

Igor Ying Zhang

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

57
papers

4,301
citations

24
h-index

60
g-index

60
ext. papers

5,106
ext. citations

4.7
avg. IF

5.26
L-index

#	Paper	IF	Citations
57	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015 , 113, 184-215	1.7	2068
56	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	11.5	280
55	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, 4963-8	11.5	280
54	Extending the reliability and applicability of B3LYP. <i>Chemical Communications</i> , 2010 , 46, 3057-70	5.8	145
53	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, 19896-900	11.5	124
52	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	3.9	115
51	OPBE: A promising density functional for the calculation of nuclear shielding constants. <i>Chemical Physics Letters</i> , 2006 , 421, 383-388	2.5	107
50	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	7	106
49	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>Journal of Chemical Physics</i> , 2012 , 136, 174103	3.9	86
48	Geometric dependence of the B3LYP-predicted magnetic shieldings and chemical shifts. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 9431-7	2.8	66
47	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	2.9	65
46	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. <i>New Journal of Physics</i> , 2013 , 15, 123033	2.9	65
45	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, 2431-42	3.5	63
44	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, 1669-75	6.4	57
43	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,	3.3	40
42	Basis set dependence of the doubly hybrid XYG3 functional. <i>Journal of Chemical Physics</i> , 2010 , 133, 104105	3.5	39
41	Polyvinylpyrrolidone-Coordinated Single-Site Platinum Catalyst Exhibits High Activity for Hydrogen Evolution Reaction. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15902-15907	16.4	38

40	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. <i>Journal of Chemical Physics</i> , 2010 , 132, 194105	3.9	37
39	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, 1462-9	6.4	37
38	Coupled Cluster Theory in Materials Science. <i>Frontiers in Materials</i> , 2019 , 6,	4	33
37	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, 1636-46	3.5	32
36	XO: an extended ONIOM method for accurate and efficient modeling of large systems. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2142-60	3.5	30
35	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12554-70	3.6	29
34	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. <i>Journal of Computational Chemistry</i> , 2011 , 32, 1824-38	3.5	25
33	Theoretical studies on thermochemistry for conversion of 5-chloromethylfurfural into valuable chemicals. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 13628-41	2.8	24
32	The X1s method for accurate bond dissociation energies. <i>ChemPhysChem</i> , 2010 , 11, 2561-7	3.2	23
31	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1759-74	3.5	20
30	Gas-phase thermodynamics as a validation of computational catalysis on surfaces: a case study of Fischer-Tropsch synthesis. <i>ChemPhysChem</i> , 2012 , 13, 1486-94	3.2	19
29	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. <i>Physical Review Letters</i> , 2016 , 117, 133002	7.4	18
28	A New-Generation Density Functional. <i>Springer Briefs in Molecular Science</i> , 2014 ,	0.6	18
27	Pyrolysis of D-Glucose to Acrolein. <i>Chinese Journal of Chemical Physics</i> , 2011 , 24, 249-252	0.9	18
26	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		17
25	Experimentally quantifying anion polarizability at the air/water interface. <i>Nature Communications</i> , 2018 , 9, 1313	17.4	16
24	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	3.9	16
23	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	6.4	15

22	Simultaneous Attenuation of Both Self-Interaction Error and Nondynamic Correlation Error in Density Functional Theory: A Spin-Pair Distinctive Adiabatic-Connection Approximation. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2617-2623	6.4	12
21	Understanding the Nonplanarity in Aromatic Metallabenzenes: A σ -Control Mechanism. <i>Inorganic Chemistry</i> , 2018 , 57, 9205-9214	5.1	12
20	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11,	7.9	12
19	Insight into organic reactions from the direct random phase approximation and its corrections. <i>Journal of Chemical Physics</i> , 2015 , 143, 144115	3.9	11
18	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. <i>New Journal of Physics</i> , 2019 , 21, 013025	2.9	10
17	Wave-function inspired density functional applied to the H ₂ /H ₂ ⁺ challenge. <i>New Journal of Physics</i> , 2016 , 18, 073026	2.9	10
16	O-atom transfer reaction from N ₂ O to CO: A theoretical investigation. <i>Chemical Physics Letters</i> , 2009 , 475, 202-207	2.5	8
15	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1798-807	3.5	8
14	Response to Comment on Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. <i>J. Chem. Phys.</i> 143, 187101 (2015)]. <i>Journal of Chemical Physics</i> , 2015 , 143, 187102	3.9	7
13	RRS-PBC: a molecular approach for periodic systems. <i>Science China Chemistry</i> , 2014 , 57, 1399-1404	7.9	7
12	Assessment of Some Density Functional Theory Methods and Force Field Models in Describing Various Interaction Modes of Benzene Dimer. <i>Chinese Journal of Chemical Physics</i> , 2011 , 24, 635-639	0.9	7
11	Exploring the Limits of the XYG3-Type Doubly Hybrid Approximations for the Main-Group Chemistry: The xDH@B3LYP Model. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2638-2644	6.4	6
10	Resolving the chemical identity of HSO derived anions on Pt(111) electrodes: they're sulfate. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 19147-19152	3.6	5
9	Identification of Water Hexamer on Cu(111) Surfaces. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6902-6906	16.4	5
8	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		4
7	Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. <i>Journal of Computational Chemistry</i> , 2019 , 40, 1113-1122	3.5	3
6	A New Generation of Doubly Hybrid Density Functionals (DHDFs). <i>Springer Briefs in Molecular Science</i> , 2014 , 25-45	0.6	2
5	Accurate Description of Catalytic Selectivity: Challenges and Opportunities for the Development of Density Functional Approximations. <i>CCS Chemistry</i> , 136-143	7.2	1

- 4 Benchmarking the Performance of DHDFs for the Main Group Chemistry. *Springer Briefs in Molecular Science*, **2014**, 47-77 0.6
- 3 An Overview of Modern Density Functional Theory. *Springer Briefs in Molecular Science*, **2014**, 1-24 0.6
- 2 XYG3 Results for Some Selected Applications. *Springer Briefs in Molecular Science*, **2014**, 79-101 0.6
- 1 Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. *Springer Series in Materials Science*, **2021**, 245-255 0.9