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	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
3	Hydrogenation of Single-Walled Carbon Nanotubes. Physical Review Letters, 2005, 95, 225507.	7.8	241
4	Hydrogen Storage in Carbon Nanotubes through the Formation of Stable Cå^'H Bonds. Nano Letters, 2008, 8, 162-167.	9.1	186
5	Spinå^'Orbit Configuration Interaction Using the Graphical Unitary Group Approach and Relativistic Core Potential and Spinå^'Orbit Operators. Journal of Physical Chemistry A, 1999, 103, 5791-5800.	2.5	163
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 Ammoniaå^'Borane. Inorganic Chemistry, 2009, 48, 1069-1081.	4.0	108
8	Câ€“H bond formation at the graphite surface studied with core level spectroscopy. Surface Science, 2008, 602, 2575-2580.	1.9	99
9	Electronic Structure and Spectra of Actinyl Ions. Journal of Physical Chemistry A, 2001, 105, 3825-3828.	2.5	95
10	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO₂ Reduction. Inorganic Chemistry, 2010, 49, 8724-8728.	4.0	70
11	Ab initiostudy of hydrogen interaction with pure and nitrogen-doped carbon nanotubes. Physical Review B, 2007, 75, .	3.2	60
12	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
13	Atomic orbital basis sets for use with effective core potentials. International Journal of Quantum Chemistry, 2000, 77, 516-520.	2.0	32
14	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
15	Energetics of Cå^'H Bonds Formed at Single-Walled Carbon Nanotubes. Nano Letters, 2009, 9, 1301-1306.	9.1	16
16	Spinâ€“orbit DFT with analytic gradients and applications to heavy element compounds. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	11
17	Spinâ€“orbit interaction with nonlinear wave functions. International Journal of Quantum Chemistry, 2007, 107, 3191-3202.	2.0	10