Igor Ying Zhang

List of Publications by Year in Descending Order

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	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	6.4	6
56	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		4
55	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of SIE and NCE. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11,	7.9	12
54	Prediction of Heats of Formation of Polycyclic Saturated Hydrocarbons Using the XYG3 Double Hybrid Functionals. *Springer Series in Materials Science*, **2021**, 245-255	0.9	
53	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
52	Polyvinylpyrrolidone-Coordinated Single-Site Platinum Catalyst Exhibits High Activity for Hydrogen Evolution Reaction. *Angewandte Chemie - International Edition*, **2020**, 59, 15902-15907	16.4	38
51	Identification of Water Hexamer on Cu(111) Surfaces. *Journal of the American Chemical Society*, **2020**, 142, 6902-6906	16.4	5
50	Resolving the chemical identity of HSO derived anions on Pt(111) electrodes: they're sulfate. *Physical Chemistry Chemical Physics*, **2019**, 21, 19147-19152	3.6	5
49	Coupled Cluster Theory in Materials Science. *Frontiers in Materials*, **2019**, 6,	4	33
48	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	6.4	12
47	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	10
46	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	6.4	15
45	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	3.5	3
44	Experimentally quantifying anion polarizability at the air/water interface. *Nature Communications*, **2018**, 9, 1313	17.4	16
43	Understanding the Nonplanarity in Aromatic Metallabenzenes: A Control Mechanism. *Inorganic Chemistry*, **2018**, 57, 9205-9214	5.1	12
42	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
41	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. *Physical Review Letters*, **2016**, 117, 133002	7.4	18

40	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,	3.3	40
39	Wave-function inspired density functional applied to the H2/${{rm{H}}}_{2}^{+}$ challenge. *New Journal of Physics*, **2016**, 18, 073026	2.9	10
38	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
37	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	65
36	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	3.9	7
35	Insight into organic reactions from the direct random phase approximation and its corrections. *Journal of Chemical Physics*, **2015**, 143, 144115	3.9	11
34	A New-Generation Density Functional. *Springer Briefs in Molecular Science*, **2014**,	0.6	18
33	RRS-PBC: a molecular approach for periodic systems. *Science China Chemistry*, **2014**, 57, 1399-1404	7.9	7
32	A New Generation of Doubly Hybrid Density Functionals (DHDFs). *Springer Briefs in Molecular Science*, **2014**, 25-45	0.6	2
31	Benchmarking the Performance of DHDFs for the Main Group Chemistry. *Springer Briefs in Molecular Science*, **2014**, 47-77	0.6	
30	An Overview of Modern Density Functional Theory. *Springer Briefs in Molecular Science*, **2014**, 1-24	0.6	
29	XYG3 Results for Some Selected Applications. *Springer Briefs in Molecular Science*, **2014**, 79-101	0.6	
28	Nonfitting protein-ligand interaction scoring function based on first-principles theoretical chemistry methods: development and application on kinase inhibitors. *Journal of Computational Chemistry*, **2013**, 34, 1636-46	3.5	32
27	Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. *Journal of Computational Chemistry*, **2013**, 34, 1759-74	3.5	20
26	Reaching a Uniform Accuracy for Complex Molecular Systems: Long-Range-Corrected XYG3 Doubly Hybrid Density Functional. *Journal of Physical Chemistry Letters*, **2013**, 4, 1669-75	6.4	57
25	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New Journal of Physics*, **2013**, 15, 123033	2.9	65
24	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	3.9	16
23	Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. *Journal of Chemical Physics*, **2012**, 136, 174103	3.9	86

22	XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. *Physical Chemistry Chemical Physics*, **2012**, 14, 12554-70	3.6	29
21	XO: an extended ONIOM method for accurate and efficient modeling of large systems. *Journal of Computational Chemistry*, **2012**, 33, 2142-60	3.5	30
20	Gas-phase thermodynamics as a validation of computational catalysis on surfaces: a case study of Fischer-Tropsch synthesis. *ChemPhysChem*, **2012**, 13, 1486-94	3.2	19
19	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		17
18	Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. *Journal of Computational Chemistry*, **2011**, 32, 1824-38	3.5	25
17	Doubly hybrid density functional for accurate description of thermochemistry, thermochemical kinetics and nonbonded interactions. *International Reviews in Physical Chemistry*, **2011**, 30, 115-160	7	106
16	Theoretical studies on thermochemistry for conversion of 5-chloromethylfurfural into valuable chemicals. *Journal of Physical Chemistry A*, **2011**, 115, 13628-41	2.8	24
15	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	0.9	7
14	Pyrolysis of D-Glucose to Acrolein. *Chinese Journal of Chemical Physics*, **2011**, 24, 249-252	0.9	18
13	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, 19896-900	11.5	124
12	XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. *Journal of Chemical Physics*, **2010**, 132, 194105	3.9	37
11	Basis set dependence of the doubly hybrid XYG3 functional. *Journal of Chemical Physics*, **2010**, 133, 104105	3.9	39
10	Extending the reliability and applicability of B3LYP. *Chemical Communications*, **2010**, 46, 3057-70	5.8	145
9	Trends in R-X Bond Dissociation Energies (R□= Me, Et, i-Pr, t-Bu, X□= H, Me, Cl, OH). *Journal of Chemical Theory and Computation*, **2010**, 6, 1462-9	6.4	37
8	The X1s method for accurate bond dissociation energies. *ChemPhysChem*, **2010**, 11, 2561-7	3.2	23
7	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, 4963-8	11.5	280
6	O-atom transfer reaction from N2O to CO: A theoretical investigation. *Chemical Physics Letters*, **2009**, 475, 202-207	2.5	8
5	Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. *Journal of Computational Chemistry*, **2008**, 29, 1798-807	3.5	8

4	Systematic studies on the computation of nuclear magnetic resonance shielding constants and chemical shifts: the density functional models. *Journal of Computational Chemistry*, **2007**, 28, 2431-42	3.5	63
3	Geometric dependence of the B3LYP-predicted magnetic shieldings and chemical shifts. *Journal of Physical Chemistry A*, **2007**, 111, 9431-7	2.8	66
2	OPBE: A promising density functional for the calculation of nuclear shielding constants. *Chemical Physics Letters*, **2006**, 421, 383-388	2.5	107
1	Accurate Description of Catalytic Selectivity: Challenges and Opportunities for the Development of Density Functional Approximations. *CCS Chemistry*,136-143	7.2	1