes. Nano Letters, 2009, 9, 1301-1306.	9.1	16
9	Câ€“H bond formation at the graphite surface studied with core level spectroscopy. Surface Science, 2008, 602, 2575-2580.	1.9	99
10	Hydrogen Storage in Carbon Nanotubes through the Formation of Stable Câˆ’H Bonds. Nano Letters, 2008, 8, 162-167.	9.1	186
11	Ab initiostudy of hydrogen interaction with pure and nitrogen-doped carbon nanotubes. Physical Review B, 2007, 75, .	3.2	60
12	Spinâ€“orbit interaction with nonlinear wave functions. International Journal of Quantum Chemistry, 2007, 107, 3191-3202.	2.0	10
13	Hydrogenation of Single-Walled Carbon Nanotubes. Physical Review Letters, 2005, 95, 225507.	7.8	241
14	High-level multireference methods in the quantum-chemistry program system COLUMBUS: Analytic MR-CISD and MR-AQCC gradients and MR-AQCC-LRT for excited states, GUGA spinâ€“orbit CI and parallel CI density. Physical Chemistry Chemical Physics, 2001, 3, 664-673.	2.8	401
15	Electronic Structure and Spectra of Actinyl Ions. Journal of Physical Chemistry A, 2001, 105, 3825-3828.	2.5	95
16	Atomic orbital basis sets for use with effective core potentials. International Journal of Quantum Chemistry, 2000, 77, 516-520.	2.0	32
17	Spinâˆ’Orbit Configuration Interaction Using the Graphical Unitary Group Approach and Relativistic Core Potential and Spinâˆ’Orbit Operators. Journal of Physical Chemistry A, 1999, 103, 5791-5800.	2.5	163