# 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 | 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 |
| 2 | Accurate Description of Catalytic Selectivity: Challenges and Opportunities for the Development of Density Functional Approximations. CCS Chemistry, 2021, 3, 136-143. | 7.8 | 11 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | Polyvinylpyrrolidoneâ€Coordinated Singleâ€Site Platinum Catalyst Exhibits High Activity for Hydrogen Evolution Reaction. Angewandte Chemie - International Edition, 2020, 59, 15902-15907. | 13.8 | 80 |
| 8 | Identification of Water Hexamer on Cu(111) Surfaces. Journal of the American Chemical Society, 2020, 142, 6902-6906. | 13.7 | 14 |
| 9 | 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 |
| 10 | Resolving the chemical identity of H<sub>2</sub>SO<sub>4</sub> derived anions on Pt(111) electrodes: they're sulfate. Physical Chemistry Chemical Physics, 2019, 21, 19147-19152. | 2.8 | 12 |
| 11 | Coupled Cluster Theory in Materials Science. Frontiers in Materials, 2019, 6, . | 2.4 | 74 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | Experimentally quantifying anion polarizability at the air/water interface. Nature Communications, 2018, 9, 1313. | 12.8 | 25 |
| 16 | Understanding the Nonplanarity in Aromatic Metallabenzenes: A Ïƒ-Control Mechanism. Inorganic Chemistry, 2018, 57, 9205-9214. | 4.0 | 18 |
| 17 | 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 |
| 18 | Wave-function inspired density functional applied to the H<sub>2</sub>/${{m{H}}}_{2}^{+}$ challenge. New Journal of Physics, 2016, 18, 073026. | 2.9 | 12 |

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|---|---|---|---|
| 19 | Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002. | 7.8 | 24 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | Insight into organic reactions from the direct random phase approximation and its corrections. Journal of Chemical Physics, 2015, 143, 144115. | 3.0 | 11 |
| 24 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 1.7 | 2,561 |
| 25 | RRS-PBC: a molecular approach for periodic systems. Science China Chemistry, 2014, 57, 1399-1404. | 8.2 | 8 |
| 26 | A New-Generation Density Functional. Springer Briefs in Molecular Science, 2014, , . | 0.1 | 20 |
| 27 | A New Generation of Doubly Hybrid Density Functionals (DHDFs). Springer Briefs in Molecular Science, 2014, , 25-45. | 0.1 | 2 |
| 28 | Benchmarking the Performance of DHDFs for the Main Group Chemistry. Springer Briefs in Molecular Science, 2014, , 47-77. | 0.1 | 0 |
| 29 | An Overview of Modern Density Functional Theory. Springer Briefs in Molecular Science, 2014, , 1-24. | 0.1 | 0 |
| 30 | XYG3 Results for Some Selected Applications. Springer Briefs in Molecular Science, 2014, , 79-101. | 0.1 | 0 |
| 31 | 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 |
| 32 | 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 |
| 33 | 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 |
| 34 | Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033. | 2.9 | 81 |
| 35 | 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 |
| 36 | Doubly hybrid density functional xDH-PBE0 from a parameter-free global hybrid model PBE0. Journal of Chemical Physics, 2012, 136, 174103. | 3.0 | 99 |

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|---|---|---|---|
| 37 | XYG3 and XYGJ-OS performances for noncovalent binding energies relevant to biomolecular structures. Physical Chemistry Chemical Physics, 2012, 14, 12554. | 2.8 | 32 |
| 38 | XO: An extended ONIOM method for accurate and efficient modeling of large systems. Journal of Computational Chemistry, 2012, 33, 2142-2160. | 3.3 | 42 |
| 39 | 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 |
| 40 | 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 |
| 41 | Theoretical Studies on Thermochemistry for Conversion of 5-Chloromethylfurfural into Valuable Chemicals. Journal of Physical Chemistry A, 2011, 115, 13628-13641. | 2.5 | 25 |
| 42 | 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 |
| 43 | Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. Journal of Computational Chemistry, 2011, 32, 1824-1838. | 3.3 | 26 |
| 44 | 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 |
| 45 | Pyrolysis of D-Glucose to Acrolein. Chinese Journal of Chemical Physics, 2011, 24, 249-252. | 1.3 | 22 |
| 46 | 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 |
| 47 | The X1s Method for Accurate Bond Dissociation Energies. ChemPhysChem, 2010, 11, 2561-2567. | 2.1 | 24 |
| 48 | XYG3s: Speedup of the XYG3 fifth-rung density functional with scaling-all-correlation method. Journal of Chemical Physics, 2010, 132, 194105. | 3.0 | 40 |
| 49 | Basis set dependence of the doubly hybrid XYG3 functional. Journal of Chemical Physics, 2010, 133, 104105. | 3.0 | 41 |
| 50 | Extending the reliability and applicability of B3LYP. Chemical Communications, 2010, 46, 3057. | 4.1 | 196 |
| 51 | 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 |
| 52 | 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 |
| 53 | O-atom transfer reaction from N2O to CO: A theoretical investigation. Chemical Physics Letters, 2009, 475, 202-207. | 2.6 | 12 |
| 54 | Systematic investigation on the geometric dependence of the calculated nuclear magnetic shielding constants. Journal of Computational Chemistry, 2008, 29, 1798-1807. | 3.3 | 9 |

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|---|---|---|---|
| 55 | Geometric Dependence of the B3LYP-Predicted Magnetic Shieldings and Chemical Shifts. Journal of Physical Chemistry A, 2007, 111, 9431-9437. | 2.5 | 70 |
| 56 | 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 |
| 57 | OPBE: A promising density functional for the calculation of nuclear shielding constants. Chemical Physics Letters, 2006, 421, 383-388. | 2.6 | 120 |