

Igor Ying Zhang

List of Publications by Year in descending order

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57
papers

5,839
citations

236833

25
h-index

161767

54
g-index

60
all docs

60
docs citations

60
times ranked

6273
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
3	Understanding band gaps of solids in generalized Kohn-Sham theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2801-2806.	3.3	423
4	Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 4963-4968.	3.3	332
5	Extending the reliability and applicability of B3LYP. <i>Chemical Communications</i> , 2010, 46, 3057.	2.2	196
6	A fast doubly hybrid density functional method close to chemical accuracy using a local opposite spin ansatz. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 19896-19900.	3.3	143
7	OPBE: A promising density functional for the calculation of nuclear shielding constants. <i>Chemical Physics Letters</i> , 2006, 421, 383-388.	1.2	120
8	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 115-160.	0.9	116
9	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>Journal of Chemical Physics</i> , 2012, 136, 174103.	1.2	99
10	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. <i>New Journal of Physics</i> , 2015, 17, 093020.	1.2	97
11	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. <i>New Journal of Physics</i> , 2013, 15, 123033.	1.2	81
12	Polyvinylpyrrolidone-Coordinated Single-Site Platinum Catalyst Exhibits High Activity for Hydrogen Evolution Reaction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15902-15907.	7.2	80
13	Coupled Cluster Theory in Materials Science. <i>Frontiers in Materials</i> , 2019, 6, .	1.2	74
14	Geometric Dependence of the B3LYP-Predicted Magnetic Shieldings and Chemical Shifts. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9431-9437.	1.1	70
15	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: The density functional models. <i>Journal of Computational Chemistry</i> , 2007, 28, 2431-2442.	1.5	68
16	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1669-1675.	2.1	63
17	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. <i>Physical Review B</i> , 2016, 94, .	1.1	52
18	XO: An extended ONIOM method for accurate and efficient modeling of large systems. <i>Journal of Computational Chemistry</i> , 2012, 33, 2142-2160.	1.5	42

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19	Basis set dependence of the doubly hybrid XYG3 functional. <i>Journal of Chemical Physics</i> , 2010, 133, 104105.	1.2	41
20	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. <i>Journal of Chemical Physics</i> , 2010, 132, 194105.	1.2	40
21	Trends in R [∞] X Bond Dissociation Energies (R = Me, Et, i-Pr, t-Bu, X = H, Me, Cl, OH). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1462-1469.	2.3	39
22	Nonfitting protein-ligand interaction scoring function based on first-principles theoretical chemistry methods: Development and application on kinase inhibitors. <i>Journal of Computational Chemistry</i> , 2013, 34, 1636-1646.	1.5	37
23	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12554.	1.3	32
24	Doubly Hybrid Functionals Close to Chemical Accuracy for Both Finite and Extended Systems: Implementation and Test of XYG3 and XYGJ-OS. <i>Jacs Au</i> , 2021, 1, 543-549.	3.6	31
25	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. <i>Journal of Computational Chemistry</i> , 2011, 32, 1824-1838.	1.5	26
26	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. <i>Journal of Computational Chemistry</i> , 2013, 34, 1759-1774.	1.5	26
27	Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13628-13641.	1.1	25
28	Experimentally quantifying anion polarizability at the air/water interface. <i>Nature Communications</i> , 2018, 9, 1313.	5.8	25
29	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of $\langle \text{scf} \rangle \text{SIE}$ and $\langle \text{scf} \rangle \text{NCE}$. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, .	6.2	25
30	The X1s Method for Accurate Bond Dissociation Energies. <i>ChemPhysChem</i> , 2010, 11, 2561-2567.	1.0	24
31	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. <i>Physical Review Letters</i> , 2016, 117, 133002.	2.9	24
32	Gas-Phase Thermodynamics as a Validation of Computational Catalysis on Surfaces: A Case Study of Fischer-Tropsch Synthesis. <i>ChemPhysChem</i> , 2012, 13, 1486-1494.	1.0	23
33	Calculations of ionization energies and electron affinities for atoms and molecules: A comparative study with different methods. <i>Frontiers of Chemistry in China: Selected Publications From Chinese Universities</i> , 2011, 6, 269-279.	0.4	22
34	Pyrolysis of D-Glucose to Acrolein. <i>Chinese Journal of Chemical Physics</i> , 2011, 24, 249-252.	0.6	22
35	Massive-Parallel Implementation of the Resolution-of-Identity Coupled-Cluster Approaches in the Numeric Atom-Centered Orbital Framework for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4721-4734.	2.3	22
36	Accurate prediction of nuclear magnetic resonance shielding constants: Towards the accuracy of CCSD(T) complete basis set limit. <i>Journal of Chemical Physics</i> , 2013, 138, 124113.	1.2	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 ĩf-Control Mechanism. Inorganic Chemistry, 2018, 57, 9205-9214.	1.9	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.	2.1	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.	2.1	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.	1.2	15
42	Identification of Water Hexamer on Cu(111) Surfaces. Journal of the American Chemical Society, 2020, 142, 6902-6906.	6.6	14
43	O-atom transfer reaction from N2O to CO: A theoretical investigation. Chemical Physics Letters, 2009, 475, 202-207.	1.2	12
44	Wave-function inspired density functional applied to the H₂/{m{H}}_{2}^{+}\$ challenge. New Journal of Physics, 2016, 18, 073026.	1.2	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.	1.3	12
46	Insight into organic reactions from the direct random phase approximation and its corrections. Journal of Chemical Physics, 2015, 143, 144115.	1.2	11
47	Accurate Description of Catalytic Selectivity: Challenges and Opportunities for the Development of Density Functional Approximations. CCS Chemistry, 2021, 3, 136-143.	4.6	11
48	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. Journal of Computational Chemistry, 2008, 29, 1798-1807.	1.5	9
49	RRS-PBC: a molecular approach for periodic systems. Science China Chemistry, 2014, 57, 1399-1404.	4.2	8
50	Response to "Comment on "Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0" [J. Chem. Phys. 143, 187101 (2015)]. Journal of Chemical Physics, 2015, 143, 187102.	1.2	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.	0.6	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.	1.5	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.	0.4	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