Igor Ying Zhang

List of Publications by Year
in descending order

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57	5,839	236925	161849
papers	citations	25 h-index	54 g-index

60	60	60	6273
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
3	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
4	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4963-4968.	7.1	332
5	Extending the reliability and applicability of B3LYP. Chemical Communications, 2010, 46, 3057.	4.1	196
6	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 19896-19900.	7.1	143
7	OPBE: A promising density functional for the calculation of nuclear shielding constants. Chemical Physics Letters, 2006, 421, 383-388.	2.6	120
8	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. International Reviews in Physical Chemistry, 2011, 30, 115-160.	2.3	116
9	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103.	3.0	99
10	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. New Journal of Physics, 2015, 17, 093020.	2.9	97
11	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033.	2.9	81
12	Polyvinylpyrrolidoneâ€Coordinated Singleâ€Site Platinum Catalyst Exhibits High Activity for Hydrogen Evolution Reaction. Angewandte Chemie - International Edition, 2020, 59, 15902-15907.	13.8	80
13	Coupled Cluster Theory in Materials Science. Frontiers in Materials, 2019, 6, .	2.4	74
14	Geometric Dependence of the B3LYP-Predicted Magnetic Shieldings and Chemical Shifts. Journal of Physical Chemistry A, 2007, 111, 9431-9437.	2.5	70
15	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: The density functional models. Journal of Computational Chemistry, 2007, 28, 2431-2442.	3.3	68
16	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. Journal of Physical Chemistry Letters, 2013, 4, 1669-1675.	4.6	63
17	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. Physical Review B, 2016, 94, .	3.2	52
18	XO: An extended ONIOM method for accurate and efficient modeling of large systems. Journal of Computational Chemistry, 2012, 33, 2142-2160.	3.3	42

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19	Basis set dependence of the doubly hybrid XYG3 functional. Journal of Chemical Physics, 2010, 133, 104105.	3.0	41
20	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. Journal of Chemical Physics, 2010, 132, 194105.	3.0	40
21	Trends in Râ˜X Bond Dissociation Energies (Râ€¢ = Me, Et, i-Pr, t-Bu, Xâ€¢ = H, Me, Cl, OH). Journal of Chemical Theory and Computation, 2010, 6, 1462-1469.	5.3	39
22	Nonfitting proteinâ€“ligand interaction scoring function based on firstâ€principles theoretical chemistry methods: Development and application on kinase inhibitors. Journal of Computational Chemistry, 2013, 34, 1636-1646.	3.3	37
23	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. Physical Chemistry Chemical Physics, 2012, 14, 12554.	2.8	32
24	Doubly Hybrid Functionals Close to Chemical Accuracy for Both Finite and Extended Systems: Implementation and Test of XYG3 and XYGJ-OS. Jacs Au, 2021, 1, 543-549.	7.9	31
25	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. Journal of Computational Chemistry, 2011, 32, 1824-1838.	3.3	26
26	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. Journal of Computational Chemistry, 2013, 34, 1759-1774.	3.3	26
27	Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. Journal of Physical Chemistry A, 2011, 115, 13628-13641.	2.5	25
28	Experimentally quantifying anion polarizability at the air/water interface. Nature Communications, 2018, 9, 1313.	12.8	25
29	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of <scp>SIE</scp> and <scp>NCE</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	14.6	25
30	The X1s Method for Accurate Bond Dissociation Energies. ChemPhysChem, 2010, 11, 2561-2567.	2.1	24
31	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002.	7.8	24
32	Gasâ€Phase Thermodynamics as a Validation of Computational Catalysis on Surfaces: A Case Study of Fischerâ€“Tropsch Synthesis. ChemPhysChem, 2012, 13, 1486-1494.	2.1	23
33	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. Frontiers of Chemistry in China: Selected Publications From Chinese Universities, 2011, 6, 269-279.	0.4	22
34	Pyrolysis of D-Glucose to Acrolein. Chinese Journal of Chemical Physics, 2011, 24, 249-252.	1.3	22
35	Massive-Parallel Implementation of the Resolution-of-Identity Coupled-Cluster Approaches in the Numeric Atom-Centered Orbital Framework for Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 4721-4734.	5.3	22
36	Accurate prediction of nuclear magnetic resonance shielding constants: Towards the accuracy of CCSD(T) complete basis set limit. Journal of Chemical Physics, 2013, 138, 124113.	3.0	20

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37	A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , .	0.1	20
38	Understanding the Nonplanarity in Aromatic Metallabenzenes: A Ïƒ-Control Mechanism. Inorganic Chemistry, 2018, 57, 9205-9214.	4.0	18
39	Simultaneous Attenuation of Both Self-Interaction Error and Nondynamic Correlation Error in Density Functional Theory: A Spin-Pair Distinctive Adiabatic-Connection Approximation. Journal of Physical Chemistry Letters, 2019, 10, 2617-2623.	4.6	17
40	Exploring the Limits of the XYG3-Type Doubly Hybrid Approximations for the Main-Group Chemistry: The xDH@B3LYP Model. Journal of Physical Chemistry Letters, 2021, 12, 2638-2644.	4.6	17
41	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. New Journal of Physics, 2019, 21, 013025.	2.9	15
42	Identification of Water Hexamer on Cu(111) Surfaces. Journal of the American Chemical Society, 2020, 142, 6902-6906.	13.7	14
43	O-atom transfer reaction from N2O to CO: A theoretical investigation. Chemical Physics Letters, 2009, 475, 202-207.	2.6	12
44	Wave-function inspired density functional applied to the H₂/${{m{H}}}_{2}^{+}$ challenge. New Journal of Physics, 2016, 18, 073026.	2.9	12
45	Resolving the chemical identity of H₂SO₄ derived anions on Pt(111) electrodes: they're sulfate. Physical Chemistry Chemical Physics, 2019, 21, 19147-19152.	2.8	12
46	Insight into organic reactions from the direct random phase approximation and its corrections. Journal of Chemical Physics, 2015, 143, 144115.	3.0	11
47	Accurate Description of Catalytic Selectivity: Challenges and Opportunities for the Development of Density Functional Approximations. CCS Chemistry, 2021, 3, 136-143.	7.8	11
48	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. Journal of Computational Chemistry, 2008, 29, 1798-1807.	3.3	9
49	RRS-PBC: a molecular approach for periodic systems. Science China Chemistry, 2014, 57, 1399-1404.	8.2	8
50	Response to â€œComment on â€˜Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0â€â€™ [J. Chem. Phys. 143, 187101 (2015)]. Journal of Chemical Physics, 2015, 143, 187102.	3.0	8
51	Assessment of Some Density Functional Theory Methods and Force Field Models in Describing Various Interaction Modes of Benzene Dimer. Chinese Journal of Chemical Physics, 2011, 24, 635-639.	1.3	7
52	Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. Journal of Computational Chemistry, 2019, 40, 1113-1122.	3.3	6
53	A New Generation of Doubly Hybrid Density Functionals (DHDFs). Springer Briefs in Molecular Science, 2014, , 25-45.	0.1	2
54	Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. Springer Series in Materials Science, 2021, , 245-255.	0.6	1

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55	Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77.	0.1	0
56	An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24.	0.1	0
57	XYG3 Results for Some Selected Applications. Springer Briefs in Molecular Science, 2014, , 79-101.	0.1	0